Thermal Quantum Field Theory

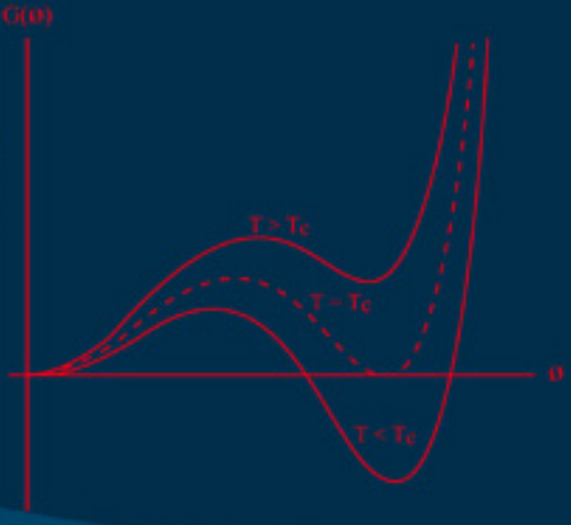
Algebraic Aspects and Applications

Faqir C. Khanna

Adolfo P. C. Malbouisson

Jorge M. C. Malbouisson

Ademir E. Santana



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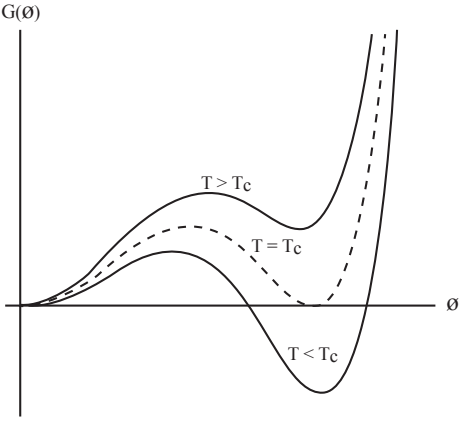
Faqir C. Khanna
University of Alberta & TRIUMF, Canada

Adolfo P. C. Malbouisson
Centro Brasileiro de Pesquisas Fisicas, Brazil

Jorge M. C. Malbouisson
Universidade Federal da Bahia, Brazil

Ademir E. Santana
Universidade de Brasilia, Brazil



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Algebraic Aspects and Applications

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Dedicated to:

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Preface

The objective of writing this book is to bring together in a coherent fashion the foundations of and recent developments in finite temperature quantum field theory and its applications to physical problems. The basic tool of our presentation is symmetry.

Symmetry is the cornerstone of contemporary physics. It has played a fundamental role in our understanding, in particular, of elementary particles and their interactions. This concept has been useful not only in *ab initio* theories, but also in heuristic formulations, such as thermodynamics. In order to appreciate this point, let us trace some elements of temperature dependent phenomena. Thermodynamics is a theory describing macroscopic properties of matter without any microscopic dynamic input. For this reason, it was considered by many as a way of systematizing the properties of measurements. However, it is quite amazing that the description of entropy, free energy, specific heat and several types of phase transitions can be related and some conceptual progress has developed. In these developments, a crucial step was taken by Landau, guided by concepts of symmetry, who set forth his theory of first and second-order phase transitions. This introduced notions such as the order parameter and spontaneous symmetry breaking. In order to advance with the Landau theory describing properties of critical phenomena in matter, the methodology of the quantum field theory was borrowed by thermodynamics. This was a two-way street. The quantum field theory, describing elementary particles, adopted the concept of spontaneous symmetry breaking to justify, for instance, the origin of mass, superconducting transitions and many other phenomena.

As the understanding of the microscopic nature of matter developed, it became imperative to introduce dynamics to describe the thermodynamic properties in terms of forces and a consistent theoretical structure. But the large number of particles made it prohibitive to carry out a real microscopic calculation. This led to ideas of statistical mechanics, starting with Boltzmann and Maxwell, and finding a synthesis by Gibbs with the ensemble theory.

The last century saw a rapid growth of ideas and sophisticated methods to treat microscopic systems. The developments of both quantum theory and relativity led to the quantum field theory that incorporated these two ideas. Then this in turn

provided results such as the spin-statistics theorem. These formulations, initially considered to be useful in developing a theory for elementary particles, proved in fact highly beneficial to an understanding of the properties and phenomena in many-body physics. However, it still lacked the notion of temperature. Part of this theoretical apparatus, such as the partition function in statistical mechanics and Green function in quantum physics, was converted into a proper microscopic theory at finite temperature by Matsubara in 1955 using the expedient of imaginary-time.

At about that time, there was a tremendous development of quantum field theory with methods due to Feynman, Tomonaga and Schwinger, among others. There were two other fundamental achievements. One was carried out by Wigner who, in the late ninteen thirties, when studying representations of the Lorentz group, found a way to classify elementary particles. The other step was due to Yang and Mills, that extended the notion of gauge symmetry (due to Weyl) to describe the basic interactions in nature. These findings of a theory at zero-temperature were enough motivation for researchers to look for an extension of the Matsubara method. This was carried out by Ezawa, Tomozawa and Umezawa, in order to describe processes in relativistic physics, settling then a strong proximation of two different areas: statistical mechanics and quantum field theory. The consequence was a diversity of developments of practical and formal interest, such as the periodicity in time described by the KMS (Kubo-Martin-Schwinger) conditions, with topological implications, and the spontaneous symmetry breaking in particle physics by Dolan and Jackiw. It is also important to state that many findings, first introduced in the zero-temperature theories, were brought to the finite temperature theory. For example, this is the case for the Ward-Takahashi (W-T) relations, where using symmetry provides a way to carry out consistent perturbative calculations. Furthermore, the W-T relations present the only non-perturbative method in quantum field theory, at both zero and finite temperature.

The imaginary-time formalism is basically a theory for thermal equilibrium. However, time is a crucial ingredient in many processes in relativistic and in many-body physics. This led Schwinger, followed by Keldysh, to propose a method using elements of the imaginary-time formalism with real time. A decade later, while studying superconductivity, Umezawa and coworkers found that to transpose zero-temperature methods to imaginary-time problems with field operators and their products was difficult and cumbersome. The attempt to solve this led Takahashi and Umezawa to propose a real-time operator field theory at finite temperature, thermofield dynamics (TFD). This required the Hilbert space to be doubled. The second Hilbert space was eventually related to the heat bath as the old thermodynamics required a heat bath to have a system at constant temperature. TFD brought to the realm of thermal theories two elements. One was the Bogoliubov transformation, describing the temperature effect as a condensate of field in the vacuum, and it was well-known for superconducting phase transitions. The other was a Hilbert space structure associated to the thermal state. The latter is, in turn,

connected to the concept of c*-algebras, the formal structure of statistical physics. As a consequence, representations of symmetry groups for thermal theories could be explored. In addition, these algebraic elements were combined with the KMS conditions giving rise to representations of quantum fields in topological manifolds, say $\mathbb{S}^1 \times \mathbb{R}^3$, describing a system in compactified regions of imaginary-time, where the dimensions of the compactification, represented by the circle $\mathbb{S}^1$, is the temperature. In this book, we explore in detail this symbiosis of symmetry and topology.

The book is divided into five parts. The first part treats fundamental principles. We start, for the sake of completeness, by considering the status of thermodynamics. Our goal is to show its connection with the elements of field theory by discussing the Landau phenomenological description of first and second-order phase transitions. Then, in the second chapter, basic elements of statistical mechanics are presented. The Louiville-von Neumann equation and the von Neumann entropy are used to arrive at the Gibbs ensembles using the variational principle. Starting again from the Louiville-von Neumann equation, the Wigner function formalism is introduced. In the third chapter the notion of partition function is explored, leading us to consider the idea of a generating functional that has proved so very useful in the perturbative approach for quantum systems; in particular the path integral method, including gauges fields. Chapter 4 deals with the theory of interacting fields at zero-temperature. Examples of scalar field and Yang-Mills theory are presented. It provides a brief look at the set-up of the canonical theory and the perturbative approach. In this brief review of so many topics, compactified in four chapters in Part One, we have focussed on concepts that will be explored and developed at finite temperature in the rest of the book.

Part Two deals with the thermal field theory. We start with some basic notions of thermofield dynamics and statistical physics to introduce the concept of representations of symmetries associated with thermal phenomena. This is called the thermo-algebra. These ideas are illustrated with examples, by considering oscillators for bosons and fermions. The doubling of operators is interpreted physically. It is followed by considering thermal groups based on kinematic symmetries: Poincaré and Galilei, leading us to thermal Lagrangians. The representations of the kinematic groups provide, in particular, relativistic Liouville-von Neumann equations for fermions and bosons. The relationship among TFD, Matsubara and Keldysh-Schwinger formalisms is discussed in terms of symmetry, providing a unified view of these diverse techniques. Finally, the path integral approach at finite temperature is introduced. This is followed with some examples of calculating decay rates and cross sections at finite temperature and these are compared with those at zero temperature. We close this Part with a discussion of topics on renormalization and Ward-Takahashi relations at finite temperature.

Part Three contains applications to quantum optics. Exploring thermal representations in TFD, various thermal states of a field mode are introduced and defined consistently. In order to study the physical nature of such states, the sta-

tistical properties are analyzed by considering the Mandel factor and Wigner and P-functions. Finally bipartite states are introduced and their entanglement is considered, taking the TFD structure as a guide.

Part Four deals with compactified fields and their application. The basic idea is to explore the topology associated with the KMS conditions to treat fields in confined spatial regions at finite temperature. Starting with topological arguments, we discuss how to generalize the Bogoliubov transfomations and the Matsubara imaginary time to allow a study of systems confined to finite regions, linear, surface and volume, consistent with topologies $\Gamma_D^d = (\mathbb{S}^1)^d \times \mathbb{R}^{D-d}$. Due to the close association of the Bogoliubov transformation and the imaginary-time method, the process of space compactification may be understood physically, in one case as in the other, as a process of condensation of the field in the vaccum. The first example is the Casimir effect for the electromagnetic field between plates, and in a parallelepiped box. The generalized discussion implies that the Casimir effect may be viewed as a condensation of the electromagnetic field in the vacuum. Then we consider the example of fermions in different configurations. Some results for a simplified QCD Lagrangian are obtained. This is followed by studying the case of the compactified $\lambda\phi^4$ theory and an analysis of spontaneous symmetry breaking for spatially confined systems at finite temperature. Then the examples of phase transitions in superconducting material in films, wires and grains are considered. This is to analyze the role of topology that may change the transition temperatures in these confined systems. The case of first order phase transition in superconducting films is also taken up. All these examples provide a strong support for the ideas, using symmetry representations with topological ingredients, to treat compactified fields.

In Part Five, first we analyze representations of thermo-algebras in the phase space. The Wigner function is then derived for relativisitic and non-relativistic fields, followed by a study of the classical version of TFD. These results give us elements of kinetic theory and stochastic processes from a perspective of the representation theory of the kinematic groups, Poincaré and Galilei. Further chapters provide some ideas about open systems, exploring methods of quantum field theory. Systems in nonequilibrium states are considered only in a simple manner. An exhaustive analysis of such a problem would require a separate monograph.

The book is structured in such a way that some topics can be studied independently. For instance, a reader sufficiently trained in quantum field theory can start from Chapter 5. Another reader interested in optics can start from reviewing some basic concepts in Chapters 1 and 2, and then jump to Chapters 5, 6, 12, 13 and 14. Beyond Part One, other basic elements are introduced throughout the book to make it convenient for beginners and students to study.

Finally, we wish to thank many colleagues and friends for contributing to the developments in this book. Over the last fifteen years, they have shared their expertise, their advice and their encouragement to undertake this project and to take it to completion. Our discussions with many of them have been invaluable

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Contents

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PART I

General Principles

Chapter 1

Elements of Thermodynamics

Thermodynamics provides a phenomenological description of nature, self-contained from an axiomatic point of view, considering, as a principle, matter in an aggregated form without any microscopic assumption. During the 20th Century, the common presentation of this theory followed the historical developments, with laws and examples fundamentally based on and explained by considering the classical problems of thermal engineering. Following this trend, it was, and still is, usual to see the formulation of the second law based on the Kelvin and Clausius prescriptions. Historically, with such a law, by using the Carnot cycle and the Clausius theorem, the existence of a state function called *entropy* (from the Greek, *transformation*) is then formulated. Tisza [1] and Callen [2], in a rigorous presentation, used the entropy function and the notion of an extremum principle as an ontological starting point to build the thermodynamic theory. This procedure equips a physicist with a readable formalism, providing a way to encompass the effect of time in the context of thermal approaches and yet bringing notions of thermal laws to the realm of the quantum field theory. We present an outline of the main elements of the equilibrium thermodynamics along the lines introduced by Tisza and Callen.

We describe four formulations of thermodynamics and the compatibility among them, that is: (i) the formulation based on the fundamental relation (or equation) in which the function of state entropy, S, or the energy, E, is given explicitly; (ii) the formulation using the Legendre transformation of S or E, giving rise to the thermodynamical potentials, such as the Helmholtz free energy and enthalpy; (iii) the formulation based on the set of equations of state, involving the first derivative of the extensive quantities as S or E. Such derivatives are zero-order homogeneous functions, and describe intensive variables such as pressure ($P = -\partial E/\partial V$), temperature ($T = \partial E/\partial S$), and so on; and (iv) the formulation based on second derivatives, describing quantities like specific heat, among others. The importance of formulations (iii) and (iv) relies on the straightforward connection with experiments.

Regarding the theoretical structure of the thermal formalism, it is worth emphasizing that it is similar to the theory of a mechanical system, in the sense that, first a definition for the notion of thermal state is introduced, and subsequently

the changes in the states are analyzed with causal laws. Although, in equilibrium, thermodynamics time does not play a role as it does in mechanics, we can still distinguish the kinematic and the dynamic aspects of the theory. The former is related to the definition of thermodynamic (thermal) variables, the measurability, the definition of the state of a thermal system, and the definition of specific processes. The dynamical aspects are related to changes in the state and laws regulating such changes. This scheme also works when time is a relevant parameter, such that nonequilibrium processes take place. For further readings, we suggest Refs. [1–7].

1.1 Kinematical aspects of thermal physics

The theoretical description of a physical system can be carried out by, first of all, defining the points in space and time where processes of measurement and tests of such a theory are supposed to take place. This leads us to the usual notion of a reference frame, defined by the of transformation from one point to another in space and time. One important aspect associated with the introduction of a reference frame is that the notion of space and time are defined simultaneously. For equilibrium thermal processes space only plays a significant role and is defined by a proper definition of a ruler. In this chapter we consider non-relativistic thermodynamics, then we have Galilean reference frames. We assume as a reference frame the laboratory system, without addressing to any change of coordinates. The characterization of a thermal system will then be given by a set of macroscopic variables selected in advance by an observer located in the laboratory. These variables are, for example, internal energy (E), pressure (P), volume (V), number of moles (N), temperature (T), among others. The definition of such thermal variables is given in association with the measurement process through the use of constraints and walls. Volume is measured by rulers; temperature, which is interpreted in a first moment as a quantity providing the degree of warmth of a body, is measured by thermometers. We say that walls define a volume when their sizes are fixed. Walls restrictive to energy of any kind give rise to an *isolated system*. When the walls of a system permit a very slow flow of energy to a system via mechanical work only, the walls are called *adiabatic*. Walls are called *diathermic* when changes of the energy between two systems are permitted via a difference of temperature.

There are two kinds of thermal variables. To realize that, consider a macroscopic homogeneous system, divided into a number of similar subsystems. For instance, a gas in a box can be seen as formed by a collection of sub-boxes. A variable is said to be *extensive* when its value is equal to the sum of values of each subsystem. Examples of such type of variables are energy, volume and number of moles. A variable is said to be *intensive* if its value is independent of subsystems. As examples we have temperature, pressure and all the densities defined from the extensive variables as energy density, volume density, number of moles density (or simply, density), and so on.

The *state* of a macroscopic system is defined by specifying a set of thermal variables, or in a more general sense, by a function of the state of the system. Usually, the evolution of an isolated system is such that, after some time, the system reaches a final state in which its variables no longer change in time. Such a state is the so-called *thermal equilibrium state,* and is defined by a set of extensive parameters, including energy necessarily. An equilibrium state will be denoted by $x = \{x_0, x_1, \ldots, x_r\}$, with $x_0 = E$. A *simple system* is defined by setting $x_1 = V$, $x_2 = N_1$, $x_3 = N_2, \ldots$, where N_1, $N_2, \ldots$ are the number of moles of different substances; this is the case, for instance, of a mixture of gases in a box with no chemical reactions.

The measurability of the variables like V and N, as we have said, follows standard methods. The measurement of the energy E, however, requires a careful discussion. To begin, we have to recall that the notion of energy has its origin in mechanics. That is, energy is defined in terms of the notion of work, measured in the MKS system in Joules, J, with 1 J = 1 Nm, such that the difference between two energy levels of a system is physically associated with the change of the mechanical state. Therefore, even treating a thermal system, the internal energy has to be measured by a process involving mechanical work. The concept of energy conservation, however, is supported by the Joule experiment.

Consider a change in a system from a state a to a state b. The Joule experiment assures that if we isolate this system by adiabatic walls, then always there exists a mechanical procedure by which we can take the system from a to b or vice versa. In this way the quantity of energy that the system receives from or liberates to its neighborhood can be measured by a well defined mechanical method. Take, for instance, a gas in a box of volume V_a at pressure P_a and temperature T_a. The system is set in contact with a block of ice, such that at the final equilibrium new values for volume, temperature and pressure are, respectively, V_b, T_b and P_b, with $T_a > T_b$. It is not so simple to generate a mechanical procedure to bring the system from a to b, but is much more trivial to find a mechanical apparatus to raise the temperature of the system from the state b, taken as the initial state, to the final state a. In both situations we assume that the energy flow is the same. This is an example where there are energy flows to or from a system conditioned by the difference of temperature, via diathermic walls. This flow is called *heat* and was initially measured in arbitrary units called *calorie* (Cal). With Joule, the energy content of each *cal* was established experimentally resulting in 1 Cal = 4.184 J.

If we treat equilibrium states, we assume that two arbitrary states can be connected to each other through a process composed of an infinity of intermediary states. Processes like that are called *quasi-static*. This notion is necessary in order to give a proper definition to a differentiable thermal quantity. The mechanical work associated with a system described by the parameters $x = \{E, x_1, \ldots, x_r\}$ can

Table 1.1 Mechanical works and generalized forces

Infinitesimal work dW	Type of force
$-PdV$	Pressure P
$\sum_{j=1}^{l} \mu_j dN_j$	Chemical potential μ_j
$\mu_0 \mathbf{H}_{ext} \cdot d\mathbf{I}_j$	Magnetic field $\mathbf{H}$
$\mathbf{E}_{ext} \cdot d\mathbf{p}$	Electric field $\mathbf{E}$

be written as

$$dW = f \cdot dx = \sum_{j=1}^{l} f_j dx_j, \quad l \leq r, \tag{1.1}$$

where f_j is the applied generalized force and x_j is the corresponding extensive parameter modified by the action of f_j. Expressions for mechanical work are given in Sec. 1.1 for different systems, where P stands for pressure; μ_j for the chemical potential; μ_0 for the vacuum permissivity; $\mathbf{H}_{ext}$ for the external magnetic field; $\mathbf{I}_j$ for the magnetic dipole moment, where $\mu_0 \mathbf{H}_{ext}$ is the force associated with the extensive variable $\mathbf{I}_j$; $\mathbf{E}_{ext}$ for the electrical field and $\mathbf{p}$ the electric dipole moment.

Up to now the characterization of a thermal system has been based on aspects involving the definition of a thermal state, without a specification of the laws describing the changes in the state. This dynamical characterization is the subject of the following section.

1.2 Dynamical aspects of thermal physics

First law of thermodynamics

In order to establish laws controlling the evolution of a thermal equilibrium state, first consider an infinitesimal energy flow to a system via work (dW) and heat (dQ), and let us assume the conservation of energy. Then from the Joule experiment we can write infinitesimal changes in the internal energy (dE) in the following way

$$dE = dQ + dW. \tag{1.2}$$

This expression is called the *first law of thermodynamics*, and it expresses the energy conservation taken as a fundamental law. Observe that the content of the mathematical differential can be assumed for dE, since E can be taken as a function of variables of the thermal system — a function of state. But this is not the case for dQ and dW, which express only small flows to or from the system.

Second law of thermodynamics

The first law is not enough to treat all the richness of thermal processes. For instance, it is a well-established experimental result that if two simple systems are

set forth in thermal contact with one another, the flow of heat will take place from the hotter system to the colder one. The reversal of this process, without any external intervention, is not observed, although it does not contradict the first law. In order to address this question, let us consider a system in a state given by the set $x = \{E, x_1, \ldots, x_r\}$ and assume the existence of a state function $S = S(E, x_1, \ldots, x_r)$ to be called *entropy*. The entropy $S(E, x_1, \ldots, x_r)$ is, by definition, an extensive, analytical and monotonically increasing function in the variable E. Besides that, in the absence of internal constraints, values of extensive variables are those that make S maximum for an equilibrium state. That is,

$$\delta S|_{\text{equilibrium}} = 0,$$
$$\delta^2 S|_{\text{equilibrium}} < 0.$$

This principle is called *the second law of thermodynamics.*

With the second law, thermal processes can be classified as *reversible* or *irreversible*. An irreversible process is that one which, if taken as reversible, would tend to minimize S, contradicting the second law. A typical example of such a process is the free expansion of a gas, which is a nonequilibrium process. In the case of equilibrium, a process is reversible when it can be recovered quasi-statically through a set of equilibrium states. In this case, the entropy is constant, in agreement with the second law.

Third law of thermodynamics

The *third law* states that by a number of finite steps, it is impossible to lower the temperature to $T = 0$. A consequence of this principle is that if a system, in a state characterized by a variable x (finite), is cooled to another state characterized by $x + \delta x$, then at $T = 0$, $\delta S|_a = 0$, or

$$\left(\frac{\partial S}{\partial x}\right)_{T\to 0} = 0. \tag{1.3}$$

An experimental result derived from this principle is that

$$\lim_{T\to 0}\left(\frac{\partial S}{\partial P}\right)_{T\to 0} = -\lim_{T\to 0}\left(\frac{\partial V}{\partial T}\right)_P = 0.$$

This law, formulated by Nerst in 1905, is interpreted sometimes in statistical mechanics as an entropy condition, fixing the value of the entropy as $S = 0$ at $T = 0$ [2, 8].

1.3 Equations of state

Due to the second law, the entropy S is an analytical function in the energy variable. Then we can write in a unique way

$$S = S(E, x_1, \ldots, x_r) \tag{1.4}$$

or equivalently

$$E = E(S, x_1, \ldots, x_r). \tag{1.5}$$

Relations given by Eqs. (1.4) and (1.5) are called *fundamental equations (*or *relations).* "Fundamental" in the sense that if we know one of these relations, the properties of a thermal system can be obtained. We write the fundamental equation as

$$\Psi = \Psi(x_0, x_1, \ldots, x_r) \equiv \Psi(x), \tag{1.6}$$

such that taking $\Psi = S$ and $x_0 = E$, Eq. (1.4) is recovered and the fundamental equation is said to be in the *entropy representation.* On the contrary, taking $\Psi = E$ and $x_0 = S$, Eq. (1.5) is obtained and the description is referred to as the *energy representation.*

Since S is an extensive function, it is a first-order homogeneous function. Indeed, for a system composed of m subsystems, the entropy can be written as

$$\begin{aligned} S &= S(E, x_1, \ldots, x_r) \\ &= \sum_{k=1}^{m} S_k, \end{aligned} \tag{1.7}$$

where S_k is the entropy of the k-th system. Then taking for instance a system characterized by the state $E, x_1, \ldots, x_r$, with the fundamental equation given by $S(E, x_1, \ldots, x_r)$, another system can be constructed by a dilation of the former one by writing $\lambda E, \lambda x_1, \ldots, \lambda x_r$ such that the new fundamental equation is λS. As a result of Eq. (1.7), the entropy of the new system is given by

$$S(\lambda E, \lambda x_1, \ldots, \lambda x_r) = \lambda S(E, x_1, \ldots, x_r). \tag{1.8}$$

The same result is true for the fundamental equation in the energy representation, that is,

$$E(\lambda S, \lambda x_1, \ldots, \lambda x_r) = \lambda E(S, x_1, \ldots, x_r). \tag{1.9}$$

We have stated that Ψ is a first-order homogeneous function, that is

$$\Psi\left(\lambda x_0, \lambda x_1, ..., \lambda x_r\right) = \lambda \Psi\left(x_0, x_1, ..., x_r\right). \tag{1.10}$$

As a consequence, differentiating Eq. (1.10) with respect to λ, we have

$$\sum_j \frac{\partial \Psi\left(...\lambda x_j\right)}{\partial\left(\lambda x_j\right)} x_j = \Psi\left(x_0, ..., x_r\right). \tag{1.11}$$

On the other hand, taking the differential of Eq. (1.6), we obtain

$$d\Psi = \sum_{j=0}^{r} F_j dx_j, \tag{1.12}$$

where

$$F_i = \left(\frac{\partial \Psi}{\partial x_i}\right)_{x_0 \ldots x_{i-1}, x_{i+1} \ldots x_r} \quad ; \quad i = 0, ..., r. \tag{1.13}$$

The notation $(\,...\,)_y$ means that y is held fixed. For simplicity, we drop this index. Notice that λ is an arbitrary parameter; then setting $\lambda = 1$ in Eq. (1.11), and using Eq. (1.13), we find

$$\Psi = \sum_{j=0}^{r} F_j x_j. \tag{1.14}$$

This is a basic result showing that if we know the set of $(r+1)$-relations given by Eq. (1.13), then we can solve, in principle, the thermodynamical problem by writing the fundamental relation as given in Eq. (1.14). The $(r+1)$-relations given by Eq. (1.13) are called the set of *equations of state.*

The interest in equations of state lies in practical aspects. To see this, let us analyze the physical content of the functions F_j . Observe that since $\Psi\left(x_0, ..., x_k\right)$ is a first-order homogeneous function, its derivatives, $F_i = (\partial\Psi/\partial x_i)$, are zero-order homogeneous functions, that is

$$F_i\left(\lambda x_0, ..., \lambda x_r\right) = F_i\left(x_0, ..., x_r\right). \tag{1.15}$$

The functions $F_i\left(x_0, ..., x_r\right)$, also called "forces," are natural candidates to stand for intensive variables, like temperature, pressure and density of moles. Then the equations of states (1.13), relating intensive variables, are directly accessible by experiment, which is not the case for Ψ.

Since F_i are zero-order homogeneous functions, we have

$$\begin{aligned} F_i &= \left(\frac{\partial\Psi}{\partial x_j}\right) = F_i\left(x_0, ..., x_r\right) \\ &= F_i(\lambda x_0, ..., \lambda x_r) \\ &= F_i\left(\frac{x_0}{x_r}, ..., \frac{x_{r-1}}{x_r}, 1\right) \ , \quad i = 0, ..., r, \end{aligned} \tag{1.16}$$

where in the last line we have taken the arbitrary quantity λ to be $\lambda = 1/x_r$. Therefore, we have $r+1$ functions F_i, each one depending on r intensive variables, since a ratio like x_{r-1}/x_r is an intensive quantity. Thus Eq. (1.16) show that the set of equations of state can be written exclusively in terms of intensive variables. The decrease in the variable number (originally Ψ required $(r+1)$ variables, while each intensive function is written in terms of r variables) reflects the fact that, for instance, the molar density, rather than the number of moles, is important in this description. The elimination of the r variables from Eq. (1.16) gives rise to a relation among the $r+1$ intensive variables. This relation can be derived from general arguments and it is called the Gibbs-Duhem relation. We proceed with the physical identification of each intensive variable $F_i\left(x_0, ..., x_r\right)$.

1.4 The meaning of intensive variables

We consider a simple isolated system composed of two subsystems, denoted by a and b, such that V_a, V_b, N_a and N_b are kept fixed. Suppose there is a virtual flow

of heat between a and b, that is E_a and E_b can suffer a variation, where the total energy is given by

$$E = E_a + E_b. \tag{1.17}$$

The *equilibrium conditions* are specified by considering S as constant at equilibrium. Notice that E is constant since the system is isolated. Let us then analyze this fact in the entropy representation. In this case we denote,

$$\Psi = S \quad \text{and} \quad F_j^{(s)} = \frac{\partial S}{\partial x_j}.$$

For the composite system, the entropy can be written as

$$S = S_a\left(E_a\right) + S_b\left(E_b\right).$$

If the system reaches equilibrium, the second law states that $\delta S = 0$; therefore

$$\frac{\partial S}{\partial E_a} = \frac{\partial S_a}{\partial E_a} + \frac{\partial S_b}{\partial E_b}\frac{\partial E_b}{\partial E_a} = 0.$$

Using Eq. (1.17) with E being constant, i.e. $\delta E_a = -\delta E_b$, we derive

$$\frac{\partial S_a}{\partial E_a} = \frac{\partial S_b}{\partial E_b}. \tag{1.18}$$

In terms of the forces we write

$$F_{0,a}^{(s)} = \frac{\partial S_a}{\partial E_a}, \quad F_{0,b}^{(s)} = \frac{\partial S_b}{\partial E_b},$$

where $F_{0,\alpha}^{(s)}$ stands for the force in the entropy representation (s), considering $\alpha = a$ or $\alpha = b$. From Eq. (1.18) we obtain

$$F_{0,a}^{(s)} = F_{0,b}^{(s)}. \tag{1.19}$$

This equation is the equilibrium condition written in terms of the intensive variable $F_{0,\alpha}^{(s)}$.

At this point, we have to analyze the stability conditions of the systems. That is, suppose the system is virtually displaced from equilibrium with $E =$ constant, such that two systems are set in thermal contact with each other. During the evolution of the system up to the final equilibrium state, S increases, and this fact can be expressed by $\delta S > 0$. Under this condition we have

$$\begin{aligned}\delta S = \delta S_a + \delta S_b &= \left(\frac{\partial S_a}{\partial E_a} - \frac{\partial S_b}{\partial E_b}\right)\delta E_a \\ &= (F_{0,a}^{(s)} - F_{0,b}^{(s)})\delta E_a > 0.\end{aligned}$$

Assuming $F_{0,a}^{(s)} > F_{0,b}^{(s)}$, it follows that $\delta E_a > 0$ and $\delta E_b < 0$. Writing

$$F_{0,\alpha}^{(s)} = \frac{1}{\tau_\alpha}\ ,$$

then we have

$$\tau_a < \tau_b. \tag{1.20}$$

Table 1.2 Extensive variables

$\partial E/\partial S = T$	temperature
$\partial E/\partial V = -P$	pressure
$\partial E/\partial N = \mu$	chemical potential

In the reverse way, assuming $F^{(s)}_{0,a} < F^{(s)}_{0,b}$, we have $\delta E_a < 0$ and $\delta E_b > 0$. As a consequence

$$\tau_a > \tau_b. \tag{1.21}$$

In conclusion, in either case, heat flows from a system with the higher τ to the one with lower τ; and at equilibrium, from Eq. (1.19) we obtain $\tau_a = \tau_b$, implying that there is no heat flow between the two systems. Therefore, since τ is an intensive quantity, it is the natural variable to represent the temperature, T, in accordance with the intuitive notion of temperature as a measure of the perception of coldness and warmness.

Recall that S increases monotonically with E, such that $(\partial E/\partial S) = T \geq 0$. This result ensures that T is positive definite. The third law fixes, as stated, $S = 0$ for the state at $T = 0$. The temperature, T, is measured in Kelvin degrees, denoted by K. Observe that this interpretation for $(\partial S/\partial E) = 1/T$ could be derived in the energy representation. In this case, we use the notation $F^{(E)}_{0,\alpha} = \partial E/\partial S = T$.

We proceed with this analysis for the sake of identification of the physical meaning of other intensive variables. Some results are given in Sec. 1.2 for a simple system. By this procedure, temperature is the "force" regulating the equilibrium for the energy flow in the form of heat. Pressure is the "force" regulating the equilibrium for the energy flow in the form of mechanical work defined via the variation of volume, and the chemical potential regulates the equilibrium for the exchange of matter among systems.

For a simple system in the energy representation, Eqs. (1.12) and (1.14) are given by

$$dE = TdS - PdV + \sum_{j=1}^{k} \mu_j dN_j \tag{1.22}$$

and

$$E = TS - PV + \sum_{j=1}^{k} \mu_j N_j. \tag{1.23}$$

Comparing Eq. (1.22) with Eq. (1.2), it results in

$$dQ = TdS. \tag{1.24}$$

Therefore, a quasi-static flow of heat to a system is associated with the increasing of the entropy.

With the result given in Eq. (1.24), the physical content of the second law as enunciated by Kelvin and Clausius is [2, 3]:

> Kelvin: *It is not possible to realize a process, in which the only effect is to remove heat from a heat bath to give rise to an equivalent quantity of work.*
>
> Clausius: *It is not possible to realize a process, in which the only effect is to transfer heat from a colder body to another one that is hotter.*

These two statements are equivalent to each other and can be derived from the second law as presented by following the Clausius procedure. Clausius introduced the entropy function as a theorem from the above enunciations. Here we have reversed the order.

Finally, Eqs. (1.12) and (1.14) in the entropy representation are given by

$$dS = \frac{1}{T}dE + \frac{P}{T}dV - \frac{1}{T}\sum_{j=1}^{k}\mu_j dN_j. \tag{1.25}$$

and

$$S = \frac{1}{T}E + \frac{P}{T}V - \frac{1}{T}\sum_{j=1}^{k}\mu_j N_j. \tag{1.26}$$

1.5 Thermodynamical potentials

We find that the set of relations given in Eq. (1.13) provides an alternative procedure to treat thermal systems. In addition, as already observed, an advantage of this formalism based on $r+1$ equations of state is that the intensive variables are more easily handled from an experimental perspective. For instance, for a dilute and hot gas, experiments shows that $P \sim \rho T$, where $\rho = N/V$ is the density. This is a state equation for the so-called *ideal gas*. The other equations for such a system are also available experimentally. A problem here is that despite experimental advantages, the full set of state equations remains inscrutable for a general situation. Such a difficulty naturally suggests a search for other formulations of thermodynamics. We can think of a thermal system considering the state defined by a set of mixed, intensive and extensive, variables. To find such a formalism, a preliminary step should be to define the fundamental equation via a function of state depending on a set of mixed variables, keeping compatibility with the aforementioned formulation.

For a specific situation, consider a system described by the fundamental equation

$$E = E(S, x_1, ..., x_r).$$

Then we look for an equivalent representation for E, such that the state of the system is characterized by the set of mixed variables $\{T, x_1, ..., x_r\}$, being the fundamental equation described by

$$F = F(T, x_1, ..., x_r).$$

Note that a formulation in terms of F is of interest to describe the process of a system with constant temperature (an *isothermal process*). In this case, the system

is no longer isolated in reaching the equilibrium state, which is quite often the experimental situation. Beyond that, we have a reduction in the number of variables from $r+1$, with the fundamental equation for E, to r, with the fundamental equation written in terms of F.

Introducing the function F, observe that the difference between E and F is in the variable S: in the function $E(S, x_1, ..., x_r)$, the variable S was changed to $T = \partial E/\partial S$ in F. Therefore, the function F can be introduced from E via a Legendre transformation. Since the motivation and the solution for the problem have been identified, there is no need to work with the specific energy representation.

Consider then the fundamental equation $\Psi = \Psi(x_0, x_1, ..., x_r)$. The Legendre transformation of Ψ in $r-k$ variables $x_{k+1}, ..., x_r$, is defined by

$$L = \Psi - \sum_{i=k+1}^{r} F_i x_i, \tag{1.27}$$

where $F_i = \partial\Psi/\partial x_i$. The differential of L is given by

$$dL = \sum_{i=0}^{k} F_i dx_i - \sum_{i=k+1}^{r} (x_i)\, dF_i. \tag{1.28}$$

This shows that L is a function in the variables $(x_0, ..., x_k, F_{k+1}, ..., F_r)$, i.e. $L = L(x_0, ..., x_k, F_{k+1}, ..., F_r)$. The functions L are the *thermodynamical potentials*, and F_i is said to be the *conjugate* of x_i. Therefore Eq. (1.27) defines the potential, while Eq. (1.28) shows its dependence on the variables. In the following the thermodynamical potentials for simple systems are identified explicitly using Eqs. (1.27) and (1.28) in the energy representation.

Helmholtz free energy

Define the Helmholtz free energy, F, as

$$F(T, V, N_1, ..., N_k) = E - TS, \tag{1.29}$$

such that

$$dF = -SdT - PdV + \sum_{j=1}^{k} \mu_j dN_j. \tag{1.30}$$

This free energy is useful to describe isothermal processes. Part of the internal energy is then used to keep the temperature constant, and only the rest can be used for the realization of mechanical work.

Enthalpy

Defining the function

$$H = H(S, P, N_1, ..., N_K) = E + PV \tag{1.31}$$

we have

$$dH = TdS + VdP + \sum_{j=1}^{k} \mu_j dN_j \ . \tag{1.32}$$

The enthalpy, $H(S, P, N_1, ..., N_K)$, is useful to describe processes at constant pressure (*isobaric process*), as for instance a chemical reaction in an open container, such that P is the atmospheric pressure.

Gibbs free energy

The Gibbs free energy is defined as

$$G(T, P, N_1, ..., N_k) = E - TS + PV, \tag{1.33}$$

so that

$$dG = -SdT + VdP + \sum_{j=1}^{k} \mu_j dN_j. \tag{1.34}$$

This free energy combines aspects of the Helmholtz free energy and enthalpy.

Grand thermodynamical potential

Finally the grand thermodynamical potential is given as

$$\Omega_G(T, V, \mu_1, ..., \mu_k) = E - TS - \sum_{i=1}^{k} \mu_i dN_i \tag{1.35}$$

with

$$d\Omega_G = -SdT - \sum_{i=1}^{k} N_j d\mu_j - PdV.$$

This potential is useful to determine the full set of state equations, as we will see in the next section.

The Legendre transformations can be introduced in the entropy representation, in which $\Psi = S$. Following the same procedure as in the energy representation, with Eqs. (1.27) and (1.28), we can derive the thermodynamical potentials in the entropy representation. These potentials are called *Massieu functions*.

Previously the thermal state was introduced by a set of extensive variable. However, if the thermodynamic formalism is given in terms of potential functions, the state is represented by a set of mixed, intensive and extensive, variables. In this case, the restriction is that the state is not described by pairs of conjugate variables. For instance (S, P, N) can be used to describe the state of a simple system. But this is not the case for (S, T, N), since S and T are conjugate variables.

1.6 Gibbs-Duhem relation

In this section we go back to the equations of state. We have seen that the fundamental equation, $\Psi = \Psi(x_0, ..., x_r)$, can be written as in Eq. (1.14), that is

$$\Psi = \sum_{i=0}^{r} F_i x_i.$$

Taking the differential of Eq. (1.14) we have

$$d\Psi = \sum_{j=0}^{r} (dF_i x_i + F_i dx_i).$$

Using the differential of $\Psi = \Psi(x_0, ..., x_r)$,

$$d\Psi = \sum_{i=0}^{r} F_i dx_i,$$

we find the following relation among the intensive variables

$$\sum_{i=0}^{r} x_i dF_i = 0. \tag{1.36}$$

This equation is the Gibbs-Duhem *relation*.

An immediate consequence of the Gibbs-Duhem relation is in the number of state equations. As mentioned before, we have to find $r + 1$ state equations for the F_j, functions of r variables. For instance, for a simple system with (S, V, N) the intensive variables are (T, P, μ). Therefore, we have to look for three equations of state. We can use experimental results to infer only two of them, since the third one can be written by using the Gibbs-Duhem relation.

For a simple system in the energy representation with $E = E(S, V, N)$, the Gibbs-Duhem relation, Eq. (1.36), reads

$$SdT - VdP + Nd\mu = 0. \tag{1.37}$$

Using Eq. (1.34), the differential for the Gibbs free energy, that is

$$dG = -SdT + VdP + \mu dN,$$

and Eq. (1.37), we find $d(\mu N) = dG$. Writing $g = G/N$, it follows that

$$g = \mu.$$

Therefore, for simple systems the density of the Gibbs free energy is the chemical potential.

In the entropy representation, where $\Psi \equiv S = S(E, V, N)$, the Gibbs-Duhem relation is given by

$$d(\mu/T) = \varepsilon d(1/T) + \frac{1}{n} d(P/T),$$

where $\varepsilon = E/N$ and $n = N/V$.

1.7 Second derivatives

We analyze in this section the formulation of thermodynamics using second derivatives of the fundamental relations. The importance of this is that it brings the formulation of thermodynamics still closer to the experimental language.

The starting point of this formulation is an attempt to establish relations involving the variation of extensive variables. Consider the variables $F_i = F_i(x_0, ..., x_j, ..., x_r)$ and $F_j = F_j(x_0, ..., x_j, ..., x_r)$. Notice that by isolating x_j in the function F_i, and using this in F_j, we obtain, for any $i, j = 0, 1, 2, ..., r$, the following equation

$$F_j = F_j(x_0, ..., x_{j-1}, F_i, x_{j+1}..., x_r);$$

or in terms of infinitesimals,

$$dF_j = dF_i \left(\frac{\partial F_j}{\partial F_i}\right)_{x_0,...,x_{j-1},x_{j+1}...,x_r}.$$

These equations can be solved for particular systems if we specify derivatives $\partial F_j/\partial F_i$, which is just a function of second derivatives of the fundamental equation, since we can write, for instance

$$dF_j = \left(\frac{\partial F_j}{\partial x_i}\right)\left(\frac{\partial x_i}{\partial F_i}\right) dF_i.$$

This result demands a carefully analysis of second derivatives and relations among them. The connection among all second derivatives is known as *Maxwell relations*. We consider a specific situation of a simple system.

Consider a simple system described by the fundamental equation

$$E = E(S, V, N), \tag{1.38}$$

in a closed container of adiabatic walls, with the number of moles, N, fixed. Initially the system is at a temperature T_i with a pressure P_i. The system is squeezed quasi-statically up to a final pressure P_f. The thermodynamical problem is then to find final values for the volume, V_f, the temperature, T_f, the internal energy, E_f, the entropy, S_f, and the chemical potential, μ_f.

As the process is quasi-static and adiabatic, then $dQ = 0$. As a consequence $dS = dQ/T = 0$, such that $S_i = S_f$. Assuming that Eq. (1.38) is given, by taking derivatives, we write equations of state, which are three in number. Two of them are written as

$$T = T(S, V, N), \tag{1.39}$$

$$P = P(S, V, N). \tag{1.40}$$

The third equation for μ is derived from the Gibbs-Duhem relation. An equation between T and P can be derived by elimination of V in Eqs. (1.39) and (1.40). The result is written as

$$T = T(S, P, N).$$

Since S and N are constant, the variation of T is

$$dT = \left(\frac{\partial T}{\partial P}\right)_{S,N} dP. \tag{1.41}$$

Besides

$$\left(\frac{\partial T}{\partial P}\right)_{S,N} = \left(\frac{\partial T}{\partial V}\right)_{S,N} \left(\frac{\partial V}{\partial P}\right)_{S,N}. \tag{1.42}$$

Similarly, we verify changes in the temperature with volume, using Eq. (1.39), that is,

$$dT = \left(\frac{\partial T}{\partial V}\right)_{S,N} dV. \tag{1.43}$$

These types of equations, as Eqs. (1.41) and (1.43), are all we need to provide an understanding of the thermodynamical problem; but above all, such relations are very useful for experimental tests. On the other hand, if we assume that Eqs. (1.41) and (1.43) are given in advance, then we can reverse the reasoning and write the state equations, as well as fundamental equations.

Relations as given by Eqs. (1.41) and (1.43) can be determined if we find a way, may be experimentally, to provide the derivatives like $(\partial T/\partial V)_{S,N}$, which are second derivatives of E or S. This requires an analysis of such second derivatives and the relations among them.

For this simple system we have only three independent second derivatives, for instance

$$\frac{\partial^2 E}{\partial S^2}; \quad \frac{\partial^2 E}{\partial V \partial S}; \quad \frac{\partial^2 E}{\partial V^2}. \tag{1.44}$$

Any other relation can be written as a combination of these three derivatives. To see that this is the case, consider for instance the derivative in Eq. (1.43), $(\partial T/\partial V)_{S,N}$, which can be written as

$$\left(\frac{\partial T}{\partial V}\right)_{S,N} = \frac{\partial}{\partial V}\left(\frac{\partial E}{\partial S}\right) = -\left(\frac{\partial P}{\partial S}\right)_{V,N}. \tag{1.45}$$

By experimental necessity, for a simple system with N being constant, the set of three independent second derivatives is usually the following.

Thermal expansion coefficient

The thermal expansion coefficient, α_P, provides a measure for the fraction of volume increased by raising the temperature, when N and P are fixed.

$$\alpha_P = -\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = -\frac{1}{v}\left(\frac{\partial v}{\partial T}\right)_P; \quad v = V/N = n^{-1}. \tag{1.46}$$

Isothermal compressibility

The isothermal compressibility, κ_T, provides a measure for the fraction of the decreasing volume by an increase of pressure, when T and N are constant.

$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T = -\frac{1}{v}\left(\frac{\partial v}{\partial P}\right)_T . \tag{1.47}$$

Specific heat

The specific heat provides a measure for the heat flow by mole, necessary to increase the temperature by one degree. As a matter of convenience, this measure is carried out at constant pressure or at constant volume, that is

$$C_p = \frac{T}{N}\left(\frac{\partial S}{\partial T}\right)_P = T\left(\frac{\partial s}{\partial T}\right)_P = \frac{1}{N}\left(\frac{dQ}{dT}\right)_P \tag{1.48}$$

and

$$C_V = \frac{T}{N}\left(\frac{\partial S}{\partial T}\right)_V = T\left(\frac{\partial s}{\partial T}\right)_V = \frac{1}{N}\left(\frac{dQ}{dT}\right)_V . \tag{1.49}$$

Observe that the second derivative $(\partial T/\partial P)_{S,N}$ in Eq. (1.41) can be written as

$$(\partial T/\partial P)_{S,N} = VT\alpha_P/C_P$$

such that

$$dT = VT\frac{\alpha_P}{C_P}dP. \tag{1.50}$$

This result shows that a knowledge of the second derivatives C_P, α_P and κ_T provides an alternative way to introducing the thermodynamical theory.

We close this section with a brief discussion about a thermal magnetic system, defined by the fundamental equation which is a function of $S, V, \mathcal{M}, N$, that is

$$E = E\left(S, V, \mathcal{M}, N\right).$$

where $\mathcal{M}$ is the magnetic dipole moment. The magnetic coefficients similar to α_P, κ_T, C_P and C_V are:

Coefficient of thermal variation of the magnetic moment (analogous to α_P)

$$\alpha = \left(\frac{\partial \mathcal{M}}{\partial T}\right)_{P,H_{ex}} . \tag{1.51}$$

Magnetic susceptibility, κ_P, and isothermal susceptibility κ_T

$$\kappa_{T,P} = \frac{1}{V}\left(\frac{\partial \mathcal{M}}{\partial H_{ex}}\right)_{T,P} = \left(\frac{\partial M}{\partial H_{ex}}\right)_{T,P} . \tag{1.52}$$

Specific heat

$$C_{P,H_{ex}} = T\left(\frac{\partial S}{\partial T}\right)_{P,H_{ex}} \quad \text{or} \quad C_{P,\mathcal{M}} = T\left(\frac{\partial S}{\partial T}\right)_{P,\mathcal{M}} , \tag{1.53}$$

$$C_{V,H_{ex}} = T\left(\frac{\partial S}{\partial T}\right)_{V,H_{ex}} \quad \text{or} \quad C_{V,\mathcal{M}} = T\left(\frac{\partial S}{\partial T}\right)_{V,\mathcal{M}}. \tag{1.54}$$

The magnetic properties are often described by the susceptibility as a function of temperature, that is

$$\chi_{T,P} = \chi_{T,P}(T, P, H_{ex}) = \left(\frac{\partial M}{\partial H}\right)_{T,P}. \tag{1.55}$$

Since the relation among H, H_{ex} and M is given, we can find the relation between $\chi_{T,P}$ and $\kappa_{T,P}$, and the state equation

$$M = M(T, P, H_{ex}), \tag{1.50}$$

by integration.

1.8 Example: ideal gas and generalizations

Now we treat an example, by considering a simple system as a model characterized by a mono-component ideal gas, to exemplify the aforementioned thermodynamical formalism. Later we treat the problem to find a prescription to derive generalized state equations.

1.8.1 *State equation for an ideal gas*

An ideal gas is a chemically inert gas satisfying the following state equation

$$P = \frac{RT}{v} \quad \text{and} \quad T = \frac{2}{3R}\varepsilon,$$

where $v = V/N$ and $\varepsilon = E/N$. The quantity $R = 1,986\ cal/mole\ K$ is called *the universal constant of gases*. Another way to write the state equations is.

$$PV = NRT \quad \text{and} \quad E = \frac{3}{2}NRT. \tag{1.56}$$

These equations were established by experiments and are usually valid for a gas at high temperature and low pressure.

In order to write the fundamental relations, thermodynamical potentials and second derivatives, observe first of all that we have two state equations, but three independent extensive variables, that is, E, V and N. Then in order to use Eq. (1.14) to write the fundamental equation we have at our disposal another state equation (since, in principle, we need three of them). The third equation can be found by integrating the Gibbs-Duhem relation, Eq. (1.36), that is

$$\frac{\mu}{T} - \left(\frac{\mu}{T}\right)_0 = -\frac{3}{2}R\ln\frac{E}{E_0} - R\ln\frac{V}{V_0}, \tag{1.57}$$

where E_0, V_0, N_0 are the values for a reference state. Let us now write Eq. (1.14) in the entropy representation. This gives rise to

$$S = \frac{1}{T}E - \frac{P}{T}V - \frac{\mu}{T}N. \tag{1.58}$$

Using the state equations, Eqs. (1.56) and (1.57), we get the entropy function in terms of extensive quantities, that is,

$$S = \frac{N}{N_0}S_0 + \frac{3}{2}NR\ln\frac{E}{E_0} + NR\ln\frac{V}{V_0} - \frac{5}{2}NR\ln\frac{N}{N_0}, \tag{1.59}$$

where

$$S_0 = \frac{5}{2}N_0R - N_0\left(\frac{\mu}{T}\right)_0.$$

From Eq. (1.59), writing in the energy representation and using the Legendre transformation, thermodynamic potentials can be introduced. We leave these steps for the reader. Let us write the second derivative functions $\alpha_P, \kappa_T, C_V, C_P$:

$$\alpha_P = \frac{1}{T}\,,\ \ \kappa_T = \frac{1}{P},$$
$$C_P = \frac{5}{2}R\,,\ \ C_V = \frac{3}{2}R.$$

Therefore with this simple example we have established the usefulness of the different thermodynamical formulations.

1.8.2 *The van der Waals equation*

Although thermodynamics presents a well-defined formal structure, it would be interesting to find some prescription, at a theoretical level, to write down the fundamental equations or the equations of state, in particular, to describe more complex systems other than the ideal gas. This situation is quite close in nature to the mechanical problem to write Lagrangians explicitly. In this case the underlying symmetries can be used as a guide to write, for instance, models for the interactions. For thermal systems, such a prescription can be found if we recall that originally thermodynamics did not say a word about the microscopic nature of matter. However, we can use this microscopic viewpoint, assuming that matter is composed of particles, i.e. molecules, atoms, and so on, to implement thermodynamics. We proceed with a naive example, just to provide some flavor to this kind of reasoning.

As we have seen, an ideal gas is described by Eq. (1.56), where V is the volume of the gas container and P is the pressure. Taking into consideration that this gas is made of particles, some corrections in the ideal gas equation should be considered, resulting in a more general theory. In the case of the volume in Eq. (1.56), we can write

$$V \to V - Nb, \tag{1.60}$$

where b is a constant measuring the volume of each particle.

Assuming a molecular attraction, we expect a decrease in the pressure. That is, due to the attraction, collisions of particles with walls induce a reduction in the change of momentum, thus reducing the force on the wall; as a consequence the

pressure is lowered. Such a decrease in pressure can be considered as proportional to the number of pairs of molecules near to the wall region, that is, proportional to $n^2 = (N/V)^2$. Then the pressure should be modified to

$$P \to P - a\frac{N^2}{V^2}, \tag{1.61}$$

where a is a parameter related to the molecular interaction. Using the results of Eq. (1.60) and (1.61) in Eq. (1.56), we find

$$(V - Nb)\left(P - \frac{N^2}{V^2}a\right) = NRT.$$

or

$$P = \frac{N\ k_B T}{V - Nb} - \frac{N^2 a}{V^2}, \tag{1.62}$$

which is called the van der Waals equation. In Eq. (1.62) instead of R we have written $k_B = R/N = 1.38065 \times 10^{-23} J/K$. And thus N is to be interpreted as particle number, not moles. There is no need to use another notation since from now on N will be taken for the particle number only. The constant k_B is the Boltzmann constant.

1.9 Stability conditions and phase transitions

The second law ensures a maximum principle for the entropy, $\delta S = 0$ and $\delta^2 S < 0$, imposing stability conditions on thermodynamic systems. If the system is forced to go along a way conflicting with these conditions, then a phase transition may take place. We analyze some of these aspects in this section.

Consider a system receiving an infinitesimal amount of heat, dQ, from a heat bath at temperature T_0 and pressure P_0. In this case, as a consequence of the second law of thermodynamics, the entropy change of the system, dS, is related to dQ by

$$dQ \leq T_0 dS.$$

The equality sign holds for reversible processes. Writing $dW = -P_0 dV$ for the work done on the system by the heat bath and using the first law of thermodynamics, $dQ = dE - dW$, we have

$$dA = dE + P_0 dV - T_0 dS \leq 0,$$

where the quantity

$$A = E + P_0 V - T_0 S,$$

called *availability* of the system, describes the maximum amount of work which may be extracted from a system in contact with a heat bath. Any process taking place in the system leads to a decrease of A, which has a minimum value at equilibrium. This

stability condition can also be stated for thermodynamic potentials, implying that Helmholtz and Gibbs free energies are a minimum at equilibrium. Such stability conditions can be used to prove that $C_V > 0$ and $C_P > 0$ [7].

The equilibrium state of a simple system is determined by specifying a set of thermodynamic variables such as (E, V, N). The specification of (E, V, N), however, is not a sufficient condition to ensure a uniform state of the system. That means, we can find different states coexisting in equilibrium, which belong to different *phases* of the system. A well-known example is the coexistence of phases in water, as liquid and vapor, or even three phases, liquid, solid and vapor. The phases can be

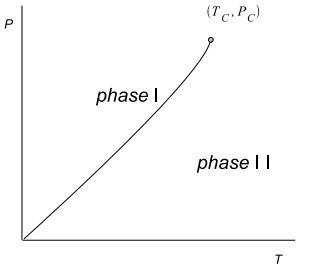


Fig. 1.1 First-order phase transition.

considered as different thermodynamic systems in equilibrium with each other; and thus, for a single system with two phases we have to state the following equilibrium phase conditions:

$$T_1 = T_2 = T, \tag{1.63}$$

$$P_1 = P_2 = P, \tag{1.64}$$

$$\mu_1(P, T) = \mu_2(P, T) = \mu. \tag{1.65}$$

We have written Eq. (1.65) with the explicit dependence on T and P to emphasize that the two phases cannot be in equilibrium at arbitrary T and P.

In a $P \times T$ diagram a phase transition can be represented by a line, as given in Fig. 1.1. If we go from region I to region II, crossing the line, we have an abrupt change in the nature of the system. That is, we find a separation of phases, at each point on the curve. The point (T_c, P_c) is called a *critical* point. Beyond that point, one can go from one region to another in a continuous way. In this case we do not meet any abrupt discontinuity among the phases.

In this type of phase transitions, we identify some specific characteristics. While the free energies of different phases are equal at the transition point, their first derivatives are discontinuous. This happens, for example, when water turns into vapor, in which case the discontinuity of entropy implies the existence of latent heat associated with the transition. This is called a *first-order phase transition*.

If the first derivatives of the free energy are continuous at the transition point, but not the thermodynamic quantities described by the second derivatives, like specific heat, compressibility and magnetization, then the system undergoes a *second-order phase transition*. Well-known examples of this transition are normal-metal to superconductor and para- to ferro-magnetic phases. In the later case, lowering the temperature below a critical value, T_c, implies a non-null magnetization, $\mathbf{M}$, appearing in the system. This ferromagnetic phase corresponds to ordered states, which have lower symmetry when compared with the disordered paramagnetic phase, where $\mathbf{M} = 0$. Distinctly from the first-order phase transition, no coexistence of phases occurs in the second-order phase transition; that is, there are no meta-stable states in either of the transition point.

The ordered phase is characterized by a non-vanishing order parameter, ϕ, which in the magnetic case can be identified with the magnetization. On the other hand, the symmetric phase has $\phi = 0$. Notice that the symmetry changes discontinuously at the transition point, since if $\phi \neq 0$ (no matter how small it is) the system presents the symmetry of the full ordered phase. Nevertheless, decreasing the temperature, ϕ changes continuously from zero to non-vanishing values at T_c. The overall behavior of order parameter with temperature is depicted in Fig. 1.2.

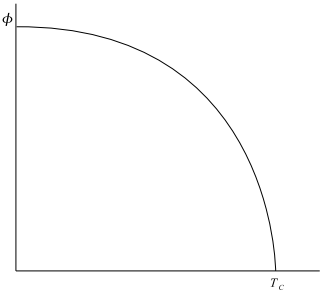


Fig. 1.2 Dependence of the order parameter with temperature.

A quantitative, phenomenological theory of second-order phase transition was proposed by Landau [7] in 1937. At a given temperature T and pressure P, for a system in equilibrium, the order parameter is determined in both phases. To describe the transition, Landau generalized the free energy allowing it to be, a function of, not only the state variables, but also of ϕ, which is taken as an independent variable. The actual value assumed by ϕ is determined by the equilibrium stability conditions, requiring that the free energy be a minimum for the given values of T and P. The next step is to assume an expansion of the generalized free energy, $\widetilde{G}(P, T, \phi)$, near the transition point, $T \sim T_c$, in powers of the order parameter, as

$$\widetilde{G}(T, \phi) = \widetilde{G}_0(T) + A(T)\phi^2 + B(T)\phi^4. \tag{1.66}$$

For simplicity, we have taken P fixed. Notice that no monomial of odd order has

been written, a fact that is justified by symmetry arguments [7]. Also the expansion is truncated at the fourth power, since the order parameter is small, $\phi \sim 0$, close to T_c and the second degree monomial alone is not enough to describe the transition. In order to guarantee that $\widetilde{G}(T,\phi)$ is bounded from below, and thus has a minimum, we take $B(T) > 0$. If $A > 0$, the minimum occurs at $\phi = 0$, the disordered phase. To have a minimum of $\widetilde{G}(T,\phi)$ for $\phi \neq 0$, corresponding to ordered phase, we should have $A < 0$. Since $\widetilde{G}(T,\phi)$ is continuous at the critical point, we must have $A(T_c) = 0$. Thus in the vicinity of T_c, we can expand $A(T)$ up to the first order in $T - T_c$, that is

$$A(T) = \alpha(T - T_c),$$

where $\alpha > 0$. With a similar reasoning, we find that at the critical point $B(T)$ is a positive constant, to be denoted by $B(T_c) = b$. Therefore, Eq. (1.66) is written as

$$\widetilde{G}(T,\phi) = \widetilde{G}_0(T) + \alpha(T - T_c)\phi^2 + b\phi^4. \tag{1.67}$$

The behavior of the Landau free energy as a function of the order parameter is illustrated in Fig. 1.3.

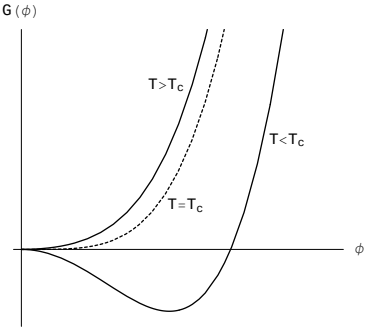


Fig. 1.3 Landau free energy, $\mathrm{G}(\phi) = \widetilde{G}(T,\phi) - \widetilde{G}_0(T)$, in a second-order phase transition.

The extrema of $\widetilde{G}(T,\phi)$ are determined by

$$\frac{\partial \widetilde{G}(T,\phi)}{\partial \phi} = 2\alpha(T - T_c)\phi + 4b\phi^3 = 0,$$

having solutions, $\phi = 0$ and

$$\phi^2 = -\frac{\alpha(T - T_c)}{2b},$$

corresponding to the minima for $T > T_c$ and $T < T_c$, respectively, since in both cases

$$\frac{\partial^2 \widetilde{G}(T,\phi)}{\partial \phi^2} = 2\alpha(T - T_c) + 12b\phi^2 > 0.$$

The entropy is given by

$$S = -\frac{\partial \widetilde{G}(T,\phi)}{\partial T} = S_0 + \alpha\phi^2;$$

and thus we observe that it varies continuously through the transition. On the other hand, the specific heat for the ordered phase, $\phi \neq 0$, is

$$C = T\frac{\partial S}{\partial T} = C_0 + \alpha^2 \frac{T_c}{2D},$$

while for the symmetric phase, $\phi = 0$, $C = C_0$. This shows that the specific heat has a discontinuity at the critical temperature.

The main features of first-order phase transitions can also be cast within a Landau thermodynamic theory. In this case, the expansion of the free energy is taken in the form

$$\widetilde{G}(T,\phi) = \widetilde{G}_0(T) + a(T)\phi^2 - b\phi^4 + c\phi^6, \tag{1.68}$$

where b and c are positive constants and $a(T) = \alpha(T - T_0)$, T_0 being a temperature parameter that does not correspond to the critical temperature. The behavior of this free energy, as a function of ϕ, is presented in Fig. 1.4.

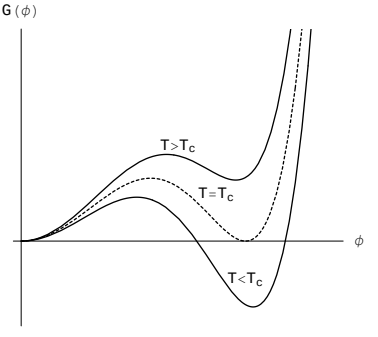


Fig. 1.4 Landau free energy, $\mathrm{G}(\phi) = \widetilde{G}(T,\phi) - \widetilde{G}_0(T)$, in a first-order phase transition.

The free energy (1.68) has two local minima occurring at $\phi = 0$ and

$$\phi_0(T) = \frac{1}{3c}\left[b + \sqrt{b^2 - 3a(T)c}\right]; \tag{1.69}$$

which minimum value of $\widetilde{G}$ is the lowest one depends on the temperature. While the absolute minimum prevails in the stable phase, the other local minimum corresponds to metastable states that show up in the supercooling. The transition temperature, at which the distinct phases can coexist in equilibrium, is determined by requiring that the two minimum values of $\widetilde{G}$ are equal, i.e. by imposing that $\widetilde{G}(T_c, \phi_0(T_c)) = 0$. This condition is equivalent to $a(T) = b^2/4c$,which implies that

$$T_c = T_0 + \frac{b^2}{4\alpha c}. \tag{1.70}$$

Note that, in a first order phase transition, the order parameter is discontinuous at T_c so that both the state and its symmetry change abruptly at the transition point. We could find the discontinuity of the entropy at the transition point, thus determining the latent heat, but we will not pursue this issue any further.

The Landau theory of phase transitions in thermodynamics can be extended to consider inhomogeneous systems, taking into account spatial fluctuations of the order parameter, such that ϕ is a field, that is $\phi = \phi(\mathbf{x})$. In this case, the expansion of $\tilde{G}(T, \phi)$ has to include derivatives of $\phi(\mathbf{x})$. For long-wavelength fluctuations, we keep only the lowest derivative terms, which has the form $(\nabla\phi)^2$. Hence, for instance, concerning a second-order phase transition we write

$$\widetilde{G}(T, \phi) = \widetilde{G}_0(T) + \alpha_0(T - T_c)\phi^2 + b\phi^4 + e(T_c)(\nabla\phi)^2. \tag{1.71}$$

Such a free energy can be viewed as an Euclidian field theory. In the quantum field theory, the thermodynamic description of the second-order phase transition is analyzed in terms of spontaneous symmetry breaking, and gives rise to new concepts such as Goldstone bosons that are related to collective states in many body systems. We will elaborate this theory including the temperature effects in the following chapters.

Chapter 2

Elements of Statistical Mechanics

Having described the macroscopic nature of matter, we turn to consider thermodynamic properties from a microscopic point of view. The main emphasis is on the microscopic definition of the Boltzmann entropy, the derivation of the Liouville-von Neumann equation and the notion of an *ensemble*. Then using the Boltzmann entropy and the second law of thermodynamics, we derive the Gibbs ensembles by a variational principle. There are many outstanding books in the literature about statistical mechanics; see for instance Refs. [2, 5–11].

2.1 Macro- and micro-physics

The heuristic derivation of the van der Waals equation in Chapter 1 has to be generalized. The ideas involved in it point to a possible extension of the thermodynamic concepts to encompass the notion of particles, such that a prescription to derive, for instance, equations of state can be available in general. This requires a set of definitions connecting the macro-physics of thermodynamics, with the micro-physics formulation of many-body systems. A theory like that is called *statistical mechanics*, describing a thermodynamical system in equilibrium or out of equilibrium. Here we concentrate on systems in equilibrium [9, 10].

In order to formulate statistical mechanics, we have to keep in mind two elements. First, considering that a macroscopic system is composed of a large number of particles, a method has to be introduced to take into account the reduction of the numerous microscopic degrees of freedom, specifying a system, to comparatively very few macroscopic variables describing a thermal state. This can be implemented by performing an average of microscopic variables. For instance, the internal energy, E, can be taken as the sum of the average energy of each particle. This requires a formulation of mechanics such that the state can be described in terms of a probability. Assuming the existence of such a formulation, the state of a system can be represented by a density operator ρ, with $\mathrm{Tr}\ \rho = 1$. A measurable macroscopic quantity, say a, can be derived from its corresponding microscopic variable, say A,

by the rule

$$a = \langle A \rangle \equiv \mathrm{Tr}(\rho A), \tag{2.1}$$

where the operation Tr stands for the trace and is responsible for the reduction of the number of degrees of freedom. For instance, in the case of energy, the microscopic variable is $A = H$, the Hamiltonian of a system of N particles, and $a = E = \langle H \rangle$ is the internal energy. The $3N$ degrees of freedom are reduced to few degrees in the dependence of E on, for instance, the variables T, V, N; three variables only! The nature of ρ is not yet fully specified, but we can assume that it is an operator acting in the same Hilbert space where A is defined. The operator ρ is called the *density operator* or *density matrix.*

The next fundamental step to formulate statistical mechanics is to find a prescription to calculate the entropy function. Entropy represents a very distinguishable quality of macroscopic world, as is the temperature, without a mechanical counterpart. Therefore, from a microscopic standpoint, entropy and temperature are collective manifestations of the system without the reduction to specific parts. This is different from any other mechanical quantity, as that described by energy or macroscopic density, which have their microscopic counterpart. It will be enough here to focus on entropy, since any other thermodynamic variable, such as temperature, can be derived from it. We then look for a way to write A in Eq. (2.1) representing entropy. In this case, one way to do this is to use the state of the system, represented by the density matrix ρ, itself to find an expression for the entropy. Observe that by definition ρ describes the microscopic properties as well as the macroscopic quantities. Thus we can think of A for the entropy as a function of ρ, that is $A = s(\rho)$, such that

$$S[\rho] = \langle s(\rho) \rangle = \quad \mathrm{Tr}[\rho s(\rho)]. \tag{2.2}$$

We can find a functional form for $s(\rho)$, considering the properties of S. Recall that S is an extensive variable; if we divide the system into two independent parts, say 1 and 2, then $S = S_1 + S_2$ while $\rho = \rho_1 \rho_2$. Using Eq. (2.2), the required extensiveness of S is satisfied if we assume that the function $s(\rho)$ has the property that

$$s(\rho) = s(\rho_a \rho_b) = s(\rho_a) + s(\rho_b),$$

resulting in

$$s(\rho) = -k_B \rho \ln \rho,$$

where k_B fixes the unit of S, and the minus sign makes S positive. As a consequence,

$$\begin{aligned} S = \langle s(\rho) \rangle &= -k_B \mathrm{Tr}(\rho \ln \rho) \\ &= S_1 + S_2, \end{aligned} \tag{2.3}$$

where

$$\begin{aligned} S_1 &= -k_B \mathrm{Tr}(\rho_1 \ln \rho_1), \\ S_2 &= -k_B \mathrm{Tr}(\rho_2 \ln \rho_2). \end{aligned}$$

This definition for S is a central point of the theory, establishing a way to derive the fundamental relation for an arbitrary thermal system in the entropy representation, using microscopic information. The remaining aspect to be developed explicitly is to find a formulation of the microscopic theory in terms of the density ρ. In quantum mechanics we use ρ, the density matrix, which is the subject of the next section. However, in classical statistical mechanics, we use the notion of distribution function in phase space as a counterpart of ρ. In this case Tr implies an integration in phase space.

2.2 Liouville-von Neumann equation

Our proposal here is to introduce the density matrix, using the notion of an *ensemble*. For a gas in a box, for instance, we expect to find a large number of microscopic states which are compatible with a given macroscopic description. Indeed,if by some process, the velocity of only few particles in the gas is changed, virtually, no change in the macroscopic condition is expected. In principle then we can think of many such states. Some of them, however, are physically unacceptable. In fact, if by some process, we change the velocity of all particles along one direction, then at some moment we expect the gas occupying one side of the box, while the other side would be empty. This situation is in contradiction with the second law. This reasoning induces us to consider the set of all states compatible with a macroscopic situation, such that each state plays a more or less important role in this case. But this characteristic can be quantified by a proper definition of weight for each state. Naturally all the microscopic states have to be compatible with macroscopic constraints.

Consider a set of representative states. Such a set is called *ensemble* and the states will be denoted by $|\psi^i\rangle, i = 1, 2, ...$, each one satisfying the Schrödinger equation

$$i\partial_t|\psi^i(t)\rangle = H|\psi^i(t)\rangle; \tag{2.4}$$

here $\hbar = 1$. The expectation value of an observable A in the state $|\psi^i(t)\rangle$ is given by

$$\langle A\rangle^i = \langle\psi^i|A|\psi^i\rangle, \tag{2.5}$$

with $\langle\psi^i|\psi^i\rangle = 1$. The thermal (macroscopic) variable, say a, is associated with the average value of the observable A by the following prescription,

$$a = \langle A\rangle = \sum_i \gamma^{(i)}\langle A\rangle^i, \tag{2.6}$$

where $\gamma^{(i)}$ is the weight for each state of the ensemble. The next step is to show that the notion of ensemble used in Eq. (2.6) gives rise to Eq. (2.1), which describes the state of the system by a density matrix.

The vector $|\psi^i(t)\rangle$ is expressed as an expansion by

$$|\psi^i\rangle = \sum_n c_n^{(i)} |n\rangle, \tag{2.7}$$

where $|n\rangle$ is an element of the Hilbert space basis. Using Eq. (2.7) in Eq. (2.6) we obtain

$$\begin{aligned}\langle A\rangle &= \sum_i \gamma^{(i)} \langle\psi^i|A|\psi^i\rangle \\ &= \sum_i \gamma^{(i)} \sum_{m,n} c_n^{(i)*} c_m^{(i)} \langle n|A|m\rangle \\ &= \sum_{m,n} \rho_{mn} A_{nm} = \mathrm{Tr}(\rho A),\end{aligned}$$

where

$$\rho_{mn} = \sum_i \gamma^{(i)} c_n^{(i)*} c_m^{(i)} = \langle m|\rho|n\rangle, \tag{2.8}$$

and $A_{nm} = \langle n|A|m\rangle$.

The matrix ρ can be written in terms of the states $|\psi^i\rangle$ by using $c_n^{(i)*} = \langle\psi^i|n\rangle$ and $c_m^{(i)} = \langle m|\psi^i\rangle$ in Eq. (2.8), that is,

$$\begin{aligned}\rho_{mn} = \langle m|\rho|n\rangle &= \sum_i \gamma^{(i)} \langle m|\psi^i\rangle\langle\psi^i|n\rangle \\ &= \langle m| \sum_i \gamma^{(i)} |\psi^i\rangle\langle\psi^i|n\rangle.\end{aligned}$$

Hence we have

$$\rho = \sum_i \gamma^{(i)} |\psi^i\rangle\langle\psi^i|. \tag{2.9}$$

From this result, the time evolution equation for $\rho(t)$ can be obtained. Taking the time derivative of Eq. (2.9), assuming $\gamma^{(i)}$ is time independent, and using the Schrödinger equation, we have

$$\begin{aligned}i\partial_t \rho(t) &= \sum_i \gamma^{(i)} [(i\partial_t|\psi^i\rangle)\langle\psi^i| + |\psi^i\rangle(\langle\psi^i|i\partial_t)] \\ &= \sum_i \gamma^{(i)} [(H|\psi^i\rangle)\langle\psi^i| - |\psi^i\rangle(\langle\psi^i|H)] \\ &= H\rho(t) - \rho(t)H;\end{aligned}$$

or

$$i\partial_t \rho(t) = [H, \rho(t)]. \tag{2.10}$$

This is the Liouville-von Neumann equation, the basic equation in non-relativistic statistical mechanics. This equation may be written as

$$i\partial_t \rho(t) = L\rho(t), \tag{2.11}$$

where $L = [H, .]$ is the Liouvillian operator. The formal solution of Eq. (2.11) is given by

$$\rho(t) = e^{-i(t-t_0)L}\rho(t_0).$$

An important aspect of the density matrix, describing the state of a quantum system, is that when $\gamma^{(i)} = \delta_{i,r}$ in Eq. (2.6), one microstate only, say $|\psi^r\rangle$, plays a role in the set of representative states of the ensemble. In this case $\rho = \sum_i \gamma^{(i)}|\psi^i\rangle\langle\psi^i| = |\psi^r\rangle\langle\psi^r|$, and there is actually no ensemble at all. Then Eq. (2.10) provides us the same information as the Schrödinger equation. In this case $\rho(t)$ describes a *pure state*. For a non-trivial ensemble, $\rho(t)$ describes a *mixed state*. It is important to note that in order to describe thermal states, $\rho(t)$ has to provide a convexity condition to S, i.e. S has to be an increasing function of E. For any thermal or non-thermal system, the convexity of an entropy function establishes that ρ stands for mixed states; otherwise, ρ describes a system in a pure state.

2.3 Gibbs ensembles

This section is devoted to finding solutions of Eq. (2.10) for the case of thermal equilibrium, such that

$$[H, \rho] = 0.$$

Then a solution for this equation is of the type $\rho = \rho(H, C)$, where C is any set of constants of motion. To find ρ, we have to recall that the prescription linking micro physics to thermodynamics is that entropy is a functional of $\rho(t)$ given by Eq. (2.2),

$$S[\rho] = -k_B \mathrm{Tr}(\rho \ln \rho); \tag{2.12}$$

in addition the equilibrium condition is characterized by the second law,

$$\delta S[\rho] = 0. \tag{2.13}$$

Then ρ can be calculated from the extremum of the functional S under some constraints, as for instance the normalization of ρ, that is, $\mathrm{Tr}\rho = 1$. Different sets of constraints give rise to different ensembles.

2.3.1 *Micro-canonical ensemble*

We consider a constraint, the normalization condition for ρ, given by

$$\phi_1 = \mathrm{Tr}\rho - 1 = 0. \tag{2.14}$$

Then the variational principle is implemented by using the notion of Lagrange multipliers, i.e. the variation of the functional $S[\rho]$ is written as

$$\delta(S + \alpha_1\phi_1) = 0,$$

where α_1 is the Lagrange multiplier independent of ρ and associated with the constraint ϕ_1. Explicitly, we obtain,

$$\delta(-k_B \mathrm{Tr}(\rho \ln \rho) + \alpha_1 \mathrm{Tr}\rho - \alpha_1) = \mathrm{Tr}[-k_B \ln \rho - k_B + \alpha_1]\delta\rho = 0.$$

Since $\delta\rho$ is arbitrary, this results in

$$-k_B \ln \rho \ - k_B + \alpha_1 = 0. \tag{2.15}$$

We have then two unknown quantities, ρ and α_1, and two equations, Eqs. (2.14) and (2.15), providing a solvable algebraic system. From Eq. (2.15), ρ can be written as

$$\rho = exp\left(\frac{\alpha_1}{k_B} - 1)\right).$$

Using Eq. (2.14), we obtain

$$\begin{aligned} \mathrm{Tr}\rho &= \exp(\frac{\alpha_1}{k_B} - 1)\mathrm{Tr}1 \\ &= \exp(\frac{\alpha_1}{k_B} - 1)\mathcal{N} = 1 \end{aligned}$$

where $\mathcal{N} = \exp(1 - \frac{\alpha_1}{k_B})$ is the total number of states of the ensemble. Hence

$$\rho = \frac{1}{\mathcal{N}},$$

expressing the fact that each representative state of the ensemble has the same probability; or all $\gamma^{(i)}$ are equal in Eq. (2.6). This is the so-called *micro-canonical ensemble,* or ensemble where each state has *a priori* equal probability.

2.3.2 *Canonical ensemble*

The canonical ensemble is derived by assuming the following set of constraints

$$\phi_1 = \mathrm{Tr}\rho - 1 = 0, \tag{2.16}$$

$$\phi_2 = \mathrm{Tr}(H\rho) - \langle H\rangle = 0. \tag{2.17}$$

The constraint ϕ_1, as before, expresses the normalization condition for ρ, whilst ϕ_2 assures that the (thermal) internal energy, which is given by $E = \langle H\rangle$, is a constant, that is, E is explicitly a function of thermal variables, but not a function of ρ. Using ϕ_1 and ϕ_2, Eq. (2.13) is written with two Lagrange multipliers, α_1 and α_2 associated to ϕ_1 and ϕ_2, respectively, that is

$$\begin{aligned} \delta(S + \alpha_1\phi_1 + \alpha_2\phi_2) &= \delta\mathrm{Tr}[-k_B\rho \ln \rho + \alpha_1(\rho - 1) + \alpha_2(H\rho - E)] \\ &= \mathrm{Tr}[-k_B \ln \rho - k_B + \alpha_1 + \alpha_2 H]\delta\rho = 0. \end{aligned}$$

Since $\delta\rho$ is arbitrary, we obtain

$$-k_B \ln \rho - k_B + \alpha_1 + \alpha_2 H = 0. \tag{2.18}$$

With the two constraint equations for ϕ_1 and ϕ_2, ρ can be calculated. Multiplying Eq. (2.18) by ρ, taking the trace and using the definition for ϕ_1 and ϕ_2, we have

$$\frac{1}{\alpha_2}S + \frac{-k_B + \alpha_1}{\alpha_2} + E = 0. \tag{2.19}$$

This equation is, by construction, a thermodynamic linear relation between S and E. It is the Legendre transformation of E in its dependence on S, giving rise to, as in Chapter 1, to the Helmholtz free energy,

$$F = E - TS. \tag{2.20}$$

Comparing Eq. (2.19) with Eq. (2.20), we find that $1/\alpha_2 = -T$,

$$F = \frac{k_B - \alpha_1}{\alpha_2} = -k_B T \ln Z, \tag{2.21}$$

where we have used a new parametrization for α_1,

$$\ln Z = (k_B - \alpha_1)/k_B.$$

But Z can be expressed by the condition ϕ_1, writing from Eq. (2.18)

$$\rho = \exp(\frac{-k_B + \alpha_1}{k_B}) \exp(\frac{-H}{k_B T}).$$

Using the normalization condition for ρ, we get

$$\exp(\frac{k_B - \alpha_1}{k_B}) = Z = \mathrm{Tr}[\exp(-\beta H)],$$

where $\beta = 1/k_B T$. The function Z is called the *partition function*, and describes the sum of states, each of which is weighted by $\exp(-\beta H)$. Finally

$$\rho = \frac{1}{Z} \exp(-\beta H). \tag{2.22}$$

This form of ρ is the density matrix for a canonical ensemble.

2.3.3 *Grand-canonical ensemble*

The *grand-canonical ensemble* can be derived with the constraints ϕ_1, ϕ_2 given respectively in Eqs. (2.16) and (2.17), and the constraint,

$$\phi_3 = \mathrm{Tr}(N\rho) - \langle N \rangle = 0,$$

expressing explicitly that the number of particles can fluctuate.

Using ϕ_1, ϕ_2 and ϕ_3, Eq. (2.13) can be calculated with three respective Lagrange multipliers, α_1, α_2 and α_3, that is

$$\begin{aligned}\delta(S + \alpha_1\phi_1 + \alpha_2\phi_2 + \alpha_3\phi_3) &= \mathrm{Tr}\delta[-k_B\rho\ln\rho + \alpha_1(\rho - 1) \\ &\quad + \alpha_2(H\rho - E) + \alpha_3(N\rho - \langle N \rangle)] \\ &= \mathrm{Tr}[-k_B \ln\rho - k_B + \alpha_1 + \alpha_2 H + \alpha_3 N]\delta\rho = 0.\end{aligned}$$

Since $\delta\rho$ is arbitrary, we obtain

$$-k_B \ln \rho - k_B + \alpha_1 + \alpha_2 H + \alpha_3 N = 0.$$

Proceeding as before, using the constraint equations and the grand thermodynamical potential, the expression for ρ in the grand-canonical ensemble is

$$\rho = \frac{1}{Z} \exp[-\beta(H - \mu N)],$$

where μ is the chemical potential, that is the Lagrange multiplier associated with ϕ_3.

Other constraints can be imposed on the variation of S, resulting in generalized ensembles. For instance, we can introduce

$$\phi_4 = \mathrm{Tr}(P\rho) - \langle P \rangle = 0,$$

where $\langle P \rangle$ is a constant macroscopic momentum of the system. This type of ensemble is appropriate to treat steady states; and the density matrix is given in the form

$$\rho = \frac{1}{Z} \exp[-\beta(H - \mu N - \nu P)], \tag{2.23}$$

where ν, the Lagrange multiplier associated with ϕ_4, is a macroscopic "force" controlling the momentum flow to the system. This density matrix describes typical cases in which the kinematical transformation of frames have to be addressed. (For a discussion of generalized ensembles see references in [11].)

2.3.4 *Equivalence among the ensembles*

Using the Boltzmann entropy, as a functional of the density matrix, we have found different expressions for ρ that, in principle, are appropriate to describe the thermal equilibrium using the average of operators like $\langle A \rangle = \mathrm{Tr}(\rho \mathrm{A})$. Of course, different results emerge by the use of different formulas for ρ in different Gibbs-ensembles. But this is not consistent with the physical situation of thermal equilibrium. We expect equivalence among ensembles in a general situation. This equivalence is achieved in the *thermodynamic limit*, the T-limit, defined as

$$\lim_{N,V \to \infty} \frac{N}{V} = n_0,$$

where n_0 is a constant finite particle density. This limit expresses the physical result that a macroscopic body, composed of a large number of particles ($\sim 10^{23}$) in a very large volume compared to the volume of each particle, has a finite density, n_0. One consequence of the T-limit is the equivalence of the ensembles. Let us discuss this fact in a heuristic way.

Consider a gas in a box of volume V_a. We can describe the gas by the microcanonical ensemble, by calculating the thermal average of an observable described by an operator A; that is we calculate $\langle A \rangle_{microcanon}$. On the other hand, consider a

volume V_b of gas within the original box, $V_a > V_b$. In the case of the volume V_b, we can use the canonical ensemble to perform the average, i.e. $\langle A\rangle_{canon}$. We expect that $\langle A\rangle_{microcanon} = \langle A\rangle_{canon}$ only in the T-limit, when $V_a, V_b \to \infty$.

Another important consequence of the T-limit is the appearance of phase transitions. We may understand this, if we consider, for instance, the canonical ensemble. In this case we have to use $\rho \sim \exp(-\beta H)$, an analytical operator function, to proceed with the thermal average. However, phase transition phenomena is characterized by the loss of analyticity of some thermal functions. That can be reached in some cases only in the T-limit.

In the following chapters other aspects about the nature of the Gibbs ensemble are discussed. Now we turn to a study of the Wigner function formalism, within quantum mechanics, leading to a consideration of quantum kinetic theory.

2.4 Wigner function formalism

The starting point of statistical mechanics is the Liouville-von Neumann equation, as given in Eq. (2.10). By a Fourier-like transform the Liouville-von Neumann equation may be expressed in phase space. This method was first presented by Wigner [12] in order to study problems in quantum kinetic theory. Since then, the usefulness of Wigner function has been established in a variety of fields. In this section we set forth definitions and properties of Wigner function, developing the approach in one dimension for simplicity. For further developments see for instance Refs. [12–20].

The matrix elements of ρ corresponding to a given state of a quantum system, in the coordinate space, are written as $\rho(q,q') = \langle q|\rho|q'\rangle$. Introducing the linear transformation

$$\begin{aligned} q &\to q - \frac{1}{2}v, \\ q' &\to q + \frac{1}{2}v, \end{aligned}$$

the Wigner function is defined by

$$f_W(q,p,t) = \frac{1}{2\pi\hbar}\int \exp\left(\frac{i}{\hbar}pv\right)\left\langle q - \frac{1}{2}v\right|\rho(t)\left|q + \frac{1}{2}v\right\rangle dv. \tag{2.24}$$

Let us analyze $f_W(q,p,t)$ exploring its physical content and its time evolution equation, using the phase-space version of Eq. (2.10). For simplicity, the Wigner function is assumed to be associated with a pure state, $\rho = |\psi\rangle\langle\psi|$, although the results may be generalized to a mixed state.

The first property to be observed is that f_W is real but not positive definite. Consider two Wigner functions, $f_W^{(\psi)}$ and $f_W^{(\phi)}$, respectively associated with the pure states $|\psi\rangle$ and $|\phi\rangle$; then

$$|\langle\psi \mid \phi\rangle|^2 = 2\pi\hbar\int f_W^{(\psi)}(q,p,t) f_W^{(\phi)}(q,p,t) dqdp. \tag{2.25}$$

The left-hand side is a positive definite number or zero. We can infer that $f_W^{(\psi)}(q,p,t)$ and $f_W^{(\phi)}(q,p,t)$, being two independent and arbitrary functions, have also to be real. Considering that $|\psi\rangle$ and $|\phi\rangle$ are two orthogonal states, i.e. $\langle\psi \mid \phi\rangle = 0$, in the general case $f_W^{(\psi)}$ and $f_W^{(\phi)}$ cannot be positive definite functions. In this sense, the Wigner function f_W cannot be interpreted as a probability distribution in phase space, despite the fact that it is normalized, that is

$$\int f_W(q,p)dqdp = 1, \tag{2.26}$$

a consequence of $\mathrm{Tr}\rho = 1$. This result implies a normalization factor, $(2\pi\hbar)^{-1}$, in Eq. (2.24).

Compatible with this normalization, and useful for practical proposes, we have

$$|\psi(q)|^2 = \int f_W(q,p)dp,$$

and

$$|\psi(p)|^2 = \int f_W(q,p)dq,$$

where $|\psi(q)|^2$ and $|\psi(p)|^2$ are, respectively, the distribution of probability in the space and momentum space. Based on this result, $f_W(q,p)$ is called a quasi-distribution of probability.

Since the average $\langle A\rangle = \mathrm{Tr}(\rho A)$ is independent of representation, an operator A can be represented in phase space as

$$A_W(q,p,t) = \int \exp\left(\frac{i}{\hbar}pv\right)\left\langle q - \frac{1}{2}v\right| A \left|q + \frac{1}{2}v\right\rangle dv, \tag{2.27}$$

such that

$$\langle A\rangle = \mathrm{Tr}(\rho A) = \int A_W(q,p,t) f_W(q,p)dqdp.$$

At this point it is interesting to note that there is another way to represent an operator in phase space. Using the identities $\int |q\rangle\langle q|\, dq = \mathbf{1}$ and $\int |p\rangle\langle p|\, dp = \mathbf{1}$, an operator A we can written as

$$A = \int |q''\rangle\langle q'' \mid p''\rangle\langle p''|\, A\, |p'\rangle\langle p' \mid q'\rangle\langle q'|\, dp'dp''dq'dq''. \tag{2.28}$$

With the change of variables,

$$\begin{aligned} 2p = p' + p'', \quad 2q = q' + q'', \\ u = p'' - p', \quad v = q'' - q', \end{aligned}$$

Eq. (2.28) becomes

$$A = \int A_W(q,p)\Delta(q,p)dqdp, \tag{2.29}$$

where

$$\Delta(q,p) = \frac{1}{2\pi\hbar}\int \exp\left(\frac{i}{\hbar}pv\right)\left|q + \frac{1}{2}v\right\rangle\left\langle q - \frac{1}{2}v\right| dv. \tag{2.30}$$

The operator $\Delta(q,p)$ is Hermitian, implying that if A is Hermitian, then A_W is real.

Using Eq. (2.29), the phase-space representation of a product of two operators A and B is written as

$$(AB)_W(q,p) = A_W(q,p)\exp\left(\frac{i\hbar}{2}\Lambda\right)B_W(q,p), \tag{2.31}$$

where Λ is the Groenewold operator given by

$$\Lambda = \frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}. \tag{2.32}$$

Defining the Moyal (or star) product by

$$A(q,p)\star B(q,p) = A(q,p)\exp\left[\frac{i\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}\right)\right]B(q,p), \tag{2.33}$$

where $A(q,p)$ and $B(q,p)$ are two arbitrary functions in phase space, Eq. (2.31) is written as

$$(AB)_W(q,p) = A_W(q,p)\star B_W(q,p). \tag{2.34}$$

The Moyal product is a mapping taking operators acting in the Hilbert space of functions defined in phase space; that is, for operators A, B, C, D and a complex constant λ, we have

$$\star : (AB + \lambda CD) \to (AB + \lambda CD)_W = A_W \star B_W + \lambda C_W \star D_W.$$

This result is important to map equations among operators in the usual Hilbert space to the equivalent relations in phase space. For the case of the Liouville-von Neumann equation, Eq. (2.10), we obtain

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}f_W(q,p,t) &= H_W(q,p,t)\star f_W(q,p,t) - f_W(q,p,t)\star H_W(q,p,t) \\ &= \{H_W, f_W\}_M, \end{aligned} \tag{2.35}$$

where

$$\{A(q,p), B(q,p)\}_M = A(q,p)\star B(q,p) - B(q,p)\star A(q,p), \tag{2.36}$$

The quantity $\{A(q,p), B(q,p)\}_M$ is called the *Moyal bracket*, which can also be written, by expanding the exponential in the definition of the star product, as

$$\{A(q,p), B(q,p)\}_M = \frac{2}{\hbar}A(q,p)\,\sin\left[\frac{\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}\right)\right]B(q,p). \tag{2.37}$$

An immediate consequence of Wigner function formalism is in the analysis of the classical limit, where $\hbar$ can be considered very small. Up to the first order, we write

$$\sin\left(\frac{\mathrm{i}\hbar}{2}\Lambda\right) \approx \frac{\mathrm{i}\hbar}{2}\Lambda = \frac{\mathrm{i}\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}\right). \tag{2.38}$$

Therefore, we find

$$\frac{\partial f_W}{\partial t} = \frac{\partial H_W}{\partial q}\frac{\partial f_W}{\partial p} - \frac{\partial H_W}{\partial p}\frac{\partial f_W}{\partial q} = \{H_W, f_W\}, \tag{2.39}$$

where $\{\cdot,\cdot\}$ is the classical Poisson bracket; and Eq. (2.39) is the Liouville equation, the starting point of the classical statistical mechanics and the kinetic theory.

It is to be noted that H_W is the phase space representation of the Hamiltonian operator, which is equal to the classical Hamiltonian for a broad class of systems, but not in general. This is a consequence of a property of the phase space representation establishing that, for an operator function of momentum, say $A(P)$, the Wigner approach leads to $A_W(P) = A(p)$, where $A(p)$ is a function in phase space depending only on p, with the same functional form as the operator $A(P)$. The same is true for a function of the position only. As an example, it is the case for the Hamiltonian in the form

$$H(Q,P) = \frac{P^2}{2m} + V(Q),$$

since $V(Q) \to V(Q)_W = V(q)$ and $P^2 \to (P^2)_W = p^2$. Then $H(Q,P)_W = H(q,p)$ is the classical Hamiltonian. Nevertheless this is not valid in general; and a counter example is the case of a potential depending on position and momentum.

In addition, for a quadratic potential, $V(Q) = a + bQ + cQ^2$, Eq. (2.35) reduces to Eq. (2.39) but we still have $f_W(q,p)$ describing a quantum harmonic oscillator. This is so since the content of the Liouville equation for such a potential is of a drift in phase space in the presence of an external field; a result that can be explicitly expressed by

$$\begin{aligned}\frac{\partial f_W}{\partial t} &= \{H_W, f_W\} \\ &= (b + 2cq)\frac{\partial}{\partial p} f_W - \frac{p}{m}\frac{\partial}{\partial q} f_W.\end{aligned}$$

This is an expected result for both classical and quantum systems. Therefore, in the analysis of the classical limit using the Wigner representation, we have to be careful with the state of the quantum system, described by $f_W(q,p)$. Due to these properties regarding the classical limit, despite the fact that $f_W(q,p)$ is only a quasi-probability, Eq. (2.35) is the natural candidate to be the starting point of the quantum kinetic theory.

In this brief summary of some aspects of the statistical mechanics we have stressed the variation method to construct ensembles and the Wigner representation. The first aspect will be used in Chapter 14 to construct maximally entangled states for boson and fermion bipartite systems, while the Wigner representation will be important in the discussion of open systems.

Chapter 3

Partition Function and Path Integral

The central goal of this chapter is to show that the partition function can be used to introduce the notion of generating functional, an important tool to carry out calculations in quantum systems, giving rise to powerful perturbative methods. This fact opens doors to bring thermodynamics to the realm of quantum field theory.

The concept of path integral was first presented by Wiener [21, 22], in the context of stochastic problems. Feynman [23, 24], based on a generalization of Dirac's work [25], developed the idea of path integral as a general scheme for quantization. The concept of generating functional was introduced by Heisenberg and Euler [26]; and Schwinger [27] used such a notion with the path integral formalism, proposing a theory of particles and sources. It was also Schwinger [28] who, intending to describe fermions through a path integral formalism, introduced the Grassmann numbers in physics.

The importance of path integral for contemporary physics, in spite of the remaining difficulties, is immeasurable. Here we present an outline for using the generating functional method, with its extension to quantum fields at zero temperature [29–33]. The effect of temperature will be analyzed in a later chapter.

3.1 Partition function and the propagator

The statistical average of an observable A, as stated in Chapter 2, in the canonical ensemble is given by

$$\langle A\rangle = \mathrm{Tr}[\rho(\beta)A] = \frac{1}{Z(\beta)}\mathrm{Tr}[e^{-\beta H}A],$$

where the partition function is

$$Z(\beta) = \mathrm{Tr}(e^{-\beta H}), \tag{3.1}$$

$\beta = 1/T$ is the inverse of temperature (we take $k_B = 1$ everywhere), and H is the Hamiltonian. The primary role played by the partition function is to work as a sum of states, supplying the normalization of ρ.

The partition function provides also a way for calculating the ground state energy at zero temperature. For a basis in which the Hamiltonian is diagonal we have

$$\begin{aligned}\langle H\rangle &= \frac{1}{Z(\beta)}\mathrm{Tr}e^{-\beta H}H = \frac{1}{Z(\beta)}\sum_{n=0}^{\infty}\langle n|\ e^{-\beta\epsilon_n}H|n\rangle \\ &= \frac{1}{Z(\beta)}[\epsilon_0 e^{-\beta\epsilon_0} + \sum_{n=1}^{\infty}\ \epsilon_n e^{-\beta\epsilon_n}]. \end{aligned} \tag{3.2}$$

Considering $\beta = 1/T \to \infty$ (equivalent to taking $T \to 0$), the leading term in Eq. (3.2) is just the ground state energy.

Some basic quantities such as free energy, pressure and entropy are calculated directly from Z. Indeed, from the definition of the internal energy, we have

$$\langle H\rangle = \frac{1}{Z(\beta)}\mathrm{Tr}(e^{-\beta H}H) = -\frac{\partial}{\partial\beta}\ln Z(\beta). \tag{3.3}$$

The Helmholtz free energy reads

$$F = -\frac{1}{\beta}\ln Z(\beta),$$

which is consistent with the entropy given by

$$\begin{aligned} S &= \frac{1}{T}F + \frac{1}{T}E = \beta^2\frac{\partial}{\partial\beta}F \\ &= -\beta^2\frac{\partial}{\partial\beta}\left(\frac{1}{\beta}\ln Z(\beta)\right). \end{aligned}$$

The pressure is then written as

$$P = -\frac{\partial}{\partial V}F = \frac{1}{\beta}\frac{\partial}{\partial V}\ln Z(\beta).$$

Another important result regarding the nature of the canonical (or even the grand canonical) ensemble is the Kubo-Martin-Schwinger (KMS) [34, 35] conditions stating that the statistical average of an operator in the Heisenberg picture, say $A_H(t) = e^{-itH}A(0)e^{itH}$, is periodic in time with a period $i\beta$ (the subscript "H" in $A_H(t)$ stands for the Heiserberg picture). This result can be proved directly from the statistical average:

$$\begin{aligned}\langle A_H(t)\rangle &= \mathrm{Tr}[\rho(\beta)A(t)] = \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}A(t)\right] \\ &= \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}e^{-itH}A(0)e^{itH}\right] \\ &= \frac{1}{Z(\beta)}\mathrm{Tr}\left[e^{-\beta H}A_H(t-i\beta)\right] \equiv \langle A_H(t-i\beta)\rangle. \end{aligned}$$

The change in the argument of $A_H,\ t \to t - i\beta$ is called a Wick rotation of the time axis.

Let us investigate the consequence of the KMS condition for the partition function. For that, take the trace in Eq. (3.1) using the position representation; i.e.

$$Z(\beta) = \mathrm{Tr} e^{-\beta H} = \int dq \, \langle q | e^{-\beta H} | q \rangle. \tag{3.4}$$

Defining

$$Z_{ba} = \langle q_b | e^{-\beta H} | q_a \rangle, \tag{3.5}$$

we find

$$Z(\beta) = \int dq_a Z_{aa}.$$

Now examine the meaning of the quantity Z_{ab}. For this purpose, introduce a Wick rotation, defined by the identification

$$\beta \to i(t_b - t_a),$$

such that

$$Z_{ba} = \langle q_b | e^{-\beta H} | q_a \rangle = \langle q_b | e^{-i(t_b - t_a)H} | q_a \rangle \equiv \langle q_b t_b | q_a t_a \rangle, \tag{3.6}$$

where

$$|q_a t_a\rangle = e^{it_a H} |q_a\rangle \ , \quad |q_b t_b\rangle = e^{it_b H} |q_b\rangle.$$

The set of states $|q \ t\rangle = e^{itH}|q\rangle$ form a complete basis, with the completeness relation

$$\int dq |q\rangle\langle q| = \int dq |q \ t\rangle\langle q \ t| = 1.$$

Such a basis may be used to build a Schrödinger-picture state $|\psi(t)\rangle$, in the position representation, from a state in the Heisenberg picture $|\psi\rangle_H$. In fact, since

$$|\psi(t)\rangle = e^{-itH}|\psi(0)\rangle = e^{-itH}|\psi\rangle_H,$$

we have

$$\psi(q,t) = \langle q|\psi(t)\rangle = \langle q \ t|\psi\rangle_H.$$

This result shows the physical content of Eq. (3.6), i.e. $Z_{ba} = \langle q_b t_b | q_a t_a \rangle$ is a transition amplitude from $|q_a t_a\rangle$ to $|q_b t_b\rangle$.

The function Z_{ba} is called the *propagator,* for considering an arbitrary amplitude at a time t_a, $\psi(q_a, t_a) = \langle q_a \ t_a | \psi \rangle$, and using the completeness relation, we obtain

$$\begin{aligned} \langle q_b \ t_b | \psi \rangle &= \int dq_a \langle q_b t_b | q_a \ t_a \rangle \langle q_a \ t_a | \psi \rangle \\ &= \int dq_a Z_{ba} \psi(q_a, t_a). \end{aligned}$$

In this expression Z_{ba} describes how the state $|\psi(t)\rangle$ evolves from $|\psi\rangle$ at t_a and q_a to $|\psi\rangle$ at t_b and q_b. With $t_b > t_a$ we insure causality. The fundamental quantity here is then the propagator Z_{ba}. With this understanding for Z_{ba}, we find that Z_{aa} is the propagator in a closed-time interval. In the case of the partition function, we have then a Wick rotation, with period β.

The results presented above show a close association of Z not only to the thermal but also to the non-thermal quantities, demanding then a detailed analysis of Z_{ba}.

3.2 Path integral in quantum mechanics

In order to calculate the propagator Z_{ba}, we split the time interval from t_a to t_b in n-point, resulting in $n+1$-pieces of size $\delta t_j = t_{j+1} - t_j$; $j = 1, 2, ..., n$, with $n \to \infty$, and $\delta t \to 0$. At each point j, characterized by t_j and q_j, we use a completeness relation $\int dq_j |q_j\ t_j\rangle\langle q_j\ t_j| = 1$ in $\langle q_b t_b | q_a\ t_a\rangle$, resulting in the expression

$$\langle q_b t_b | q_a\ t_a\rangle = \int dq_1 ... dq_n \langle q_b t_b | q_n\ t_n\rangle\langle q_n t_n | q_{n-1} t_{n-1}\rangle ... \langle q_1 t_1 | q_a\ t_a\rangle. \tag{3.7}$$

The propagator in an arbitrary small interval δt_j results in

$$\begin{aligned} Z_{j+1,j} &= \langle q_{j+1} t_{j+1} | q_j\ t_j\rangle \\ &= \langle q_{j+1} | e^{-i\delta t_j H} | q_j\ \rangle = \langle q_{j+1} | 1 - i\delta t_j H | q_j\ \rangle \\ &= \delta(q_{j+1} - q_j) - i\delta t_j \langle q_{j+1} | H | q_j\ \rangle. \end{aligned} \tag{3.8}$$

For simplicity we consider one-dimensional one-particle system in a potential $V(\widehat{q})$. Then the Hamiltonian reads

$$H(\widehat{q}, \widehat{p}) = \frac{\widehat{p}^2}{2m} + V(\widehat{q}),$$

where $\widehat{q}|q_j\ \rangle = q_j |q_j\ \rangle$ and $\widehat{p}|p_j\ \rangle = p_j |p_j\ \rangle$, with

$$\langle q_j | p_i \rangle = \frac{1}{\sqrt{2\pi}} e^{i q_j p_i},$$

and

$$\langle q_j | q_i \rangle = \delta(q_j - q_i) = \frac{1}{2\pi} \int dp e^{ip(q_j - q_i)} \tag{3.9}$$

Hence we obtain,

$$\langle q_{j+1} | \frac{\widehat{p}^2}{2m} | q_j\ \rangle = \frac{1}{2\pi} \int dp e^{ip\delta q_j} \frac{p^2}{2m},$$

$$\langle q_{j+1} | V(\widehat{q}) | q_j\ \rangle = V(Q_j) \frac{1}{2\pi} \int dp e^{ip\delta q_j}$$

where $\delta q_j = q_{j+1} - q_j$, and $Q_j = (q_{j+1} + q_j)/2$. Gathering together these results, we get

$$\langle q_{j+1} | H | q_j\ \rangle = \frac{1}{2\pi} \int dp e^{ip\delta q_j} H(Q_j, p).$$

Using the integral representation for the δ-function, Eq. (3.9), we obtain from Eq. (3.8),

$$\begin{aligned} Z_{j+1,j} &= \frac{1}{2\pi} \int dp e^{ip\delta q_j} - i\delta t_j \frac{1}{2\pi} \int dp e^{ip\delta q_j} H(Q_j, p) \\ &= \frac{1}{2\pi} \int dp e^{ip\delta q_j} [1 - i\delta t_j H(Q_j, p)] \\ &= \frac{1}{2\pi} \int dp e^{i\delta t_j [p\delta q_j / \delta t_j - H(Q_j, p)]} \\ &= \frac{1}{2\pi} \int dp e^{i\delta t_j [pv_j - \frac{p^2}{2m} - V(Q_j)]}\ . \end{aligned}$$

Completing the square in the integration variable p, and using the Gaussian integral

$$\int_{-\infty}^{\infty} dx e^{-ax^2+bx+c} = \exp\left(\frac{b^2}{4ac}+c\right)\sqrt{\frac{\pi}{a}},$$

we obtain

$$Z_{j+1,j} = \left(\frac{m}{2\pi i\delta t_j}\right)^{1/2} \exp\left\{i\delta t_j\left[\frac{1}{2}mv_j^2 - V(Q_j)\right]\right\}.$$

Substituting this result in Eq. (3.7), and taking the limit $n \to \infty$, we obtain

$$Z_{ba} = \langle q_b t_b | q_a\ t_a\rangle = \lim_{n\to\infty}\left(\frac{m}{2\pi i\delta\tau}\right)^{(n+1)/2} \times \int \prod_{j=1}^{n} dq_j \exp\left\{i\sum_{j=0}^{n}\delta\tau\left[\frac{1}{2}m\dot{q}_j^2 - V(Q_j)\right]\right\}, \tag{3.10}$$

where we have defined: $\delta\tau \equiv \delta t_j$, $q_b \equiv q_{n+1}$ and $q_a \equiv q_0$. This limit leads to

$$Z_{ba} = \langle q_b t_b | q_a\ t_a\rangle = \mathcal{N}\int Dq\ e^{iS_{ab}}, \tag{3.11}$$

where $\mathcal{N}$ is a normalization factor,

$$Dq \equiv \lim_{n\to\infty}\prod_{j=1}^{n} dq_j$$

is the measure od integration and

$$S_{ab} = \int_{t_a}^{t_b} dt\ L(q,\dot{q}) \tag{3.12}$$

is the action defined by the Lagrangian

$$L(q,\dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q). \tag{3.13}$$

It is worth emphasizing that this derivation of Z_{ba} expresses a sum (a functional integration) over different trajectories of a classical system; and in turn a quantization scheme is provided by using the classical action S_{ab}. Such a procedure is called the *path integral formalism* and can be generalized to quantum fields.

3.3 Classical fields

The action given in Eq. (3.12) is, in classical physics, the fundamental tool for deriving equations of motion through an extremum principle. Indeed, assuming the condition $\delta S_{ab} = 0$, we obtain

$$\delta S_{ab} = \int_{t_a}^{t_b} dt\ \delta L(q,\dot{q}) \ = \int_{t_a}^{t_b} dt[L(q+\delta q, \dot{q}+\delta\dot{q}) \ - L(q,\dot{q})]$$

$$= \int_{t_a}^{t_b} dt(\frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\ \delta\dot{q}) = 0, \tag{3.14}$$

where we define $\delta q(t) = \varepsilon\sigma(t)$, with ε being an infinitesimal quantity and $\sigma(t)$ is an arbitrary but analytical function of t, such that

$$\delta\dot{q}(t) = \delta\frac{dq(t)}{dt} = \frac{d}{dt}\delta q(t).$$

Using this result in Eq. (3.14) and performing an integral by parts, we obtain

$$\delta S_{ab} = \int_{t_a}^{t_b} dt[\frac{\partial L}{\partial q} - \frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}\ )]\delta q = 0,$$

where the fixed extremum condition, that is, $\delta q(t_a) = \delta q(t_a) = 0$, has been used. Since $\delta q(t) = \varepsilon\sigma(t)$ is an arbitrary quantity, we get the Euler-Lagrange equation,

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}\ ) = \frac{\partial L}{\partial q}.$$

For L given in Eq. (3.13) we obtain the Newton's second law: $m\ddot{q} = -\partial V/\partial q$.

This procedure can be generalized for an arbitrary number of parameters, considering $q(\tau) = q(\tau^0, \tau^1, ..., \tau^r)$, and $\mathcal{L}(q, \partial q) = \mathcal{L}(q, \partial_0 q, \partial_1 q, ..., \partial_r q)$, where $\partial_\alpha q = \partial q/\partial\tau^\alpha$. The action is written as

$$S = \int_\Gamma d^r\tau\ \mathcal{L}(q, \partial q), \tag{3.15}$$

where $\mathcal{L}(q, \partial q)$ is the Lagrangian density. As before, assume the extremum condition now defined by a hyper-surface Γ, $\delta q(\tau)|_\Gamma = 0$. From $\delta S = 0$, we derive

$$\partial_\alpha \frac{\partial \mathcal{L}}{\partial(\partial_\alpha q)} \ = \frac{\partial \mathcal{L}}{\partial q}; \quad \alpha = 0, 1, ..., r, \tag{3.16}$$

where there is a sum over the repeated indices. If q, has more than one component, then in Eq. (3.16) we have to replace q by q_j, where the subindex $j = 1, 2, ...$ stands for the number of components of q.

A physical interpretation of this method is realized when we specify the nature of the parameters τ and the function q. For that, we assume that τ is a 4-vector in the Minkowski space-time ($\mathcal{M}^{3+1}$) with $\tau^0 \equiv x^0 = ct$; $\tau^1 \equiv x^1$, $\tau^2 \equiv x^2$, $\tau^3 \equiv x^3$, that is $x = (x^0, x^1, x^2, x^3)$. The metric tensor is given by

$$(g^{\mu\nu}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

such that $g = g^{-1}$; with $(g^{\mu\nu})^{-1} \equiv g_{\mu\nu}$, $x_\mu = g_{\mu\nu}x^\nu$, and $x^\mu = g^{\mu\nu}x_\nu$. The generalized canonical coordinate, $q(x)$, is then a field, defining some quantity at a point x of space-time. For a scalar field, instead of q, a Greek letter $\phi(x) = \phi(t, \mathbf{x})$ is used. In this case, Eq. (3.16) reads

$$\partial_\alpha \frac{\partial \mathcal{L}}{\partial(\partial_\alpha \phi)} = \frac{\partial \mathcal{L}}{\partial \phi}; \tag{3.17}$$

where $\alpha = 0, 1, 2, 3$. The Lagrangian density is specified by symmetry conditions, imposing restrictions on the form of different models. For relativistic fields the Lorentz invariance is the basic symmetry to be taken into account. This corresponds to invariance under a set of linear transformations in $\mathcal{M}^{3+1}$ that preserves the scalar product between vectors, $x \cdot y = g_{\mu\nu}x^\nu x^\mu$. Writing the linear transformation as

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu,$$

the invariance of the scalar product requires the invariance of the metric, $\Lambda^T g \Lambda = g$, where Λ^T is the transpose of the matriz Λ, with components given by

$$\Lambda^\mu{}_\nu = \frac{\partial x'^\mu}{\partial x^\nu}.$$

Then we have $\det \Lambda = \pm 1$. For $\det \Lambda = 1$ the Lorentz map is called *the proper Lorentz transformations*, which is the group connected to the identity. For proper infinitesimal transformations we write

$$x'^\mu = x^\mu + \omega^\mu{}_\nu x^\nu$$

where $\omega_{\rho\nu} = g_{\rho\mu}\omega^\mu{}_\nu$ is an anti-symmetric matrix. In this case, a finite Lorentz transformation in an infinite-dimensional representation (i.e. acting on, for example, analytical functions defined in $\mathcal{M}^{3+1}$) can be written as

$$\Lambda = \exp[\omega_{\mu\nu} M^{\mu\nu}],$$

where $M^{\mu\nu}$ are the generators of Lorentz transformations given by

$$M^{\mu\nu} = i(x^\mu \partial^\nu - x^\nu \partial^\mu).$$

Using this symmetry and requiring that the Lagrangian density be a real Lorentz scalar, a variety of models can be proposed. A simple one, for a real scalar field, is

$$\mathcal{L} = \frac{1}{2}\partial_\alpha \phi \partial^\alpha \phi - \frac{1}{2}m^2\phi^2 + J\phi. \tag{3.18}$$

Using the Euler-Lagrange equation, we derive

$$\partial_\alpha \partial^\alpha \phi + m^2 \phi = J,$$

which is the Klein-Gordon equation describing a particle with a mass m, with a source term, J.

We have then identified a general scheme to treat a classical field as a mechanical system described by a Lagrangian. Our goal here is to extend the path integral approach to various fields, and then to construct a quantum field theory. For this purpose it is useful, first of all, to analyze the canonical quantization of fields, based on the Dirac correspondence principle. The central ingredient to develop this method is the Hamiltonian theory.

3.4 Canonical quantization of scalar fields

In order to introduce the Hamiltonian formalism for a field theory, we define the canonical momentum density in terms of the Lagrangian density by

$$\pi(x) = \frac{\partial \mathcal{L}(\phi, \partial\phi)}{\partial \dot{\phi}} = \dot{\phi}(x).$$

The Hamiltonian is defined by a generalization of the usual Legendre transformation of the Lagrangian, that is,

$$H = \int d^3x \mathcal{H}(\phi, \pi) = \int d^3x [\pi(x)\dot{\phi}(x) - \mathcal{L}(\phi, \partial\phi)], \tag{3.19}$$

where $d^3x = dx^1 dx^2 dx^3 = d\mathbf{x}$. For the Klein-Gordon field in the presence of a source, J, the Hamiltonian density is

$$\mathcal{H}(\phi, \pi) = \frac{1}{2}\pi^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{1}{2}m^2\phi^2 - J\phi.$$

A quantum field theory is introduced following the Dirac's prescription for the pair of canonical variables, that in the case of a real scalar field are ϕ and π. We then demand that at a time t the following commutation relations are fulfilled,

$$[\phi(t, \mathbf{x}), \pi(t, \mathbf{y})] = i\delta(\mathbf{x} - \mathbf{y}), \tag{3.20}$$

$$[\phi(t, \mathbf{x}), \phi(t, \mathbf{y})] = [\pi(t, \mathbf{x}), \pi(t, \mathbf{y})] = 0. \tag{3.21}$$

The fields ϕ and π are now operators defined in a Hilbert space to be specified (we keep the notation for the case of c-number functions for simplicity, since there is no risk of confusion). The energy spectrum of the scalar field is analyzed by introducing Fourier components. Thus the real scalar field, $\phi(x)$, is written as

$$\phi(x) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2k_0} \left(a(k)e^{-ikx} + a^\dagger(k)e^{ikx}\right) \tag{3.22}$$

and

$$\pi(x) = \dot{\phi}(x) = \int \frac{d^3k}{(2\pi)^3}(-i)\ \frac{1}{2}\left(a(k)e^{-ikx} - a^\dagger(k)e^{ikx}\right);$$

such that from Eqs. (3.20) and (3.21), we require

$$[a(k), a^\dagger(k')] = (2\pi)^3 2k_0 \delta(\mathbf{k} - \mathbf{k}'),$$

and all other commutation relations being zero. The four-vector $k = (k^0, k^1, k^2, k^3) = (k_0, \mathbf{k})$ satisfies the mass-shell condition

$$k_0^2 = \mathbf{k}^2 + m^2.$$

Here $a(k)$ and $a^\dagger(k)$ are the annihilation and creation operators, respectively, for particles with momentum k.

In terms of operators $a(k)$ and $a^\dagger(k)$, the Hamiltonian is

$$H = \int \frac{d^3k}{(2\pi)^3} k_0 [a^\dagger(k)a(k) + a(k)a^\dagger(k)].$$

Using the commutation relations, it can be shown that this Hamiltonian is defined up to an infinite constant. The suppression of this is achieved by *normal ordering*, which is defined by taking all creation operators to the left, keeping in mind the sign from the commutation relations, in a product of basic operators. For instance, $: a(k)a^\dagger(k): \; = a^\dagger(k)a(k)$. The normal ordering is indicated by the colons. With this ordering, the Hamiltonian is written as

$$H = \int \frac{d^3k}{(2\pi)^3} k_0 \; a^\dagger(k)a(k).$$

The vacuum (ground) state, $|0\rangle$, for a free field in the Minkowski space is defined by $\langle 0|H|0\rangle = 0$. Requiring

$$a(k)|0\rangle = 0 \;\text{ and }\; \langle 0|0\rangle = 1,$$

a basis in this Hilbert space, called the Fock space, is built from vectors given by $[a^\dagger(k_1)]^n ... [a^\dagger(k_N)]^m|0\rangle$.

Let us define, for a real field, the following function

$$G_0(x-y) = -i\langle 0|T[\phi(x)\phi(y)]|0\rangle,$$

where T is the time ordering operator, such that $G_0(x-y)$ can be written as

$$G_0(x-y) = \theta(x^0-y^0)G(x-y) + \theta(y^0-x^0)G(y-x),$$

with the step function $\theta(x)$ defined by $\theta(x) = 1$, for $x > 1$, $\theta(x) = 0$, for $x < 1$, and $G(x-y) = -i\langle 0|\phi(x)\phi(y)|0\rangle$. Using Eq. (3.22), $G(x-y)$ reads

$$\begin{aligned} G(x-y) &= (-i)\langle 0| \int \frac{d^3p}{(2\pi)^3}\frac{1}{2\omega_p} \; \left(a(p)e^{-ipx} + a^\dagger(p)e^{ipx}\right) \\ &\quad \times \int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k} \; \left(a(k)e^{-iky} + a^\dagger(k)e^{iky}\right)|0\rangle \\ &= \int \frac{d^3k}{(2\pi)^3}\frac{(-i)}{2\omega_k} e^{-ik(x-y)}, \end{aligned}$$

and then

$$\begin{aligned} G_0(x-y) = -i \int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k} [&\theta(x^0-y^0)e^{-i\omega_k(x^0-y^0)} \\ &+\theta(y^0-x^0)e^{i\omega_k(x^0-y^0)}]e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}. \end{aligned}$$

Using Cauchy theorem, the θ-functions in these expressions can be written as

$$\begin{aligned} \int dp^0 \frac{e^{-ip_0(x^0-y^0)}}{p_0 - (w_k - i\varepsilon)} &= -2\pi i e^{-iw_k(x^0-y^0)}\theta(x^0-y^0), \\ \int dp^0 \frac{e^{-ip_0(x^0-y^0)}}{p_0 - (-w_k + i\varepsilon)} &= 2\pi i e^{iw_k(x^0-y^0)}\theta(y^0-x^0), \end{aligned}$$

with infinitesimal ε resulting in

$$\begin{aligned} G_0(x-y) &= (-i)\int \frac{d^4k}{(2\pi)^4}\frac{1}{2k_0}e^{-ik(x-y)} \\ &\quad\times\left[\frac{-1}{k_0-(w_k-i\varepsilon)}+\frac{1}{k_0-(-w_k+i\varepsilon)}\right] \\ &= \frac{-i}{(2\pi)^4}\int d^4k\frac{e^{-ik(x-y)}}{k^2-m^2+i\varepsilon}. \end{aligned} \tag{3.23}$$

Then $G_0(x-y)$ is the Green's function for the inhomogeneous Klein-Gordon equation with a point source

$$(\Box+m^2)G_0(x-y) = -i\delta(x-y), \tag{3.24}$$

where $\Box = \partial_\alpha\partial^\alpha = \partial_0\partial^0 - \nabla$.

For $m=0$, using the integrals

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dx e^{ix^2a} = \frac{1}{2}\sqrt{\frac{i}{\pi a}}, \qquad \int_0^{\infty} dx e^{ixa} = \frac{i}{a},$$

the Green's function for a scalar particle takes the simple form

$$G_0(x-y) = \frac{i}{(2\pi)^2}\frac{1}{(x-y)^2+i\varepsilon}. \tag{3.25}$$

3.5 Path integral for a scalar field

In this section we generalize Eq. (3.11) to a scalar field, using S given in Eq. (3.15) and the Lagrangian in Eq. (3.18), resulting in

$$\begin{aligned} Z_0[J] &= \mathcal{N}\int D\phi e^{iS_{ab}} = \mathcal{N}\int D\phi\ \exp\left\{i\int d^4x\left[\frac{1}{2}\partial_\alpha\phi\partial^\alpha\phi - \frac{1}{2}m^2\phi^2 + J\phi\right]\right\} \\ &= \mathcal{N}\int D\phi\ \exp\left\{-i\int d^4x[\frac{1}{2}\phi(\Box+m^2)\phi - J\phi]\right\}, \end{aligned} \tag{3.26}$$

where we have used the index 0 in $Z_0[J]$ to indicate free fields. To handle this expression, we develop some elements of the functional integration.

The product of r Gaussian integrals is given by

$$\int e^{-a_1w_1^2/2}e^{-a_2w_2^2/2}\cdots e^{-a_rw_r^2/2}dw_1\cdots dw_r = \frac{(2\pi)^{r/2}}{\prod_{i=1}^{r} a_i^{1/2}}, \tag{3.27}$$

where $a_i > 0$, for $i = 1,\ldots,r$. Defining

$$A = (A_{ij}) = \begin{pmatrix} a_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & a_r \end{pmatrix}; \quad w = \begin{pmatrix} w_1 \\ \vdots \\ w_r \end{pmatrix},$$

$$(w, Aw) = \sum_{i,j=1}^{r} w_i A_{ij} w_j = \sum_{i=1}^{r} a_i w_i^2 \tag{3.28}$$

and Eq. (3.27) reads

$$\int e^{-(w,Aw)/2} dw = \frac{1}{(\det A)^{1/2}}, \tag{3.29}$$

where the measure of the integral is given by $dw = dw_1 \cdots dw_r/(2\pi)^{r/2}$.

Let us go further by analyzing integrals of the type $\int dw \exp(-f(w))$, where

$$f(w) = \frac{1}{2}(w, Aw) + (b, w) + c, \tag{3.30}$$

with b and c being r-component vectors. The minimum of $f(w)$ is calculated by

$$df = \sum_{i=1}^{r} \frac{\partial f}{\partial w_i} dw_i = \sum_{i,j=1}^{r} w_i A_{ij} + \sum_{i=1}^{r} c_i = 0,$$

that has the solution $w^0 = -A^{-1}b$. Then Eq. (3.30) is written as

$$f(w) = f(w^0) + \frac{1}{2}(w - w^0, A(w - w^0)),$$

and from Eq. (3.29) we have

$$\int e^{-[(w,Aw)/2 + (b,w) + c]} dw = e^{(b, A^{-1}b)/2 - c} \frac{1}{(\det A)^{1/2}}.$$

Taking the continuum limit, we write $w_i \to w(x)$; $A_{ij} \to A(x, y)$ such that

$$(Aw)_j = \sum_{i=1}^{r} w_i A_{ij} \to (Ab)(x) = \int A(x, y) b(y) dy,$$

$$(w, Aw) = \sum_{i,j=1}^{r} w_i A_{ij} w_j \to \int w(x) A(x, y) w(y) dx dy$$

and

$$\int dw ... = \int dw_1 \cdots dw_r/(2\pi)^{r/2} \to \int Dw(x) ...$$

These results are generalized to more than one parameter, such that x can be taken as a four-vector. Therefore Eq. (3.26) by identifying: $w(x) = \phi(x)$; $A = i(\Box + m^2)$; $b = -iJ$; $c = 0$, becomes,

$$Z_0[J] = \mathcal{N} \exp\left[\frac{i}{2} \int J(x)(\Box + m^2)^{-1} J(y) d^4x d^4y\right] [\det i(\Box + m^2)]^{1/2}, \tag{3.31}$$

where

$$[\det i(\Box + m^2)]^{1/2} = \int D\phi \ \exp\left\{-i \int d^4x [\frac{1}{2}\phi(\Box + m^2)\phi]\right\}.$$

This factor can be incorporated in the normalization factor $\mathcal{N}$. In addition, using the notation above, Eq. (3.24) is written in an operator form as

$$G_0(x-y) = -(\Box + m^2)^{-1}.$$

Then Eq. (3.31) reads

$$Z_0[J] = \mathcal{N} \exp\left[\frac{-i}{2}\int J(x)G_0(x-y)J(y)d^4xd^4y\right].$$

Here J is arbitrary. This fact is used to take $Z_0[J]$ as a generating functional for the propagator. This is achieved by taking functional derivatives.

A functional $F[w(x)]$ is a mapping of analytical functions in the real field. The derivative of $F[w(x)]$ with respect to $w(y)$ is defined as a generalization of the ordinary derivative of functions, by

$$\frac{\delta F[w(x)]}{\delta w(y)} = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\{F[w(x)+\varepsilon\delta(x-y)] - F[w(x)]\}.$$

Let us test the consistency of such a definition using two examples.

Consider

$$F[w(x)] = \int H(x,y)w(x)dx,$$

where $H(x,y)$ is a given arbitrary function. Then we have

$$\begin{aligned}\frac{\delta F[w(x)]}{\delta w(z)} &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\{\int H(x,y)[w(x)+\varepsilon\delta(x-z)]dx - \int H(x,y)w(x)dx\\ &= \int H(x,y)\varepsilon\delta(x-z)dx = H(z,y).\end{aligned}$$

Now take

$$F[w] = F[w(x)] = \exp[\int H(x,y)w(x)dx].$$

In this case we have

$$\begin{aligned}\frac{\delta F[w]}{\delta w(z)} &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left\{\exp\left[\int H(x,y)[w(x)+\varepsilon\delta(x-z)]dx\right] - \exp\left[\int H(x,y)w(x)dx\right]\right\}\\ &= H(z,y)\exp\left[\int H(x,y)w(x)dx\right] = H(z,y)F[w].\end{aligned}$$

These results can be applied to calculate the derivatives of $Z_0[J]$ with respect to J, involving now a double integral:

$$\begin{aligned}\frac{\delta Z_0[J]}{\delta J(z)} &= \left\{\frac{\mathcal{N}}{\varepsilon}\exp\left[\frac{-i}{2}\int[J(x)+\varepsilon\delta(x-z)]G_0(x-y)[J(y)+\varepsilon\delta(y-z)]d^4xd^4y\right]\right.\\ &\quad\left. - \frac{\mathcal{N}}{\varepsilon}\exp\left[\frac{-i}{2}\int J(x)G_0(x-y)J(y)d^4xd^4y\right]\right\}_{\varepsilon\to 0}\\ &= \left[\frac{-i}{2}\int J(x)G_0(x-y)\delta(y-z)d^4xd^4y\right.\end{aligned}$$

$$-\frac{i}{2}\int \delta(x-z)G_0(x-y)J(y)d^4xd^4y\Big] Z_0[J]$$
$$= -i\int J(x)G_0(x-z)d^4x\ Z_0[J]$$

and

$$\frac{\delta^2 Z_0[J]}{\delta J(z)\delta J(z')} = -iG_0(z-z')Z_0[J] + (-i)^2\left[\int J(x)G_0(x-z)d^4x\right]^2 Z_0[J].$$

From these expressions, $Z_0[J]$ is considered a generating functional for $G_0(z-z')$ if we define the normalization constant as $\mathcal{N}=1$, such that, $Z_0[J=0]=1$; then we find

$$\frac{\delta^2 Z_0[J]}{i\delta J(z) i\delta J(z')}|_{J=0} = iG_0(z-z') = \langle 0|T[\phi(z)\phi(z')]|0\rangle.$$

3.6 Canonical quantization of the Dirac field

The Klein-Gordon equation expresses the mass-shell condition, since it is written in the momentum representation as $(p^2-m^2)\phi(x)=0$, which implies $p^2=m^2$. As a result of the Lorentz invariance, the Lagrangian is a scalar. These facts are used to search for other Lorentz invariant equations. Let us assume a Lorentz invariant form $i\gamma^\mu\partial_\mu$. Then we compose the equation

$$i\gamma^\mu\partial_\mu\psi(x) = k\psi(x). \tag{3.32}$$

The meaning of the 4-vector γ^μ and the constant k are determined by requiring consistency of this equation with the mass-shell condition. Multiplying Eq. (3.32) by $i\gamma^\mu\partial_\mu$ we get

$$-(\gamma^\mu\partial_\mu)^2\psi(x) = k\ i\gamma^\mu\partial_\mu\psi(x),$$

or

$$(\gamma^\mu\gamma^\nu\partial_\mu\partial_\nu + k^2)\psi(x) = 0.$$

Since $\partial_\mu\partial_\nu$ is symmetric, only the symmetric part of $\gamma^\mu\gamma^\nu$, i.e. $\frac{1}{2}\{\gamma^\mu,\gamma^\nu\}$, gives a non-null contribution

$$(\frac{1}{2}\{\gamma^\mu,\gamma^\nu\}\partial_\mu\partial_\nu + k^2)\psi(x) = 0,$$

where

$$\{\gamma^\mu,\gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu.$$

Consistency with the mass-shell condition is obtained by identifying

$$\{\gamma^\mu,\gamma^\nu\} = 2g^{\mu\nu} \tag{3.33}$$

and $\gamma_\mu k^\mu = m$. Thus we obtain the Dirac equation

$$(i\gamma^\mu \partial_\mu - m)\psi(x) = 0. \tag{3.34}$$

To study this equation, representations of Eq. (3.33), establishing a Clifford algebra, have to be presented. An irreducible representation of γ^μ is given in terms of the following 4×4 matrices,

$$\gamma^0 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \gamma^1 = \begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix}, \quad \gamma^2 = \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, \quad \gamma^3 = \begin{pmatrix} 0 & \sigma^3 \\ \sigma^3 & 0 \end{pmatrix}$$

where

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

In this case $\psi(x)$ is a 4-component object called the *Dirac spinor*.

To obtain a similar equation in the dual space, the adjoint spinor is defined by

$$\overline{\psi}(x) = \psi^\dagger(x)\gamma^0,$$

and the adjoint Dirac equation is given by

$$\overline{\psi}(x)(i\gamma \overleftarrow{\partial} + m) = 0. \tag{3.35}$$

To assure the invariance of Eqs. (3.34) and (3.35) under the Lorentz transformation, specified by $x'^\mu = \Lambda^\mu{}_\nu x^\nu$, we take

$$\psi'(x') = S(\Lambda)\psi(x),$$

where

$$S(\Lambda) = \exp\left(\frac{-i}{4}\sigma_{\mu\nu}\omega^{\mu\nu}\right),$$

with $\omega^{\mu\nu}$ being an antisymmetric tensor determining the 6 parameters of the Lorentz transformation and

$$\sigma^{\mu\nu} = \frac{i}{2}[\gamma^\mu, \gamma^\nu] = \frac{i}{2}(\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu).$$

Each Dirac matrix is transformed as

$$S(\Lambda)\gamma^\mu S^{-1}(\Lambda) = (\Lambda^{-1})^\mu{}_\nu \gamma^\nu$$

and from Eq. (3.35), $\overline{\psi}(x)$ is transformed as $\overline{\psi}'(x') = \overline{\psi}(x)S^{-1}(\Lambda)$.

In order to introduce Lorentz invariant terms that take into account interactions, it is interesting at this point to evaluate the different ways that a bilinear form of the type $\overline{\psi}(x)F(\gamma)\psi(x)$ is transformed by a Lorentz transformation, where $F(\gamma)$ is some function of γ-matrices. For instance, for $F(\gamma) = 1$, it is easy to find that $\overline{\psi}(x)\psi(x)$ is a Lorentz scalar. In general we have

$$\overline{\psi}'(x')F(\gamma)\psi'(x') = \overline{\psi}(x)S^{-1}(\Lambda)F(\gamma)S(\Lambda)\psi(x)\ ,$$

with a basic set of combinations that have different properties under the transformation. These are

$$\begin{aligned}
\overline{\psi}'(x')\psi'(x') &= \overline{\psi}(x)\psi(x) && scalar\\
\overline{\psi}'(x')\gamma^\mu\psi'(x') &= \Lambda^\mu{}_\nu\overline{\psi}(x)\gamma^\nu\psi(x) && vector\\
\overline{\psi}'(x')\sigma^{\mu\nu}\psi'(x') &= \Lambda^\mu{}_\rho\Lambda^\nu{}_\varsigma\overline{\psi}(x)\sigma^{\rho\varsigma}\psi(x) && antisymmetic\ tensor\\
\overline{\psi}'(x')\gamma^5\psi'(x') &= \det(\Lambda)\overline{\psi}(x)\gamma^5\psi(x) && pseudo-scalar\\
\overline{\psi}'(x')\gamma^5\gamma^\mu\psi'(x') &= \det(\Lambda)\Lambda^\mu{}_\nu\overline{\psi}(x)\gamma^5\gamma^\nu\psi(x) && pseudo-vector
\end{aligned}$$

where

$$\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix},$$

satisfying the properties

$$\{\gamma^\mu, \gamma^5\} = 0, \quad (\gamma^5)^2 = 1.$$

The Lagrangian density for the Dirac field is given by

$$\mathcal{L} = \frac{1}{2}\overline{\psi}(x)\gamma\cdot i\overleftrightarrow{\partial}\psi(x) - m\overline{\psi}(x)\psi(x),$$

where

$$\overline{\psi}(x)\gamma\cdot i\overleftrightarrow{\partial}\psi(x) = i\overline{\psi}(x)\gamma^\mu\partial_\mu\psi(x) - i\partial_\mu\overline{\psi}(x)\gamma^\mu\psi(x).$$

The canonical field momentum densities are derived from the Lagrangian density,

$$\begin{aligned}
\pi(x) &= \frac{\partial\mathcal{L}}{\partial\dot{\psi}(x)} = i\psi^\dagger(x),\\
\overline{\pi}(x) &= \frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}(x)} = -i\overline{\psi}^\dagger(x),
\end{aligned}$$

and the Hamiltonian density reads

$$\mathcal{H} = \pi(x)\dot{\psi}(x) + \overline{\pi}(x)\dot{\overline{\psi}}(x) - \mathcal{L}. \tag{3.36}$$

The quantization is introduced by equal-time anti-commutation relations,

$$\{\psi(t,\mathbf{x}),\pi(t,\mathbf{y})\} = i\delta(\mathbf{x}-\mathbf{y}), \tag{3.37}$$

$$\{\pi(t,\mathbf{x}),\pi(t,\mathbf{y})\} = \{\psi(t,\mathbf{x}),\psi(t,\mathbf{y})\} = 0. \tag{3.38}$$

Equal-time anti-commutation relations are needed to introduce a positive definite Hamiltonian in the theory.

A general solution of the free Dirac equation is written in terms of plane waves, a Fourier basis, and a basis for the spinor, i.e.,

$$\psi(x) = \int \frac{d^3k}{(2\pi)^3}\frac{m}{k_0}\sum_{\lambda=1}^{2}[b_\lambda(k)u^{(\lambda)}(k)e^{-ikx} + d^\dagger_\lambda(k)v^{(\lambda)}(k)e^{ikx}] \tag{3.39}$$

and

$$\overline{\psi}(x) = \int \frac{d^3k}{(2\pi)^3}\frac{m}{k_0}\sum_{\lambda=1}^{2}[b^\dagger_\lambda(k)\overline{u}^{(\lambda)}(k)e^{ikx} + d_\lambda(k)\overline{v}^{(\lambda)}(k)e^{-ikx}], \tag{3.40}$$

where $b_\lambda(k)$ ($d_\lambda(k)$) and $b^\dagger_\lambda(k)$ ($d^\dagger_\lambda(k)$) are annihilation and creation operators for particles (antiparticles), with momentum k, respectively, and satisfy the anti-commutation relations:

$$\{b_\lambda(k),b^\dagger_\xi(k')\} = \{d_\lambda(k),d^\dagger_\xi(k')\} = (2\pi)^3\frac{k_0}{m}\delta(\mathbf{k}-\mathbf{k}')\delta_{\lambda\xi}.$$

All the other anti-commutation relations are zero.

The spinor basis in Eqs. (3.39) and (3.40) is given by

$$u^{(1)}(k) = A(k_0;m)\begin{pmatrix} 1 \\ 0 \\ \frac{k^3}{k_0+m} \\ \frac{k^1+ik^2}{k_0+m} \end{pmatrix}, \quad u^{(2)}(k) = A(k_0;m)\begin{pmatrix} 1 \\ 0 \\ \frac{k^1-ik^2}{k_0+m} \\ \frac{-k^3}{k_0+m} \end{pmatrix}, \tag{3.41}$$

$$v^{(1)}(k) = A(k_0;m)\begin{pmatrix} \frac{k^3}{k_0+m} \\ \frac{k^1+ik^2}{k_0+m} \\ 1 \\ 0 \end{pmatrix}, \quad v^{(2)}(k) = A(k_0;m)\begin{pmatrix} \frac{k^1-ik^2}{k_0+m} \\ \frac{-k^3}{k_0+m} \\ 0 \\ 1 \end{pmatrix}, \tag{3.42}$$

with $A(k_0;m) = \sqrt{(k_0+m)/2}$, and

$$\overline{u}^{(\lambda)}(k) = u^{\dagger(\lambda)}(k)\gamma^0; \;\; \overline{v}^{(\lambda)}(k) = v^{\dagger(\lambda)}(k)\gamma^0.$$

These spinors satisfy the orthonormalization conditions

$$\begin{aligned} \overline{u}^{(\lambda)}(k)u^{(\xi)}(k) &= \delta_{\lambda\xi}, \\ \overline{v}^{(\lambda)}(k)v^{(\xi)}(k) &= \delta_{\lambda\xi}, \\ \overline{u}^{(\lambda)}(k)v^{(\xi)}(k) &= 0, \\ \overline{v}^{(\lambda)}(k)u^{(\xi)}(k) &= 0, \end{aligned}$$

and the projection operators are

$$\begin{aligned} \sum_{\lambda=1}^{2} u^{(\lambda)}(k)\overline{u}^{(\lambda)}(k) &= \frac{\gamma\cdot k+m}{2m}, \\ \sum_{\lambda=1}^{2} v^{(\lambda)}(k)\overline{v}^{(\lambda)}(k) &= \frac{\gamma\cdot k-m}{2m}. \end{aligned}$$

These results can be obtained by analyzing the free Dirac equation in momentum space.

Now the Hamiltonian is obtained. Here the normal ordering, respecting the sign of the anti-commutation relations, is used changing the sign for each change of operator order; for instance, $: b_\lambda(k)b^\dagger_\xi(k') : = -b^\dagger_\xi(k')b_\lambda(k)$. Then from Eq. (3.36) we get

$$\begin{aligned} H &= : \int d^3x\, \mathcal{H}(x) : \\ &= \int \frac{d^3k}{(2\pi)^3}\, m \sum_{\lambda=1}^{2} [b^\dagger_\lambda(k)b_\lambda(k) + d^\dagger_\lambda(k)d_\lambda(k)]. \end{aligned}$$

The charge is calculated from the charge density operator $j_0 = :\psi^\dagger(x)\psi(x):$, resulting in

$$\begin{aligned} Q &= \int d^3x :\psi^\dagger(x)\psi(x): \\ &= \int \frac{d^3k}{(2\pi)^3}\frac{m}{k_0}\sum_{\lambda=1}^{2}[b_\lambda^\dagger(k)b_\lambda(k) - d_\lambda^\dagger(k)d_\lambda(k)]\,. \end{aligned}$$

The vacuum is defined by

$$b_\lambda(k)|0\rangle = d_\lambda(k)|0\rangle = 0.$$

Since $[b_\lambda(k)]^2 = [d_\lambda(k)]^2 = 0$, there are only states with 0 or 1 particle or antiparticle, respectively, with the same momentum k and the same spin label λ. One particle states are introduced by $b_\lambda^\dagger(k)|0\rangle$ and $d_\lambda^\dagger(k)|0\rangle$.

The propagator is given as

$$\begin{aligned} S(x-y) &= -i\langle 0|T[\psi(x)\overline{\psi}(y)]|0\rangle \\ &= \int \frac{d^4k}{(2\pi)^4}e^{-ik(x-y)}\frac{\gamma\cdot k + m}{k^2 - m^2 + i\varepsilon} \\ &= (i\gamma\cdot\partial + m)G_0(x-y), \end{aligned}$$

where $G_0(x-y)$ is given by Eq. (3.23).

3.7 Path integral for the Dirac field

In order to construct a generating functional for the Dirac field a crucial observation has to be made: the Dirac field satisfies anti-commutation relations. The nature of a generating functional is to work with c-number functions instead of operators. Then we have to be careful in the case of fermions, due to the anti-commuting property. This difficulty is overcome with the use of Grassmann numbers.

A set of Grassmann numbers is denoted by $G = \{\alpha, \eta, \chi, \dots\}$; a one-mode fermion operator is described by the algebra $\{a, a^\dagger\} = 1$; complex number will be denoted by c. The Grassmann variables are characterized by the following properties:

$$\begin{aligned} \alpha\eta &= -\eta\alpha, \\ \alpha(\eta + c\chi) &= \alpha\eta + c\alpha\chi. \end{aligned}$$

Concerning the operators a and $a^\dagger$ we have

$$\alpha a = -a\alpha, \quad \alpha a^\dagger = -a^\dagger\alpha.$$

The complex conjugation of Grassmann variable is defined by an anti-linear mapping fulfilling the property,

$$(\alpha + ca\eta a^\dagger\chi^*)^\dagger = \alpha^* + \chi a\eta^* a^\dagger c^*.$$

The Grassmann variables α and α^* are considered independent of each other. When $\alpha = \alpha^*$, α is a real Grassmann variable.

An arbitrary function $f(\alpha)$ of a Grassmann variable is of the form

$$f(\alpha) = f_0 + f_1\alpha,$$

where f_0 and f_1 are complex numbers. This is indeed like that, since $\alpha^2 = 0$. The integration is defined by

$$\int \alpha d\alpha = 1, \quad \int d\alpha = 0,$$

where the symbol $\int$ is linear. From this result we have

$$\int f(\alpha)d\alpha = \int (f_0 + f_1\alpha)d\alpha = f_1$$

This definition for integration is equivalent to a right-side derivative, defined by the linear operation

$$\frac{\partial f(\alpha)}{\partial \alpha} = f_1.$$

This integration is also enough to define in a consistent way a δ-function. Indeed, a δ-function of the Grassmann variables, $\delta(\alpha - \eta)$, is defined by

$$\int \delta(\alpha - \eta) f(\alpha) d\alpha = f(\eta).$$

Then $\delta(\alpha - \eta) = \alpha - \eta$, which is no longer an even function.

The scalar product involving two Grassmann functions $f(\alpha)$ and $g(\alpha)$ is defined by

$$(f, g) = \int f^*(\alpha) g(\alpha) e^{-\alpha^*\alpha} d\alpha,$$

where $f^*(\alpha) = f_0^* + f_1^*\alpha$. A basis is given by $\varphi_0 = 1$ and $\varphi_1 = \alpha^*$, such that

$$\begin{aligned} (\varphi_n, \varphi_m) &= \delta_{nm}, \\ \alpha^*\varphi_0 = \varphi_1, \ \alpha^*\varphi_1 &= 0, \\ \frac{\partial}{\partial \alpha^*}\varphi_0 = 0, \ \frac{\partial}{\partial \alpha^*}\varphi_1 &= \varphi_0. \end{aligned}$$

This provides a representation for the operators $a \equiv \frac{\partial}{\partial \alpha^*}$ and $a^\dagger \equiv \alpha^*$.

Consider a normal-ordered general operator written as

$$: A(a, a^\dagger): \ = \mathcal{A}_{00} + \mathcal{A}_{01}a^\dagger + \mathcal{A}_{01}a + \mathcal{A}_{11}a^\dagger a,$$

with $\mathcal{A}_{nm} \in \mathbb{C}$, $m, n = 0, 1$ In terms of Grassmann variables two functions can be defined and associated with $: A(a, a^\dagger) :$. The first is the normal ordering symbol and the other is the kernel, given respectively by

$$\begin{aligned} \mathcal{A}(\alpha, \alpha^*) &= \sum_{m,n=0,1} \mathcal{A}_{nm}(\alpha^*)^n(\alpha)^m, \\ A(\alpha, \alpha^*) &= \sum_{m,n=0,1} A_{nm}(\alpha^*)^n(\alpha)^m, \end{aligned}$$

where $A_{nm} = (\varphi_n, A\varphi_m)$ is the matrix element of the operator A in the Grassmann basis. The relation between $A(\alpha, \alpha^*)$ and $A(\alpha, \alpha^*)$ is

$$A(\alpha, \alpha^*) = e^{\alpha^* \alpha} \mathcal{A}(\alpha, \alpha^*),$$

and the representation of the normal-ordered product of two operators $A_1 A_2$ in the normal order is given by

$$A_1 A_2(\alpha, \alpha^*) = \int A_1(\alpha^*, \eta) A_2(\eta^*, \alpha) e^{-\eta^* \eta} d\eta^* d\eta,$$

where we have used the relation

$$\int (\eta^*)^n \eta^m e^{-\eta^* \eta} d\eta^* d\eta = \delta_{nm}.$$

Another important result is

$$\int e^{-\eta^* A \eta} d\eta^* d\eta = \det A.$$

An infinite-dimensional Grassmann function in the Minkowski space-time is denoted by $\eta(x)$ and satisfies:

$$\{\eta(x), \eta(y)\} = 0; \quad \int \eta(x) d\eta(x) = 1, \quad \int d\eta(x) = 0,$$

$$\frac{\partial \eta(x)}{\partial \eta(y)} = \delta(x - y),$$

and

$$\frac{\partial \eta(x)\eta(y)}{\partial \eta(z)} = \delta(x - z)\eta(y) - \eta(x)\delta(y - z).$$

These results give rise to a definition of the functional derivative.

Let us write the Lagrangian for the Dirac field as

$$\mathcal{L} = \frac{1}{2}\overline{\psi}(x)\gamma \cdot i\partial\psi(x) - m\overline{\psi}(x)\psi(x) + \overline{\eta}(x)\psi(x) + \overline{\psi}(x)\eta(x),$$

where $\eta(x)$ and $\overline{\eta}(x)$ are the sources for the independent fields $\overline{\psi}(x)$ and $\psi(x)$, respectively. The generating functional for the fermion field is defined by

$$Z_0[\eta, \overline{\eta}] = \mathcal{N} \int D\overline{\psi} D\psi \exp\{i \int dx f[\overline{\psi}, \psi]\},$$

where

$$\begin{aligned} f[\overline{\psi}, \psi] &= \overline{\psi}(x)(i\gamma \cdot \partial - m)\psi(x) + \overline{\eta}(x)\psi(x) + \overline{\psi}(x)\eta(x) \\ &= -\overline{\eta}(x)(i\gamma \cdot \partial - m)^{-1}\eta(x) \\ &\quad + (\overline{\psi}(x) - \overline{\psi}_0(x))(i\gamma \cdot \partial - m)(\psi(x) - \psi_0(x)). \end{aligned}$$

The functional $Z_0[\eta, \overline{\eta}]$ reads

$$Z_0[\eta, \overline{\eta}] = \exp\left\{-i \int dx[\overline{\eta}(x) S(x - y)\eta(x)\right\} \mathcal{N} \det(-iS^{-1}),$$

where

$$S(x-y) = (i\gamma \cdot \partial + m)G_0(x-y).$$

The normalized functional is defined by $Z_0[\eta, \overline{\eta}]_{\eta=0,\overline{\eta}=0} = 1$, such that

$$Z_0[\eta, \overline{\eta}] = \exp\left\{-i \int dx[\overline{\eta}(x)S(x-y)\eta(x)\right\}.$$

As a result we obtain

$$\frac{\delta^2 Z_0[\eta, \overline{\eta}]}{\delta\eta(x)\delta\overline{\eta}(y)}|_{\eta,\overline{\eta}=0} = iS(x-y) = \langle 0|T[\phi(x)\phi(y)]|0\rangle.$$

These results provides a practical tool for calculations, that can be generalized to more intricate interactions.

The path integral formalism and generating functionals will be the fundamental tools to construct quantum theories for boson, fermion and gauge fields both at zero and finite temperature. Given a specific interaction, perturbative series for physical quantities are obtained. In the following chapter the generating function will lead to the Green function to be used to calculate the scattering amplitudes. Methods for working at finite temperature will be elaborated in Chapter 8.

Chapter 4

Zero Temperature Interacting Fields

We generalize here the notion of generating functional developed in the previous Chapter to treat interacting fields [30–33, 36–39]. Initially the basic elements are developed for the $\lambda\phi^4$-theory. Subsequently fermions and gauge fields are considered.

4.1 Generating functional for bosons

For a system of noninteracting bosons, the generating functional is given, up to a normalization factor, by

$$Z_0 \simeq \int D\phi e^{i\mathcal{S}} = \int D\phi \exp[i \int dx \mathcal{L}_0(\phi)] \tag{4.1}$$

$$= \exp\{\frac{i}{2} \int dxdy[J(x)G_0(x-y)J(y)]. \tag{4.2}$$

Considering the interacting Lagrangian density in the form

$$\mathcal{L}(\phi; J) = \mathcal{L} + J\phi = \frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) - \frac{m^2}{2}\phi^2 + \mathcal{L}_I(\phi) + J\phi,$$

we define the generating functional as

$$Z[J] \simeq \int D\phi e^{i\mathcal{S}}$$

$$= \int D\phi \exp[i \int dx \mathcal{L}(\phi; J)].$$

This functional satisfies the following equation

$$(\Box + m^2)\frac{\delta Z[J]}{i\delta J(x)} + \mathcal{L}_{int}\left(\frac{1}{i}\frac{\delta}{\delta J}\right) Z[J] = J(x)Z[J];$$

with a solution

$$Z[J] = \exp\left[i \int dx \mathcal{L}_{int}\left(\frac{1}{i}\frac{\delta}{\delta J}\right)\right] Z_0[J].$$

The n-point Green function is written as,

$$G^{(n)}(x_1, x_2, ..., x_n) = \frac{1}{i^n} \left.\frac{\partial^n Z[J]}{\partial J(x_1)\partial J(x_2)\cdots\partial J(x_n)}\right|_{J=0}.$$

Let us study the specific example where

$$\mathcal{L}_{int}(\phi) = \frac{\lambda}{4!}\phi^4.$$

The 2-point and the 4-point functions to first-order in λ are given respectively by

$$G^{(2)}(x_1, x_2) = G_0(x_1 - x_2) - \frac{1}{2}i\lambda \int dx G_0(x_1 - x)G_0(x - x)G_0(x - x_2) \tag{4.3}$$

and

$$\begin{aligned} G^{(4)}(x_1, x_2, x_3, x_4) = G_0^{(4)}(x_1, x_2, x_3, x_4) - \frac{1}{2}i\lambda \Bigg(& G_0(x_1 - x_2) \int dx \\ & \times G_0(x_3 - x)G_0(x - x)G_0(x - x_4) \\ & + G_0(x_3 - x_4) \int dx G_0(x_1 - x)G_0(x - x)G_0(x - x_2) \\ & + G_0(x_1 - x_3) \int dx G_0(x_2 - x)G_0(x - x)G_0(x - x_4) \\ & + G_0(x_2 - x_4) \int dx G_0(x_1 - x)G_0(x - x)G_0(x - x_3) \\ & + G_0(x_1 - x_4) \int dx G_0(x_2 - x)G_0(x - x)G_0(x - x_3) \\ & + G_0(x_2 - x_3) \int dx G_0(x_1 - x)G_0(x - x)G_0(x - x_4) \\ & - i\lambda \int dx G_0(x_1 - x)G_0(x_2 - x)G_0(x_3 - x)G_0(x_4 - x) \end{aligned}$$

where $G_0^{(4)}(x_1, x_2, x_3, x_4)$ is the 4-point function for the free field theory,

$$\begin{aligned} G_0^{(4)}(x_1, x_2, x_3, x_4) = (i)^2[& G_0(x_1 - x_2)G_0(x_3 - x_4) \\ & + G_0(x_1 - x_3)G_0(x_2 - x_4) \\ & + G_0(x_1 - x_4)G_0(x_2 - x_3)]. \end{aligned} \tag{4.4}$$

We may represent these expressions in a diagrammatic way: we use a line with the end points x_1 and x_2 to represent the propagator $G_0(x_1 - x_2)$, Fig. 4.1. Then the

$G_0(x_1 - x_2)$:

Fig. 4.1 Free propagator.

Green function $G^{(2)}(x_1 - x_2)$, up to the first order, given in Eq. (4.3), is represented diagrammatically in Fig. 4.2. A factor $-i\lambda$ at each vertex is included, as indicated in Fig. 4.3, to recover the expressions. The free 4-point function $G_0^{(4)}(x_1 - x_2)$, given in Eq. (4.4), is presented in Fig. 4.4. For a closed line, a loop, as in the second diagram in Fig. 4.2, the expression of the Green function includes an integration over x of $G(x - x)$.

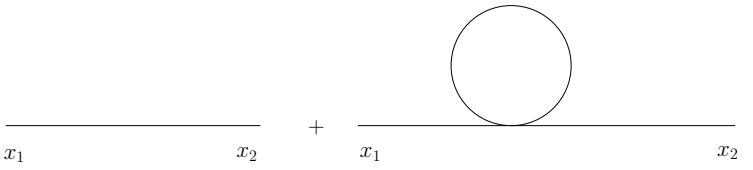


Fig. 4.2 Propagator $G^{(2)}(x_1 - x_2)$ up to first order in λ.

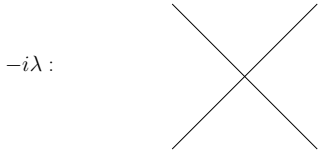


Fig. 4.3 Vertex.

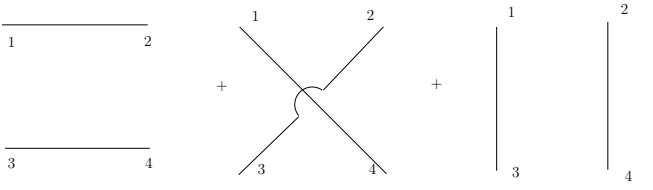


Fig. 4.4 4-point function $G_0^{(4)}(x_1 - x_2)$ at zero order.

We find from these examples that there are two classes of diagrams: the connected, like each diagram in Fig. 4.2 and the unconnected, as each of the diagrams in Fig. 4.4. All the connected Green functions can be derived from a function, say, $W[J]$, defined by

$$iW[J] \equiv \ln Z[J].$$

The connected n-point Green functions are obtained by functional derivative, i.e.

$$G_c^{(n)}(x_1, x_2, ..., x_n) = \frac{1}{i^n} \left. \frac{i\partial^n W[J]}{\partial J(x_1)\partial J(x_2)...\partial J(x_n)} \right|_{J=0}.$$

These are the relevant Green functions for the calculation of cross sections. To first order, $G^{(2)}$ given in Fig. 4.2 contains only connected parts, and so $G_c^{(2)} = G^{(2)}$. The connected 4-point function, up to the first order, is given by the vertex diagram, in Fig. 4.3.

4.1.1 *Feynman rules in momentum space*

Taking the Fourier transform of $G^{(n)}(x_1, x_2, \ldots, x_n)$, the Green function in momentum space is defined. Considering translation invariance, we have

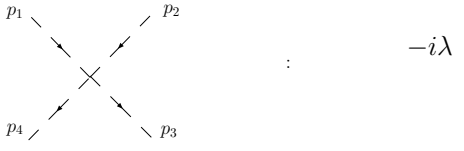
$$G^{(n)}(p_1, \ldots, p_n)(2\pi)^4 \delta(p_1 + \cdots + p_n) = \int d^n x G^{(n)}(x_1, \ldots, x_n) e^{-i(p_1 x_1 + \cdots + p_n x_n)},$$

where $d^n x = dx_1 \cdots dx_n$. The diagrammatic representation of Feynman rules in the momentum space are,

(1) Each oriented line carries a momentum p and a factor $-(p^2 - m^2 + i\varepsilon)^{-1}$,

(2) Each vertex has a factor of $-i\lambda$ and has momentum conservation:

$$p_1 + p_2 - p_3 - p_4 = 0,$$



(3) Integrate over each internal loop momentum, k, with the factor $(2\pi)^{-4} d^4 k$.

Consider as an example the 2-point Green function up to first order, i.e.

$$G_c^{(2)}(p, -p) = \frac{-1}{p^2 - m^2 + i\varepsilon} - \frac{i\lambda}{2} \int \frac{d^4 k}{(2\pi)^4} \frac{-1}{p^2 - m^2 + i\varepsilon} \frac{-1}{k^2 - m^2 + i\varepsilon} \frac{-1}{p^2 - m^2 + i\varepsilon}.$$

This is represented in Fig. 4.5.

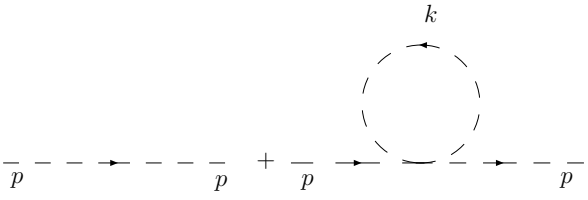


Fig. 4.5 2-point function $G_c^{(2)}(p, -p)$ at first order.

4.2 The effective action

Using a Legendre transform of the functional $W[J]$ in the variable J, the functional $\Gamma[\phi_c]$ is defined,

$$\Gamma[\phi_c] = W[J] - \int dx J(x)\phi_c(x), \tag{4.5}$$

where the *classical field* (see below) is,

$$\phi_c(x) = \frac{\delta X[J]}{\delta J(x)}. \tag{4.6}$$

Let us analyze the meaning of $\phi_c(x)$ and $\Gamma[\phi_c]$ from a physical point of view. The field $\phi_c(x)$, from Eq. (4.6), is given by

$$\phi_c(x) = \frac{\langle 0|\phi(x)|0\rangle_J}{\langle 0|0\rangle_J},$$

where $\langle 0|0\rangle_J = Z_0[J]$. Now consider a free-field theory. Then

$$iW[J] = -\frac{1}{2}\int d^4x d^4y J(y)G_0(x-y)J(x),$$

such that

$$\phi_c(x) = -\int d^4x G_0(x-y)J(x),$$

which is a solution of the inhomogeneous Klein-Gordon equation,

$$(\Box + m^2)\phi_c(x) = J(x).$$

Thus $\phi_c(x)$ is a classical field.

Using these results in Eq. (4.5), the functional $\Gamma[\phi_c]$ is written as

$$\Gamma[\phi_c] = \frac{1}{2}\int d^4x \phi_c(x)(\Box + m^2)\phi_c(x),$$

describing the classical action for the field $\phi_c(x)$. The functional $\Gamma[\phi_c]$ is called the effective action.

Expanding $\Gamma[\phi_c]$ in terms of ϕ_c, we have

$$\Gamma[\phi_c] = \sum_{n=1}^{\infty}\frac{i^n}{n!}\int d^4x_1\cdots d^4x_n\Gamma^{(n)}(x_1,\ldots,x_n)\phi_c(x_1)\cdots\phi_c(x_n), \tag{4.7}$$

where the $\Gamma^{(n)}(x_1,...,x_n)$ are called one-particle irreducible (1PI) Green functions. The Feynman diagram of an 1PI Green function is a connected graph such that it cannot be made disconnected by cutting just one of its internal lines. The 1PI Green functions are basic structures to be used to construct classes of other connected diagrams. For the free field theory the only non-trivial 1PI Green function is

$$\Gamma^{(2)}(x_1,x_2) = (\Box + m^2)\delta(x_1 - x_2).$$

In momentum space, the 1PI Green function is given by

$$\Gamma^{(n)}(p_1,\ldots,p_n)(2\pi)^4\delta(p_1+\cdots+p_n)=\int d^nx\Gamma^{(n)}(x_1,\ldots,x_n)e^{-i(p_1x_1+\cdots+p_nx_n)}. \tag{4.8}$$

This equation is used to expand $\Gamma^{(n)}$ around zero-momentum. Reverting to the space-time coordinates, such an expansion is written in the form,

$$\Gamma[\phi_c]=\int d^4x\left(-V(\phi_c)+\frac{A(\phi_c)}{2}\partial_\mu\phi_c\partial^\mu\phi_c+\cdots\right),$$

where the quantity $V(\phi_c)$ is called the *effective potential*. For a constant classical field, ϕ_c, $\Gamma[\phi_c]=\int d^4x[-V(\phi_c)]$, and from Eq. (4.5)

$$J(x)=-\frac{\delta\Gamma[\phi_c]}{\delta\phi_c}=\frac{dV(\phi_c)}{d\phi_c}.$$

If the source term is zero, then

$$\frac{dV(\phi_c)}{d\phi_c}=0.$$

This equation is solved to find the vacuum expectation value of the field operator. Using Eqs. (4.7) and (4.8), we obtain

$$V(\phi_c)=-\sum_{n=1}^{\infty}\frac{(i\hbar)^n}{n!}\Gamma^{(n)}(0,\ldots,0)\phi_c^n,$$

where we have introduced for later convenience, the Plack constant $\hbar$. As an example, consider the scalar free field. We have

$$\Gamma^{(2)}(p,-p)=-(p^2-m^2),$$

such that $\Gamma^{(2)}(0,0)=m^2$ and

$$V(\phi_c)=\frac{m^2}{2}\phi_c^2.$$

This gives the potential for the classical field; this is why $V(\phi_c)$ is called the effective potential.

Now we wish to calculate the effective potential to order $\hbar$, i.e. one-loop order. We start from the generating functional,

$$Z[J]=\mathcal{N}\int D\varphi e^{-\frac{i}{\hbar}(\mathcal{L}+J\varphi)}, \tag{4.9}$$

where $\mathcal{N}$ is a normalization factor, and we shift the integration variable φ by,

$$\varphi(x)=\varphi_c+\varphi_1(x) \tag{4.10}$$

where φ_c is the zeroth order approximation in $\hbar$, the classical field. Then we substitute this expression in

$$\begin{aligned}\int d^4x(\mathcal{L}+J\varphi)=&\int d^4x(\mathcal{L}_0+J\varphi_c)+\int d^4x\left[\partial_\mu\varphi_1\partial^\mu\varphi_1-m^2\varphi_1\varphi_c\right.\\&\left.-\frac{\lambda}{6}\varphi_1\varphi_c^3+J\varphi_1\right]\\&+\int d^4x\left[\mathcal{L}_2(\varphi_1,\varphi_c)-\frac{\lambda}{6}\varphi_1^3\varphi_c-\frac{\lambda}{24}\varphi_1^4\right],\end{aligned} \tag{4.11}$$

where

$$\mathcal{L}_2 = \frac{1}{2}\partial_\mu\varphi_1\partial^\mu\varphi_1 - \frac{1}{2}m^2\varphi_1^2 - \frac{\lambda}{24}\varphi_c^2\varphi_1^2. \tag{4.12}$$

We rescale the field φ_1 by $\varphi_1 = \hbar^{\frac{1}{2}}\varphi$, and use Eq. (4.11), so that the functional integral, Eq. (4.9), is written as

$$\begin{aligned} Z[J] = \mathcal{N}\int D\varphi \exp\left\{-\frac{i}{\hbar}\int d^4x\,[\mathcal{L}(\varphi_c) + J\varphi_c]\right\} \\ \times \int D\varphi \exp\left\{-\frac{i}{\hbar}\int d^4x\left[\mathcal{L}_2(\varphi\varphi_c) - \frac{\lambda}{6}\hbar^{\frac{1}{2}}\varphi^3\varphi_c - \frac{\hbar\lambda}{24}\varphi_c^4\right]\right\}. \end{aligned} \tag{4.13}$$

Neglecting terms proportional to $\hbar^{\frac{1}{2}}$ and $\hbar$ we write

$$\int d^4x\mathcal{L}_2(\varphi,\varphi_c) = -\frac{i}{2}\int d^4x\,d^4x'\varphi(x')A(x',x,\varphi_c)\varphi(x), \tag{4.14}$$

where

$$A(x',x,\varphi_c) = \left(-\partial_{x'\mu}\partial_x^\mu + m^2 + \frac{\lambda}{2}\varphi_c^2\right)\delta(x'-x). \tag{4.15}$$

Then to one-loop order, the generating functional of connected Green functions, $W[J]$, is $W[J] = W_0[J] + W_1[J]$, where

$$\begin{aligned} W_0[J] &= \int d^4x\,[\mathcal{L}_0(\varphi_c) + J\varphi_c] \\ W_1[J] &= \frac{1}{2}\mathrm{Tr}\ln\left[A(x',x,\varphi_c)/A(x',x,0)\right]. \end{aligned} \tag{4.16}$$

We diagonalize the matrix $A(x',x,\varphi_c)$ by using in Eq. (4.15) the Fourier representation of the δ-function,

$$A(x',x,\varphi_c) = \int \frac{d^4k}{(2\pi)^4}\left(-\partial_{x'\mu}\partial_x^\mu + m^2 + \frac{\lambda}{2}\varphi_c^2\right)e^{ik\cdot(x'-x)}.$$

We have

$$\mathrm{Tr}\ln A = \int d^4x\int\frac{d^4k}{(2\pi)^4}\ln\left(-k^2 + m^2 + \frac{\lambda}{2}\varphi_c^2\right). \tag{4.17}$$

Hence, dividing by the total volume $\int d^4x$, we get the one-loop correction to the effective potential,

$$\begin{aligned} V_1(\varphi_c) &= -\frac{i}{2}\ln\left(\frac{-k^2 + m^2 + \frac{\lambda}{2}\varphi_c^2}{-k^2 + m^2}\right) \\ &= -\frac{i}{2}\ln\left(1 - \frac{\lambda}{2}\frac{\varphi_c^2}{k^2 - m^2}\right). \end{aligned} \tag{4.18}$$

The total effective potential to one-loop order is,

$$\begin{aligned} V(\varphi_c) &\equiv V_0(\varphi_c) + V_1(\varphi_c) \\ &= \frac{m^2}{2}\varphi_c^2 + \frac{\lambda}{24}\varphi_c^4 - \frac{i}{2}\ln\left(1 - \frac{\lambda}{2}\frac{\varphi_c^2}{k^2 - m^2}\right). \end{aligned} \tag{4.19}$$

Under the assumption that λ is small, we develop the logarithm term. The one-loop correction to the effective potential is written as,

$$V_1(\varphi_c) = -\frac{i\hbar}{2}\sum_{s=1}^{\infty}\frac{(-1)^s}{2s}\left(\frac{\lambda\varphi_c^2}{2}\right)^s \int \frac{d^4k}{(2\pi)^4}\frac{1}{(k^2 - m^2 + i\varepsilon)^s}. \tag{4.20}$$

In Euclidian space we have,

$$V_1(\varphi_c) = \frac{\hbar}{2}\sum_{s=1}^{\infty}\frac{(-1)^s}{2s}\left(\frac{\lambda\varphi_c^2}{2}\right)^s \int \frac{d^4k}{(2\pi)^4}\frac{1}{(k^2 + m^2)^s}. \tag{4.21}$$

The s-order contribution to the sums in these equations is represented diagramatically in Fig. 4.6.

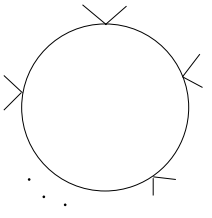


Fig. 4.6 Effective potential: s-vertex term.

4.3 Gauge fields

The study of gauge symmetries started with Weyl [40] as an attempt to write the electromagnetic field in a geometrical way, following the scheme of general relativity. The use of gauge transformations in particle physics was introduced by Yang and Mills [41]. The gauge invariance of the electromagnetic field described by the group $U(1)$ was generalized to the $SU(2)$ symmetry, the isospin group describing the nucleon. The formal results achieved by Yang and Mills were then analyzed from a geometric point of view [29]. Significant advances with the Yang-Mills fields occurred with the proof of renormalizabibity of such theories. Yang-Mills fields provides a general unified structure for the description of all known elementary particles in the context of the the standard model.

The Lagrangian density of N free Dirac fermions is written as

$$\begin{aligned} \mathcal{L}_0(\psi, \partial\psi) &= \overline{\psi}(x)[\gamma \cdot i\partial - m]\psi(x) \\ &= \sum_{i,j=1}^{N} \overline{\psi}_i(x)[\gamma \cdot i\partial - m]\delta_{ij}\psi_j(x), \end{aligned} \tag{4.22}$$

where the indices i and j stand for the N types of fermions. This Lagrangian is invariant under the Poincaré group. Besides we find that $\mathcal{L}_0$ is also invariant under the global phase transformation $\psi'(x) = U\psi(x)$, where $U = e^{i\Lambda}$, with Λ being a real constant quantity. The central characteristics of U are the following: (i) $U(\Lambda)$ is unitary and is an element of the $U(1)$ group; (ii) the phase transformation does not affect the space-time coordinates. This last aspect results in the fact that the indices of the γ-matrices are unchanged by the transformation U. These characteristics are present in any Lagrangian of a complex field describing matter. We implement two generalizations of this symmetry. One is associated with the components of $\psi_j(x)$, since we have analyzed the phase transformation $U = e^{i\Lambda}$ as being the same for any type of fermions, that is for all $i = 1, 2, \ldots, N$. In this case, U is an $N \times N$ matrix. The other possible extension is to consider U as being dependent on points of space-time. With these characteristics, a transformation of $\psi_j(x)$ can be formally written as

$$\psi_i'(x) = U_{ij}(x)\psi_j(x) \quad \text{and} \quad \overline{\psi}_i(x) = \overline{\psi}_j(x)U^{\dagger}_{ji}(x), \tag{4.23}$$

where we have assumed the sum over repeated Latin indices. This *gauge transformation*, $U_{ij}(x)$, has to be connected to the identity; thus we write it as

$$U(x) = e^{-ig\Lambda(x)} = e^{-ig\Lambda_r(x)t_r},$$

where $\Lambda_r(x)$ are real functions of space-time coordinates, g is a constant to fix the units and the operators t_j are the generators of the gauge group. These generators satisfy the Lie algebra

$$[t_r, t_s] = c_{rsl}t_l,$$

where c_{rsl} are the structure constants of the Lie group, with $r, s, l = 1, 2, \ldots, \ell$. The quantity ℓ specifies the maximal number of independent elements in the Lie algebra; or equivalently, the dimension of the algebra. The simplest finite dimensional representation for a Lie algebra is its adjoint representation. In the case of the gauge group, each matrix t_i reads

$$(t_r)_{sl} = (c_{rsl}).$$

For instance, for the the $su(2)$ algebra we have $c_{ijk} = i\varepsilon_{ijk}$ $i, j = 1, 2, 3$, such that

$$S_1 = (i\varepsilon_{1ik}) = i\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad S_2 = (i\varepsilon_{2,ik}) = i\begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$S_3 = (i\varepsilon_{3,ik}) = i\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

The transformation given by Eq. (4.23) does not leave the Lagrangian $\mathcal{L}_0$ invariant, i.e.

$$\mathcal{L}_0(\psi', \partial\psi') = \mathcal{L}_0(\psi, \partial\psi) + \overline{\psi}_i(x)\gamma^{\mu}[U^{-1}(x)i\partial_{\mu}U(x)]_{ij}\psi_j(x).$$

In order to cancel the extra term,

$$\mathcal{L}_{ext} = \overline{\psi}_i(x)\gamma^\mu[U^{-1}(x)i\partial_\mu U(x)]_{ij}\psi_j(x),$$

another term has to be added to the original Lagrangian. This new term involves a new field, say A, defined in such a way that: (i) the Lagrangian describing the field A is invariant under the gauge transformation and the Poicaré group, then the components of the field A are written as A^μ_{ij}; (ii) the field A^μ_{ij} transforms under the gauge transformation in such a way so as to cancel any non-gauge invariant term coming from $\mathcal{L}_0$. This requires a third term in the original Lagrangian with the interaction between A and $\psi_j(x)$. To take into account the extra term $\mathcal{L}_{ext}$, we introduce the Lagrangian term,

$$\mathcal{L}_1(\psi, \partial\psi) = -\overline{\psi}_i(x)g(A_\mu)_{ij}\gamma^\mu\psi_j(x),$$

requiring that under the gauge transformation the new field is

$$A'_\mu(x) = U(x)A_\mu(x)U^{-1}(x) + \frac{i}{g}\partial_\mu U(x)U^{-1}(x).$$

If we consider an infinitesimal transformation, Λ_a, $U(x)$ can be written as

$$U(x) = I + ig\Lambda_a t_a.$$

Then we write

$$A'_\mu(x) = A_\mu(x) - \partial_\mu\Lambda(x) + ig[\Lambda(x), A_\mu(x)]. \tag{4.24}$$

Observe that $\Lambda(x) = \Lambda_r(x)t_r$. The field $A_\mu(x)$ is

$$A_\mu(x) = A^r_\mu(x)t^r,$$

such that

$$\begin{aligned}[\Lambda(x), A_\mu(x)] &= [\Lambda_r(x)t_r, A_{\mu,s}(x)t_s] \\ &= \Lambda_r(x)A_{\mu,s}(x)[t_r, t_s] = \Lambda_r(x)A_{\mu,s}(x)c_{rsl}t_l.\end{aligned}$$

This is a matrix equation, since each t_l is an $N \times N$-matrix. The partial gauge-invariant Lagrangian is

$$\begin{aligned}\mathcal{L}_0 + \mathcal{L}_1 &= \overline{\psi}_i(x)[i\delta_{ij}\partial_\mu\gamma^\mu - g(A_\mu)_{ij}\gamma^\mu - m\delta_{ij}]\psi_j(x) \\ &= \overline{\psi}(x)[i\gamma^\mu D_\mu - m]\psi(x),\end{aligned}$$

where $D_\mu(A)$, the *covariant derivative*, is

$$D_\mu = \partial_\mu + igA_\mu.$$

This derivative is such that $D_\mu\psi$ transforms as ψ in Eq. (4.23); that is, the covariant derivative does not change the phase factor in a term with $D_\mu\psi$ (as it was the case of ∂_μ for Λ independent of x), such that

$$(D_\mu\psi)' = (\partial_\mu + igA'_\mu)\psi' = UD_\mu\psi.$$

Then the term $i\overline{\psi}(x)\gamma^\mu D_\mu\psi(x)$ is invariant.

Another term in the Lagrangian is needed to derive the equation of motion for $A'_\mu(x)$. This extra term has to be Poincaré and gauge invariant. Using the fact that D_μ is gauge invariant, we define

$$F_{\mu\nu} = D_\mu A_\nu - D_\nu A_\mu = \partial_\mu A_\nu - \partial_\nu A_\mu + g[A_\mu(x), A_\nu(x)]. \tag{4.25}$$

Then the simplest gauge invariant Lagrangian is

$$\mathcal{L}_2 = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}.$$

The full invariant Lagrangian, $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1 + \mathcal{L}_2$, is given by

$$\mathcal{L} = \overline{\psi}(x)(iD_\mu \gamma^\mu - m)\psi(x) - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}.$$

This expression is written in terms of quantities involving different matrix indices. Indeed we have indices describing the space-time $(\mu, \nu, ..)$, generators of the gauge group $(r, s, ..)$ and for the representation of the generators $(i, j, ...)$. Considering these indices, the explicit expressions for D_μ and $F_{\mu\nu}$, using $A_\mu(x) = A^r_\mu(x) t^r$, are

$$D_\mu = \partial_\mu + igA_\mu = \partial_\mu + igA^r_\mu(x) t^r,$$

or

$$(D_\mu)_{ij} = \delta_{ij}\partial_\mu + igA^r_\mu(x) t^r_{ij},$$

such that

$$[D_\mu, D_\nu] = igF^r_{\mu\nu} t^r,$$

where

$$F^r_{\mu\nu} = \partial_\mu A^r_\nu(x) - \partial_\nu A^r_\mu(x) + gc^{rsl} A^s_\mu(x) A^l_\nu(x).$$

In Eq. (4.25) $F_{\mu\nu}$ is

$$F_{\mu\nu} = F^r_{\mu\nu} t^r$$

and $g[A_\mu(x), A_\nu(x)]$ reads

$$g[A_\mu(x), A_\nu(x)] = gA^s_\mu(x) A^l_\nu(x)[t^s, t^l] = igc^{rsl} A^s_\mu(x) A^l_\nu(x) t^r.$$

Now Eq. (4.24) becomes

$$A'^r_\mu(x) = A^r_\mu(x) - \partial_\mu \Lambda^r(x) + gc^{rsl} \Lambda^s_\mu(x) A^l_\nu(x). \tag{4.26}$$

Observe that there is an arbitrariness in the definition of A_μ due to its Λ-dependence in the gauge transformation. It can be fixed by a proper choice of $\Lambda^r(x)$, that means, imposing some constraints on the field $A^r_\mu(x)$. The Lorentz invariance gives us a simple option,

$$\partial^\mu A^r_\mu(x) = 0.$$

This is called the Lorentz gauge condition.

We include the gauge fixing condition in the Lagrangian using an arbitrary Lagrange multiplier, say, $1/2\alpha$. Therefore, the full Lagrangian, is

$$\mathcal{L} = \overline{\psi}(x)[iD_\mu\gamma^\mu - m]\psi(x) - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{1}{2\alpha}(\partial^\mu A^r_\mu(x))^2.$$

Using this Lagrangian, the physical results have to be independent of the arbitrary constant α. For $\alpha = 1$, the condition is called the Feynman gauge; for $\alpha \to 0$, one has the Landau gauge. This term in the Lagrangian establishing the gauge condition is called *gauge fixing* term. This Lagrangian is useful, for example, to obtain the quantization of the electromagnetic field, where the gauge group is $U(1)$. However, as the gauge fixing term is not gauge invariant, in general, we find inconsistencies. This type of difficulty is overcome with a proper definition of a generating functional. In the next section we address this problem.

4.4 Generating functional for gauge fields

Consider the following generating functional for a gauge field

$$Z[J] = \int DA \exp(iS[J]), \tag{4.27}$$

with

$$S[J] = \int dx^4[\mathcal{L} + A_\mu J^\mu] \ , \quad \mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$$

and $DA = \prod_{\mu,r} DA^r_\mu$. Let us analyze the gauge invariance of $Z[J]$. $\mathcal{L}$ is gauge invariant, and so is DA. Indeed,

$$DA' = DA \det\left(\frac{\partial A'^s}{\partial A^r}\right).$$

But up to the first order in the gauge parameter Λ^r, we have

$$\det\left(\frac{\partial A'^s}{\partial A^r}\right) = \det(\delta^{rs} - c^{rsl}\Lambda^l) = 1 + O(\Lambda^2).$$

Observe that the source term is not gauge invariant, but it is not a major problem since at the end of the calculations $J \to 0$. Then we can work with $Z[0]$ first. The basic problem is how to take into account the gauge fixing term in a gauge invariant way. We proceed as follows. The gauge condition is written as

$$h^\mu A^r_\mu = b^r,$$

where h^μ and b^r are to be specified As an example, in the case of the Lorentz gauge $h^\mu = \partial^\mu$ and $b^r = 0$. Define the functional relation

$$\Delta_G[A] \int \prod_r d\Lambda^r \delta^n(h^\mu A'^r_\mu - b^r) = 1, \tag{4.28}$$

where $A'^r_\mu = A'^r_\mu(\Lambda)$ is given in Eq. (4.26) and the integration is carried over the elements of the gauge group manifold. Each element is characterized by the set

of parameters Λ^r, and the measure $\prod d\Lambda^r$ is gauge invariant. In the integral, A^r_μ acts on Λ, in such a way that $\Delta_G[A]$, defined in Eq. (4.28), is also gauge invariant. Inserting Eq. (4.28) into Eq. (4.27), we obtain

$$Z[0] = \int DA \prod_r d\Lambda^r \delta^n(h^\mu A'^r_\mu - b^r)\Delta_G[A]\exp(iS[0]).$$

All terms in this functional integral are gauge invariant. Then by a proper gauge transformation, $Z[0]$ is written as

$$Z[0] = \left(\prod_r d\Lambda^r\right)\int DA\delta^n(h^\mu A^r_\mu - b^r)\Delta_G[A]\exp(iS[0]).$$

The quantity $\prod_r d\Lambda^r$ provides only an overall factor to the generating functional, and thus it can be discarded. Therefore, we take the functional in the form

$$Z[0] = \int DA\delta^n(h^\mu A^r_\mu - b^r)\Delta_G[A]\exp(iS[0]). \tag{4.29}$$

For a generating functional this is not sufficient, since we expect to have a functional integral of the exponential of an action. For that we have to treat the δ-function and the functional Δ_G appropriately.

In Eq. (4.29), we have to specify Δ_G and fix the parameters b^r. From the definition of Δ_G, Eq. (4.28), we have

$$\Delta_G[A]\int\prod_r d\Lambda^r\delta^n(h^\mu A'^r_\mu - b^r) = \frac{\Delta_G[A]}{\det M_G} = 1;$$

i.e. $\Delta_G[A] = \det M_G$, with

$$M^{rs}_G(x,y) = \frac{\delta(h^\mu A'^r_\mu(x))}{\delta(\Lambda^s(y))}.$$

Using Eq. (4.26), let us write the matrix M_G for some gauges.

Coulomb gauge: $h^\mu = (0,\nabla)$,

$$M^{rs}_G(x,y) = (\delta^{rs}\nabla^2 - gc^{rsl}\mathbf{A}^l\cdot\nabla)\delta(x-y). \tag{4.30}$$

Lorentz gauge: $h^\mu = \partial^\mu$,

$$M^{rs}_G(x,y) = (\delta^{rs}\Box - gc^{rsl}\partial^\mu A^l_\mu)\delta(x-y). \tag{4.31}$$

Temporal gauge: $h^\mu = \widehat{\eta}^\mu = (1,0,0,0)$,

$$M^{rs}_G(x,y) = (\delta^{rs}\Box - gc^{rsl}\partial^\mu A^l_\mu)\delta(x-y). \tag{4.32}$$

We use the arbitrariness of b^r in Eq. (4.29), to rewrite the δ-function as an exponential function. We multiply Eq. (4.29) by the factor

$$\exp\left(\frac{-i}{2\alpha}\int d^4x b^2\right)$$

and integrate over b. The result is

$$Z[0] = \int DA \det M_G \exp\left(iS[0] - \frac{i}{2\alpha}\int d^4x (g^\mu A^r_\mu)^2\right).$$

The final step is to write $\det M_G$ as an exponential. This can be achieved by using the Grassmann variables. For the operator M_G, we write

$$\det M_G = \int d\chi d\chi^* \exp\left\{-i\int d^4x d^4y \chi^{r*}(x) M^{rs}_G(x,y)\chi^s(y)\right\},$$

where $\chi(x)$ is an ancillary field, called the Faddeev-Popov ghost [42]. It is a scalar field, but satisfies anti-commutation relation, i.e. it behaves like a fermion. Using $M^{rs}_G(x,y)$ in the Lorentz gauge, Eq. (4.31), an integration is carried out in the exponential, resulting in

$$\det M_G = \int d\chi d\chi^\star \exp\left\{i\int d^4x d^4y \partial^\mu \chi^{r*}(x) D^{rs}_\mu \chi^s(y)\right\},$$

where D^{rs}_μ is the covariant derivative.

The Faddeev-Popov ghost, although non-physical, is a field with a dynamics of its own. The Lagrangian is

$$\begin{aligned} L_{FP} &= \partial^\mu \chi^{r*}(x) D^{rs}_\mu \chi^s(y) \\ &= \partial^\mu \chi^{r*}(x)\partial_\mu \chi^r(y) + ig\partial^\mu \chi^{r*}(x) c^{rsl} A^l_\mu \chi^s(y). \end{aligned}$$

Discarding the interaction term in this Lagrangian, we find that the ghost field satisfies a massless Klein-Gordon equation, that shows its bosonic characteristic. On the other hand, χ is a Grassmann variable, playing the role of a fermion-like field. So to write the final expression for the generating functional, including sources, we have to take sources for ghosts in terms of Grassmann variables as it is the case for fermions. The final result, including the gauge, fermion and ghost fields, the gauge-fixing term and sources, is

$$\begin{aligned} Z[J,\eta,\overline{\eta},\xi,\xi^*] = &\int DAD\psi D\overline{\psi} D\chi D\chi^* \\ &\times \exp\left[i\int d^4x \left(\mathcal{L} + AJ + \overline{\eta}\psi + \overline{\psi}\eta + \xi^*\chi + \chi^*\xi\right)\right], \end{aligned}$$

where ξ^* and ξ are Grassmann variables describing sources for ghost fields. In $Z[J,\eta,\overline{\eta},\xi,\xi^*]$, the Lagrangian density is

$$\begin{aligned} \mathcal{L} = &\overline{\psi}(x)(iD_\mu\gamma^\mu - m)\psi(x) - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} \\ &-\frac{i}{2\alpha}(g^\mu A^r_\mu)^2 + \partial^\mu \chi^{r*}(x) D^{rs}_\mu \chi^s(y). \end{aligned}$$

4.5 $U(1)$ gauge theory

Let us consider the $U(1)$-gauge theory, quantum electrodynamics (QED). In this case $c^{rst} = 0$, i.e. the theory is abelian, and $gt^r_{ij} = -e$, where e is the magnitude of the charge of the particle. For spin 1/2 particles, the QED Lagrangian density is $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_I$ with $\mathcal{L}_0 = \mathcal{L}^G_0 + \mathcal{L}^F_0$, $\mathcal{L}^G_0$ being the free gauge field,

$$\mathcal{L}^G_0 = -\frac{1}{4}(\partial_\mu A_\nu - \partial_\nu A\mu\ )(\partial^\mu A^\nu - \partial^\nu A^\mu) - \frac{1}{2\alpha}(\partial^\mu A_\mu)^2,$$

where $A_\mu(x)$ is the vector potential and α is the electromagnetic gauge parameter. $\mathcal{L}^F_0$ describes the matter field.

$$\mathcal{L}^F_0 = \overline{\psi}(x)[\gamma \cdot i\partial - m]\psi(x).$$

The interaction Lagrangian density is

$$\mathcal{L}_I = -e\overline{\psi}\gamma^\mu A_\mu(x)\psi.$$

For the free gauge field the generating functional is

$$Z^G_0[J] = \exp\left\{\frac{i}{2}\int dxdy\, J^\mu(x)D_{0\mu\nu}(x-y)J^\nu(y)\right\},$$

where

$$D^{\mu\nu}_0(x) = \frac{1}{(2\pi)^4}\int d^4k e^{-ikx} d^{\mu\nu}(k)\frac{1}{k^2+i\varepsilon},$$

with

$$d^{\mu\nu}(k) = g^{\mu\nu} - (1-\alpha)\frac{p^\mu p^\nu}{p^2}. \tag{4.33}$$

The generating functional for the interacting fields is given by

$$Z[J,\overline{\eta},\eta] = \frac{\exp\left[i\int dx\mathcal{L}_I\left(\frac{1}{i}\frac{\delta}{\delta J}, \frac{1}{i}\frac{\delta}{\delta\overline{\eta}}, \frac{1}{i}\frac{\delta}{\delta\eta}\right)\right] Z_0[J,\overline{\eta},\eta]}{\exp\left[i\int dx\mathcal{L}_I\left(\frac{1}{i}\frac{\delta}{\delta J}, \frac{1}{i}\frac{\delta}{\delta\overline{\eta}}, \frac{1}{i}\frac{\delta}{\delta\eta}\right)\right] Z_0[J,\overline{\eta},\eta]|_{J,\overline{\eta},\eta=0}},$$

with $Z_0[J,\overline{\eta},\eta] = Z^G_0[J]Z^F_0[J,\overline{\eta},\eta]$, where $Z^F_0[J,\overline{\eta},\eta]$ is the generating functional for fermions, given in Chapter 3.

The Feynman rules in the momentum space for QED are given in Fig. 4.7. The basic loops in QED are the fermion-photon, which corresponds to an integral $-i\int d^4p/(2\pi)^4$, and the pure fermion-loop, giving an integral $i\int d^4p/(2\pi)^4$. These loops are represented in Fig. 4.8. Sum over spin-projection for the final state and spin average for the initial state must be done.

Another model for the $U(1)$-gauge theory describes the interaction of photons with charged scalar mesons, with the interaction Lagrangian given by

$$\mathcal{L}_{int} = -ieA^\mu\phi^\dagger\overleftrightarrow{\partial}_\mu\phi + e^2A^\mu A_\mu\phi^\dagger\phi.$$

There are two vertices in this theory. One with scalar mesons interacting with a single photon and a second where the interaction is with two photons. The Feynman rules for these vertices are presented in Fig. 4.9 [36].

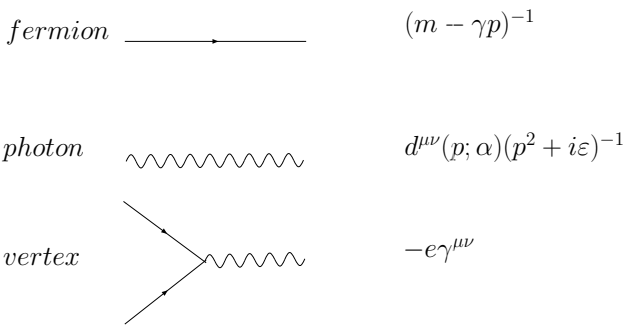


Fig. 4.7 Feynman rules for the Green functions in QED.

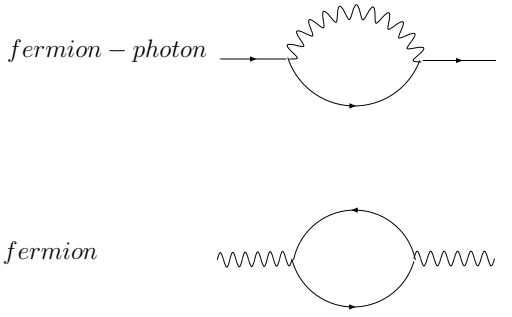


Fig. 4.8 Basic loops in QED.

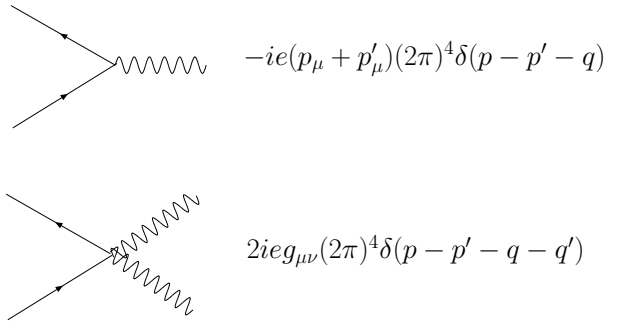


Fig. 4.9 Feynman rules for charged scalar mesons.

4.6 $SU(3)$ gauge theory

Now we turn to a study of the non-abelian gauge theory where the commutator of generators are non-zero. Taking now the SU(3) gauge theory in particular, the

Lagrangian density is

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_I,$$

where the non-interacting Lagrangian density is,

$$\mathcal{L}_0 = \mathcal{L}_0^G + \mathcal{L}_0^{FP} + \mathcal{L}_0^F,$$

with

$$\mathcal{L}_0^G = -\frac{1}{4}(\partial_\mu A_\nu^r - \partial_\nu A\mu^r)(\partial^\mu A^{\nu r} - \partial^\nu A^{\mu r}) - \frac{1}{2\alpha}(\partial^\mu A_\mu^r)^2.$$

$\mathcal{L}_0^{FP}$ is the Faddeev-Popov term [42],

$$\mathcal{L}_0^{FP} = (\partial^\mu \chi_\mu^{r*})(\partial^\mu \chi_\mu^r),$$

and $\mathcal{L}_0^F$ describes the matter field,

$$\mathcal{L}_0^F = \overline{\psi}(x)[\gamma \cdot i\partial - m]\psi(x).$$

The interaction Lagrangian density is

$$\begin{aligned}\mathcal{L}_I = &-\frac{g}{2}c^{rsl}(\partial_\mu A_\nu^r - \partial_\nu A_\mu^r)A^{s\mu}A^{l\nu} \\ &-\frac{g^2}{2}c^{rst}c^{ult}A_\mu^r A_\nu^s A^{u\mu}A^{l\nu} \\ &-gc^{rsl}(\partial^\mu \chi^{r*})A_\mu^l \chi^s(y) + g\overline{\psi}t^r\gamma^\mu A_\mu^r\psi,\end{aligned}$$

where c^{rsl} are the structure constants of the $SU(3)$ gauge group. The superscripts r, s and l vary from 1 to 8 and refer to the quantum number for color. In addition the fermion (quark) field ψ has six known flavors (the different types of fermions, indicated by $i, j = 1, 2, \ldots, N$). In the Lagrangian density $\mathcal{L}$, we refer to fermions with color and flavor; the gauge field quanta being called gluons. Such a formulation provides the non-abelian theory of quarks and gluons, called Quantum Chromodynamics (QCD), the theory of strong interactions.

The generating functional for the non-interacting gauge field is

$$Z_0^{G(rs)}[J] = \exp\left\{\frac{i}{2}\int dxdy\, J^\mu(x)D_{0\mu\nu}^{(rs)}(x-y)J^\nu(y)\right\},$$

where

$$D_0^{(rs)\mu\nu}(x) = \frac{1}{(2\pi)^4}\int d^4k e^{-ikx}D_0^{(rs)\mu\nu}(k)$$

with

$$D_0^{(rs)\mu\nu}(k) = \delta^{rs}d^{\mu\nu}(k)\frac{1}{k^2 + i\varepsilon},$$

where $d^{\mu\nu}(k)$ is given by Eq. (4.33). For the Fadeev-Popov fields the generating functional is

$$Z_0^{FP(rs)}[\overline{\xi}, \xi] = \exp\left\{\frac{i}{2}\int dxdy\,\overline{\xi}(x)D_0^{(rs)}(x-y)\xi(y)\right\},$$

where $\overline{\xi}$ and ξ are Grassmann variables and $D_0^{(rs)}(x-y) = \delta^{rs}G_0(x-y)$ is the propagator for the Fadeev-Popov field. The full generating functional for the non-abelian gauge field is

$$Z[J,\overline{\xi},\xi,\overline{\eta},\eta] = \frac{\exp\left[i\int dx\mathcal{L}_I\left(\frac{1}{i}\frac{\delta}{\delta J},\frac{1}{i}\frac{\delta}{\delta\overline{\xi}},\frac{1}{i}\frac{\delta}{\delta\xi},\frac{1}{i}\frac{\delta}{\delta\overline{\eta}},\frac{1}{i}\frac{\delta}{\delta\eta}\right)\right]Z_0[J,\overline{\xi},\xi,\overline{\eta},\eta]}{\exp\left[i\int dx\mathcal{L}_I\left(\frac{1}{i}\frac{\delta}{\delta J},\frac{1}{i}\frac{\delta}{\delta\overline{\xi}},\frac{1}{i}\frac{\delta}{\delta\xi},\frac{1}{i}\frac{\delta}{\delta\overline{\eta}},\frac{1}{i}\frac{\delta}{\delta\eta}\right)\right]Z_0[0]},$$

with $Z_0[J,\overline{\xi},\xi,\overline{\eta},\eta] = Z_0^{G(rs)}[J]Z_0^{FP(rs)}[\overline{\xi},\xi]Z_0^{F(rs)}[\eta,\overline{\eta}]$.

As an example, the contribution of the 3-gluon coupling to first order is

$$D^{r_1r_2r_3}_{\alpha_1\alpha_2\alpha_3}(x_1,x_2,x_3) = (-i)^2\frac{\delta^3}{\delta J_1\delta J_2\delta J_3}\int d^4x\mathcal{L}_I^{3G}(\frac{1}{i}\frac{\delta}{\delta J^{r\alpha}})Z_0^G[J]|_{J=0}$$

where $J_i = J^{r_i\alpha_i},\ i=1,2,3$. The 3-point function for the gluon field is

$$\begin{aligned}
D^{r_1r_2r_3}_{\mu_1\mu_2\mu_3}(x_1,x_2,x_3) = igc^{rst}&\int d^4x\{\partial_\mu D^{rr_1}_{\nu\mu_1}(x-x_1) - \partial_\nu D^{rr_1}_{\mu\mu_1}(x-x_1)\}\\
&\times D^{sr_2\mu}_{\mu_2}(x-x_2)\ D^{tr_3\nu}_{\mu_3}(x-x_3)\\
&+gc^{rst}\int d^4x\{\partial_\mu D^{rr_2}_{\nu\mu_2}(x-x_2) - \partial_\nu D^{rr_2}_{\mu\mu_2}(x-x_2)\}\\
&\times D^{sr_3\mu}_{\mu_3}(x-x_3)\ D^{tr_1\nu}_{\mu_1}(x-x_1)\\
&+gc^{rst}\int d^4x\{\partial_\mu D^{rr_3}_{\nu\mu_3}(x-x_3) - \partial_\nu D^{rr_3}_{\mu\mu_3}(x-x_3)\}\\
&\times D^{sr_1\mu}_{\mu_1}(x-x_1)D^{tr_2\nu}_{\mu_2}(x-x_2).
\end{aligned}$$

In momentum space, this propagator is written as

$$\begin{aligned}
D^{r_1r_2r_3}_{\mu_1\mu_2\mu_3}(x_1,x_2,x_3) = igc^{r_1r_2r_3}&\int\frac{d^4p_1}{(2\pi)^4}\frac{d^4p_2}{(2\pi)^4}e^{i(p_1x_1+p_2x_2+p_3x_3)}\\
&\times\frac{d_{\mu_1\lambda_1}(p_1)d_{\mu_2\lambda_2}(p_2)d_{\mu_3\lambda_3}(p_3)}{p_1^2p_2^2p_3^2}\\
&\times[(p_1-p_2)^{\lambda_3}g^{\lambda_1\lambda_2} + (p_2-p_3)^{\lambda_1}g^{\lambda_2\lambda_3}\\
&+(p_3-p_1)^{\lambda_2}g^{\lambda_1\lambda_3}],
\end{aligned}$$

with $p_3 = -p_1 - p_2$.

The Feynman rules for the $SU(3)$ gauge theory are given below. The three propagators, for the quark, gluon and ghost fields, are diagramatically represented in Fig. 4.10.

In this theory we have four types of vertices, that are given in Fig. 4.11 where

$$\begin{aligned}
V^{\lambda_1\lambda_2\lambda_3}(p_1,p_2,p_3) = &[(p_1-p_2)^{\lambda_3}g^{\lambda_1\lambda_2} + (p_2-p_3)^{\lambda_1}g^{\lambda_2\lambda_3}\\
&+(p_3-p_1)^{\lambda_2}g^{\lambda_1\lambda_3}]
\end{aligned}$$

and

$$\begin{aligned}
W^{r_1r_2r_3r_4}_{\mu_1\mu_2\mu_3\mu_4} = &(c^{13,24}-c^{14,32})g_{\mu_1\mu_2}g_{\mu_3\mu_4}\\
&+(c^{12,34}-c^{14,23})g_{\mu_1\mu_3}g_{\mu_2\mu_4}\\
&+(c^{13,42}-c^{12,34})g_{\mu_1\mu_4}g_{\mu_3\mu_2},
\end{aligned}$$

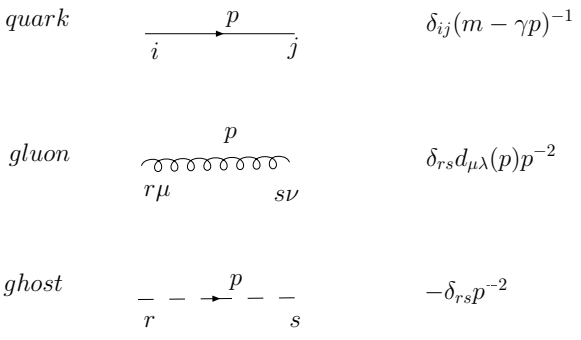


Fig. 4.10 Quark, gluon and ghost propagators.

with $c^{ij,kl} = f^{r_i r_j r} f^{r_k r_l r}$.

For the loops, shown in Fig. 4.12, we have to integrate over the internal momenta, k, as $-i \int d^4k/(2\pi)^4$. For each type of loop we have an additional symmetry factor as indicated in Fig. 4.13. There is a sum over the indices for the final state and an average over the indices of the initial state.

4.7 Scattering amplitudes

In order to calculate transition amplitudes, we have to estimate the behavior of fields as the interaction turns off asymptotically. We consider here only scalar fields such that $\phi(t, \mathbf{x}) \sim \phi_{in}(t, \mathbf{x})$, as $t \to -\infty$, $\phi(t, \mathbf{x}) \sim \phi_{out}(t, \mathbf{x})$, as $t \to \infty$, where $\phi_{in}(t, \mathbf{x})$ and $\phi_{out}(t, \mathbf{x})$ satisfy the free Klein-Gordon equation

$$(\Box + m^2)\phi_{in,out}(t, \mathbf{x}) = 0.$$

These fields are associated with the positive and negative frequencies, respectively [39], such that

$$\phi_{in}(t, \mathbf{x}) = \int \frac{d^3p}{(2\pi)^3 2p_0} a(p) e^{-ipx}$$

and

$$\phi_{out}(t, \mathbf{x}) = \int \frac{d^3p}{(2\pi)^3 2p_0} a^*(p) e^{ipx}.$$

The underlying idea for the introduction of *in* and *out* asymptotic fields relies on the fact that interacting fields obey in general coupled non-linear equations which cannot be solved analytically. So, no realistic possibility of having closed solutions for problems in field theory is actually available. The main analytical method used to deal with situations in field theory is, except for a few special cases, perturbation theory. Actually this is not a particular situation of quantum theories. In fact this method has been used since the 19th century in problems of celestial mechanics;

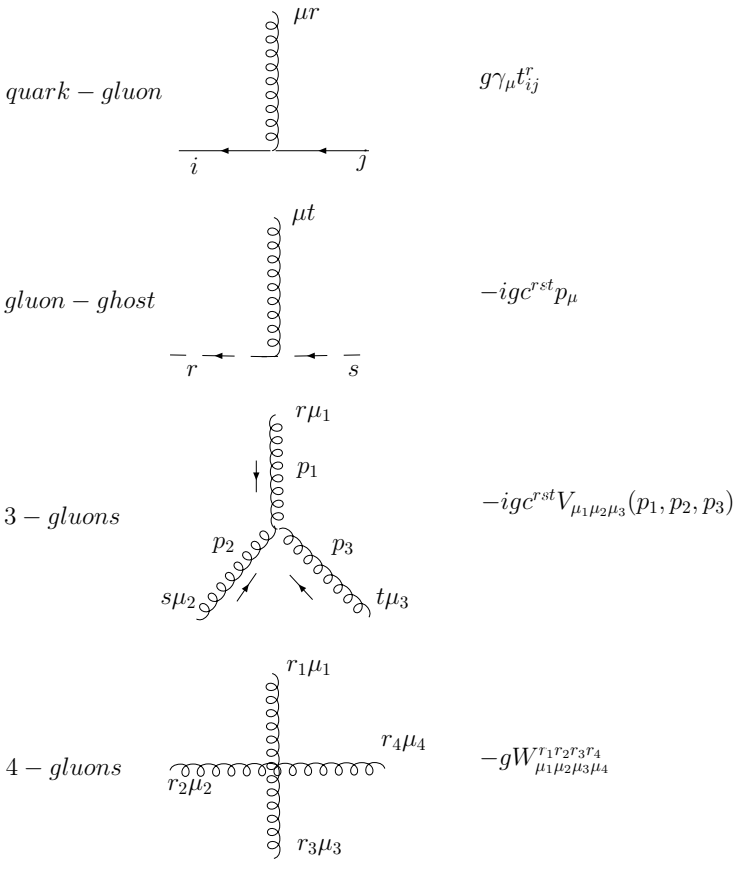


Fig. 4.11 The basic vertices in QCD.

the discovery of Neptune by Le Verrier as a "perturbation" to the orbit of Uranus is an outstanding example. In this framework, the approach is carried out by means of the definition of free fields; the interaction being introduced order by order in powers of the coupling constant in the perturbative series for the observables, in the present case, cross-sections for collision processes. This happens at both quantum and classical levels. Indeed perturbation theory was originally introduced to solve problems in celestial mechanics in the 19th century.

Using the definition of $Z[J]$, the generating functional, we introduce

$$Z[J,\phi] \equiv \int D\phi \, \exp\left[i \int d^4x(\mathcal{L} + J\phi)\right],$$

where the interacting field ϕ is such that

$$\phi(x) = \phi_{in}(x) \quad \text{as} \quad t \to -\infty,$$
$$\phi(x) = \phi_{out}(x) \quad \text{as} \quad t \to \infty.$$

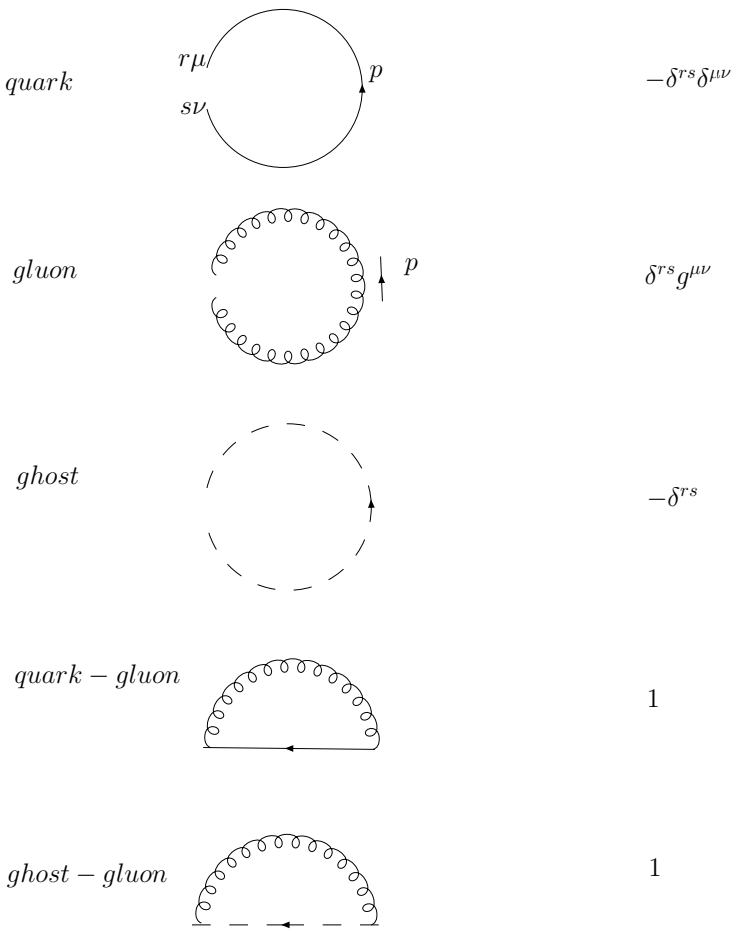


Fig. 4.12 The basic loops in QCD.

Consider the $\lambda\phi^4$ theory. Define a field $\phi_0(x)$, such that $\phi_0(x) \to \varphi_{in}(x)$ as $t \to -\infty$ and $\phi_0(x) \to \phi_{out}(x)$ as $t \to +\infty$. Then we write

$$S[J, \phi_0] \equiv \exp\left[i \int d^4x \mathcal{L}_I \left(\frac{\delta}{i\delta J(x)}\right) S_0[J, \phi_0]\right],$$

where

$$S_0[J, \phi_0] = \int D\phi \, \exp\left[i \int d^4x (\mathcal{L}_0 + J\phi_0)\right]. \tag{4.34}$$

Define

$$\phi(x) = \overline{\phi}(x) + \phi_0(x),$$

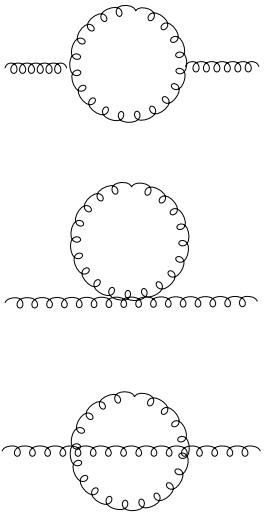


Fig. 4.13 Symmetry factors for basic diagrams in QCD.

where $\overline{\phi}(x) \to 0$ as $t \to \pm\infty$. Hence, from Eq. (4.34), we obtain

$$\begin{aligned} S_0[J,\phi_0] &= \int D\overline{\phi}\, \exp\left[-i\frac{1}{2}\int d^4x\overline{\phi}(\ \Box + m^2\ )\overline{\phi} + J\overline{\phi}\right] \\ &\quad \times \exp\left[i\int d^4y J(y)\phi_0(y)\right] \\ &= \exp\left[i\int d^4y J(y)\phi_0(y)\right]\ Z_0[J]. \end{aligned}$$

From the definition of $Z_0[J]$, we write

$$(\ \Box + m^2\ )\frac{\delta Z_0[J]}{i\delta J(x)} = J(x)Z_0[J].$$

Then

$$S_0[J,\phi_0] = \exp\left(\int d^4x\phi_0(\ \Box + m^2\ )\frac{\delta}{\delta J(x)}\right) Z_0[J]$$

and

$$\begin{aligned} S[J,\phi_0] &= \exp\left(\int d^4x\phi_0(\ \Box + m^2\ )\frac{\delta}{\delta J(x)}\right) \\ &\quad \times \exp\left[i\int d^4x\mathcal{L}_I\left(\frac{\delta}{i\delta J(x)}\right)\right] Z_0[J], \end{aligned}$$

or

$$S[J,\phi_0] = \exp\left(\int d^4x\phi_0(\ \Box + m^2\ )\frac{\delta}{\delta J(x)}\right) Z[J]. \tag{4.35}$$

This expression gives the transition between incoming and outgoing states, in the presence of the source $J(x)$.

Expanding the exponential in Eq. (4.35), we obtain

$$S[J,\phi_0] = \sum_{n=0}^{\infty} \frac{1}{n!} \int d^4x_1 \dots d^4x_n \phi_0(x_1) \cdots \phi_0(x_n) \\ \times K_{x_1} \cdots K_{x_n} G^{(n)}(x_1, \dots, x_n),$$

where $K_x = \Box_x + m^2$. In the momentum space this expression is given by

$$S[J,\phi_0] = \sum_{n=0}^{\infty} \frac{1}{n!} \int \frac{d^4p_1}{(2\pi)^4} \cdots \frac{d^4p_n}{(2\pi)^4} G^{(n)}(p_1, \dots, p_n) \\ \times (2\pi)^4 \delta(p_1 + \cdots + p_n)(m^2 - {p_1}^2) \cdots (m^2 - {p_n}^2) \\ \times \int d^4x_1 \dots d^4x_n e^{ip_1x_1 + \cdots + ip_nx_n} \phi_0(x_1) \cdots \phi_0(x_n).$$

In this expression, each field $\phi_0(x_i)$ is expressed as

$$\frac{1}{(2\pi)^4} \int d^4x e^{ipx} \phi_0(x) = \int d^3k \rho(k) [a(k)\delta(p-k) + a^*(k)\delta(p+k)],$$

where $p^2 = m^2$, $k^2 = m^2$ and $\rho(k) = [(2\pi)^3 2k_0]^{-1}$.

For a scattering process, with m initial particles, with momenta $p_1, ..., p_m$, and $n-m$ outgoing particles with momenta $p_{m+1}, .., p_n$, the amplitude is given as

$$S_{fi} = \frac{1}{\rho(p_1) \cdots \rho(p_n)} \left. \frac{\delta^n S[J,\phi_0]}{\delta a(p_1) \cdots \delta a(p_m) \delta a^*(p_{m+1}) \cdots \delta a^*(p_n)} \right|_{a=a^*=0}.$$

Notice that $S[J,\phi_0]$ describes all the transition processes; while S_{fi} represents a specific scattering process from $S[J,\phi_0]$, such that the mass-shell condition for ingoing and outgoing particles as well as the conservation of energy and momentum are satisfied. The expression is explicitly Lorentz covariant due to the factor $[\rho(p_1)...\rho(p_n)]^{-1}$. Finally, S_{fi} is an element of the S-matrix. From the definition of S_{fi} we obtain

$$S_{fi} = (2\pi)^4 \delta(p_1 + \cdots + p_m - p_{m+1} - \cdots - p_n) T_{fi}, \\ = (2\pi)^4 \delta(\sum_i p_i - \sum_f p_f) T_{fi},$$

where

$$T_{fi} = (i)^n (m^2 - {p_1}^2) \cdots (m^2 - {p_n}^2) \\ \times G^{(n)}(p_1, \dots, p_m, -p_{m+1}, \dots, -p_n).$$

The transition probability is given by

$$|S_{fi}|^2 = (2\pi)^8 \delta(0) \delta(\sum_i p_i - \sum_f p_f) |T_{fi}|^2,$$

where $(2\pi)^4\delta(p) = \int d^4x e^{ipx}$; this gives us $(2\pi)^4\delta(0) = \int d^4x = VT$, the infinite space-time volume. Therefore the transition probability per unit volume per unit time is given as

$$P_{fi} = (2\pi)^4\delta(\sum_i p_i - \sum_f p_f)|T_{fi}|^2.$$

The differential cross section is defined by

$$d\sigma_{fi} = \frac{1}{F} dN_{fi},$$

where dN_{fi}, the number of particles scattered by a single target particle, is

$$dN_{fi} = \frac{1}{2p_{10}} P_{fi} \prod_f \frac{d^3p_f}{(2\pi)^3 2p_{f0}},$$

and the incident flux of particles, F, is

$$F = 2|\mathbf{p}_1|.$$

Let us consider the simpler situation of a single incident particle of momentum $\mathbf{p}_1$ scattered by a target particle of mass m_2. The differential cross section in the laboratory frame is,

$$d\sigma_{fi} = (2\pi)^4\delta(\sum_i p_i - \sum_f p_f)\frac{1}{2m_2}\frac{1}{2|\mathbf{p}_1|}|T_{fi}|^2 \prod_f \frac{d^3p_f}{(2\pi)^3 2p_{f0}}.$$

This relation is valid for spin-zero particles. For particles with non-null spin we have to average over the initial spin directions and sum over the final spin directions. The factor $m_2|\mathbf{p}_1|$ may be written in a Lorentz covariant form as

$$m_2|\mathbf{p}_1| = m_2\sqrt{(p_{10})^2 - m_1^2} = \sqrt{(\mathbf{p}_1 \cdot \mathbf{p}_2)^2 - m_1^2 m_2^2},$$

where $p_2 = (m_2, 0, 0, 0)$ in the laboratory frame. Let us consider some examples [36, 38]

- The scattering of two scalar particles
  In the $\lambda\phi^4$ theory, up to order λ the 4-point Green functions are given by the Feynman diagrams in Fig. 4.3. Observe that only the connected diagram contributes to the transition matrix element, which is then given by $T_{fi} = -i\lambda$. Then the differential cross-section reads

  $$\frac{d\sigma_{fi}}{d\Omega_3} = \frac{\lambda^2}{64\pi^2 s},$$

  where $s = (p_1 + p_2)^2 = 4E^2$. Here E is the centre-of-mass energy, such that $p_1 = (E, \mathbf{p})$ and $p_2 = (E, -\mathbf{p})$.

- Scattering of two charged scalar particles
  In the center-of-mass frame, the scattering of two charged bosons is described by the differential cross-section, that up to order α^2, is given as

$$\frac{d\sigma_{fi}}{d\Omega_3} = \frac{\alpha^2}{16E^2}|T_{fi}|^2,$$

  where

$$|T_{fi}|^2 = 4\frac{p_1\cdot p_2 - p_1\cdot p_2'}{(p_1-p_1')^2} + 4\frac{p_1\cdot p_2 - p_1\cdot p_1'}{(p_1-p_2')^2},$$

  and $\alpha = e^2/4\pi\hbar c$ is the fine-structure constant.
- Electron-electron scattering
  Considering the scattering process given in Fig. 4.14, in the center-of-mass frame, the differential cross-section to order α^2 is [36]

$$\frac{d\sigma_{fi}}{d\Omega_3} = \frac{m^2\alpha^2}{E^2}|T_{fi}|^2,$$

  with

$$\begin{aligned}|T_{fi}|^2 = \frac{1}{2m^4}\Bigg\{&\frac{(p_1\cdot p_2)^2 + p_1\cdot p_2')^2 + 2m^2(p_1\cdot p_2' - p_1\cdot p_2)}{[(p_1'-p_1)^2]^2}\\ &+\frac{(p_1\cdot p_2)^2 + p_1\cdot p_1')^2 + 2m^2(p_1\cdot p_1' - p_1\cdot p_2)}{[(p_2'-p_1)^2]^2}\\ &+2\frac{(p_1\cdot p_2)^2 - 2m^2(p_1\cdot p_2)}{(p_1'-p_1)^2-(p_2'-p_1)^2}\Bigg\}.\end{aligned} \tag{4.36}$$

  Writing all invariants in terms of the energy E and the scattering angle θ,

$$\begin{aligned}p_1\cdot p_2 = 2E^2 - m^2,\quad p_1\cdot p_1' = E^2(1-\cos\theta) + m^2\cos\theta\,,\\ p_1\cdot p_2' = E^2(1+\cos\theta) - m^2\cos\theta,\end{aligned} \tag{4.37}$$

  results in the Möller formula

$$\begin{aligned}\frac{d\sigma_{fi}}{d\Omega_3} = \frac{\alpha^2(2E^2-m^2)^2}{4E^2(E^2-m^2)^2}\Bigg[&\frac{4}{\sin^4\theta} - \frac{3}{\sin^2\theta}\\ &+\frac{(E^2-m^2)^2}{(2E^2-m^2)^2}\left(1+\frac{4}{\sin^2\theta}\right)\Bigg].\end{aligned} \tag{4.38}$$

- e^+e^- annihilation ($e^+e^- \to q\overline{q}$)
  Consider the Feynman graph given in Fig. 4.15, in the center-of-mass frame, describing the lowest order approximation to the e^+e^- annihilation. The scattering amplitude is given by

$$\begin{aligned}|T_{fi}| = \langle q\overline{q}|T|e^+e^-\rangle = &\overline{u}_{\lambda_1'}(p_1')(-Qe)\gamma^\mu v_{\lambda_2'}(p_2')\\ &\frac{d_{\mu\nu}}{q^2}\overline{v}^e_{\lambda_2}(p_2)e\gamma^\nu u_{\lambda_1}(p_1),\end{aligned}$$

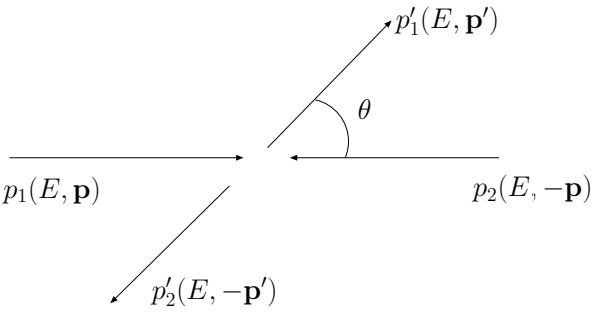


Fig. 4.14 Electron-electron scattering.

where Qe is the charge of the quark and $q = p_1 + p_2$. The total cross-section is written as,

$$\sigma = \frac{1}{8\sqrt{s(s-4m^2)}} \sum_{\lambda_1\lambda_2\lambda_1'\lambda_2'} \int \frac{d^3p_1'}{(2\pi)^3 2p_{10}'} \frac{d^3p_2'}{(2\pi)^3 2p_{20}'} \times (2\pi)^4 \delta^4(p_1' + p_2' - p_1 - p_2) |\langle q\overline{q}|T|e^+e^-\rangle|^2$$

The differential cross-section to order α^2 reads,

$$\frac{d\sigma}{d\Omega} = \frac{Q^2\alpha^2}{4s} \sqrt{\frac{s-4m^2}{s-4m_e^2}} \left[1 + \frac{4(m^2+m_e^2)}{s} + \left(1 - \frac{4m^2}{s}\right)\left(1 - \frac{4m_e^2}{s}\right)\cos^2\theta\right]$$

The total cross-section is,

$$\sigma = \frac{4\pi Q^2\alpha^2}{3s} \sqrt{\frac{s-4m^2}{s-4m_e^2}} \left(1 + \frac{2m^2}{s}\right)\left(1 + \frac{2(m_e^2}{s}\right), \tag{4.39}$$

where $q^\mu = (\sqrt{s}, 0, 0, 0)$, $m(m_e)$ is the mass of the quark (electron), $s = q^2$ and $k^\mu = (0, \mathbf{k})$.

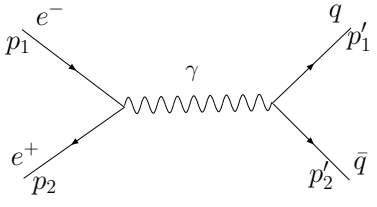


Fig. 4.15 e^+e^- annihilation.

4.8 *S*-matrix in the canonical approach

In this section we briefly review the notion of S-matrix in the canonical formalism. Consider a field operator $\phi(x)$ such that

$$\lim_{t\to-\infty}\phi(x)=\phi_{in}(x),$$
$$\lim_{t\to\infty}\phi(x)=\phi_{out}(x),$$

where $\phi_{in}(x)$ and $\phi_{out}(x)$ stand for the field before and after interaction takes place. For a discussion on how these limites are performed and precise definitions we refer to [37]. These two fields are assumed to be related to each other by a canonical transformation

$$\phi_{out}(x)=S^{-1}\phi_{in}(x)S,$$

where S is an unitary operator.

Now we define the evolution operator, $U(t,t')$, which relates the interacting field to the incoming and outgoing fields, that is

$$\begin{aligned}\phi(x)&=U^{-1}(t,-\infty)\phi_{in}(x)U(t,-\infty)\\ \phi(x)&=U^{-1}(+\infty,t)\phi_{out}(x)U(+\infty,t).\end{aligned}\tag{4.40}$$

The operator U reduces to the unit operator for $t=t'$, $U(t,t)=1$. The field operator $\phi(x)$ satisfies the Heisenberg equation

$$-i\partial_t\phi(x)=[H,\phi(x)],$$

where $H=H_0+H_I$,with H_0 being the free-particle Hamiltonian and H_I the interaction. The fields $\phi_{in}(x)$ and $\phi_{out}(x)$ satisfy

$$-i\partial_t\phi_{in}(x)=[H_0,\phi_{in}(x)]\tag{4.41}$$

and

$$-i\partial_t\phi_{out}(x)=[H_0,\phi_{out}(x)]\tag{4.42}$$

Requiring the unitarity of $U(t,t')$, we obtain

$$\partial_t(U(t,t')U^{-1}(t,t'))=0.$$

In addition, from Eq. (4.40) we obtain

$$\begin{aligned}\partial_t\phi_{in}(x)=&\ \partial_t[U^{-1}(t,-\infty)\phi(x)U(t,-\infty)]\\ &=[U(t,-\infty)\partial_tU^{-1}(t,-\infty)+iH,\phi_{in}(x)].\end{aligned}$$

Comparing with Eq. (4.41), we get

$$i\partial_tU(t,t')=H_I(t)U(t,t').$$

This equation is solved by iteration of the integral equation,

$$U(t,t')=I-i\int_{t'}^{t}dt_1H(t_1)U(t_1,t')$$

resulting in

$$U(t,t') = I - i\int_{t'}^{t} dt_1 H(t_1) + (-i)^2 \int_{-\infty}^{t}\int_{-\infty}^{t_1} dt_1 dt_2 H(t_1)\ H(t_2) + \cdots$$
$$+(-i)^n \int_{t'}^{t}\cdots\int_{t'}^{t_{n-1}} dt_1\cdots dt_n\, H(t_1)\cdots H(t_n) + \cdots$$

Each product of the interaction Hamiltonian terms in Eq. (4.43) is time ordered, since $t_1 \geq t_2 \geq \cdots \geq t_n$. Then we can write $T(H(t_1)\cdots H(t_n))$ for $H(t_1)\cdots H(t_n)$ in Eq. (4.43) and

$$U(t,t') = T\exp\left[-i\int_{t'}^{t} dt' H(t')\right], \tag{4.43}$$

where T is the time-ordering operator.

The S-matrix operator is defined by

$$S = U(\infty,-\infty) = T\exp\left[-i\int_{-\infty}^{\infty} dt' H(t')\right].$$

The transition operator is defined by $\mathrm{T} = S - I$. The expectation values of the operator T between incoming and outgoing states are elements of the transition matrix. To obtain explicit expressions for these, the use of the LSZ reduction formulas is required [37]. The elements of the S-matrix give the probability amplitudes for specific scattering processes, defined by the incoming and outgoing fields and states we choose.

With this chapter, we close the brief review of the fundamental grounds we have to rely on to build thermal quantum field theories. Such a construction starts in the next chapter by introducing the algebraic basis of the operator formalism known as thermofield dynamics.

PART II

Thermal Fields

Chapter 5

Thermofield Dynamics: Kinematical Symmetry Algebraic Basis

The derivation of statistical mechanics, based on a constrained variational method, provides an elegant structure ready to be applied to any system since we are able to define the density matrix and solve the Liouville-von Neumann equation. This is not feasible when we have a system described by an interacting quantum field theory, like many-body systems and relativistic objects in particle physics. One way to proceed is to look for methods paralleling temperature-independent formalisms ($T = 0$ theories). For instance, if we take the Liouville-von Neumann equation as the equation of motion for the state of a system, then pure and mixed states can, in principle, be considered at the same level. This observation suggests that for equilibrium we can think of the operation $\langle A\rangle = \mathrm{Tr}(A\rho) = Z^{-1}(\beta)\mathrm{Tr}(Ae^{-\beta H})$, with a Wick rotation $\beta \to -i\tau$, as an alternative way to solve problems using, for instance, perturbative and diagramatic techniques. Another possibility is that the operator average $\langle A\rangle$ would be performed in a Hilbert state, with temperature dependent states $|0(\beta)\rangle$, such that $\langle A\rangle = \langle 0(\beta)|A|0(\beta)\rangle$.

Using these ideas, several methods have been proposed. The first systematic approach to treat a quantum field theory at finite temperature was presented by Matsubara [43], the *imaginary-time* formalism, using the Wick rotation. Since then the development of the thermal quantum field formalism has followed the achievements of the $T = 0$ quantum field theory. The first generalization of the imaginary-time formalism was carried out by Ezawa, Tomozawa and Umezawa [44], who extended the Matsubara's work to the relativistic quantum field theory, and discovered, in particular, periodicity (anti-periodicity) conditions for the Green functions of boson (fermion) fields, a concept that later became known as the KMS (Kubo, Martin and Schwinger) condition. Some ideas, developing the imaginary-time approach, have been proposed [45–48], and others, originally introduced in $T = 0$ theories, have been considered with the counterpart notions at finite temperature. We can list, as examples, the thermal Ward-Takahashi relations, the Goldstone theorem, renormalization procedures, the notion of non-abelian gauge field among others, with all its consequences for particles physics [49–52].

Despite the successes, even with its generalizations, difficulties in thermal field theory remain to be overcome in order to treat experimental and theoretical de-

mands. In fact, numerous studies particularly in lattice quantum chromodynamics (QCD) [53], have been carried out in attempts to understand, for instance, the quark-gluon plasma at finite temperature; and in this effort, some underlying aspects have been identified. For example, the coupling constants for π, σ, w and ρ mesons decrease to zero at certain critical temperatures, which are, respectively, given by: $T_c^{\pi} = 360$ MeV, $T_c^{\sigma} = 95$ MeV, $T_c^{w} = 175$ MeV and $T_c^{\rho} = 200$ MeV [54, 55]. These results require general and consistent calculations to establish the existence of a phase transition. This reinforces the need for the development of a finite temperature field theory for the standard model, which would provide answers about the transition from hadrons to the quark-gluon plasma. In this realm, effective models have been largely employed in trials to obtain clues to the behavior of interacting particles. This is the case of the Gross-Neveu model [56], dealing with the direct four-fermion interaction, which has also been analyzed at finite temperature, as an effective model for QCD and for superconducting systems [57–59]. Along these lines, some achievements have been seminal, as the paper by Dolan and Jackiw [60], which performs the calculations for the effective potential at finite temperature to study spontaneous symmetry breaking.

Beyond that, despite the numerous instances in high energy physics and in condensed matted physics where (real) time dependance is essential, a nonequilibrium theory has not been fully developed as yet. This difficulty was recognized early as a flaw in the Matsubara equilibrium formalism and has been motivating attempts to construct real-time formalisms at finite temperature [61–66].

One of these real-time methods is the closed-time path formulation due to Schwinger [67], Mahanthapa and Bakshi [68, 69], and Keldysh [70]. The approach uses a closed path in the complex-time plane such that the contour goes along the real axis and then back. From this procedure an effective doubling of the degrees of freedom emerges, such that the Green functions are represented by 2×2 matrices. Actually, this type of doubling has been recognized as an intrinsic characteristic of real-time theories, providing in turn a correct definition for perturbative series, which is not the case of the Matsubara method [51].

The fact that a quantum formalism is strongly founded on the basis of representations of linear algebras suggests that a $T \neq 0$ field theory needs a real-time *operator* structure. Such a theory, based on the state $|0(\beta)\rangle$, was presented by Takahashi and Umezawa [71–73] and they called it *Thermofield Dynamics* (TFD). As a consequence of the real-time requirement, a doubling is defined in the original Hilbert space of the system, such that the temperature is introduced by a Bogoliubov transformation.

The Takahashi and Umezawa approach has been developed for practical purposes and some results should be mentioned, as the proof of the Goldstone theorem within this formalism with a quite amazing physical and mathematical appeal, and the perturbative scheme with Feynman rules established to carry out calculations completely in parallel with the zero-temperature quantum field theory [72]. Thus it

has been successfully applied to study magnetic superconductors [73], magnetic systems like ferromagnets and paramagnets [74], in quantum optics [75–79], transport phenomena [80] and d-branes [81, 82], among others. Furthermore, the propagators are 2×2 matrices; from this fact the association of the Matsubara and Schwinger-Keldysh methods has been analyzed in a unified way [72, 83].

Formally the thermal theory can be established, via TFD, within c^* algebras [84, 85, 18] and symmetry groups [87, 18, 86], opening a broad spectrum of possibilities for the study of thermal effects. For instance, the kinetic theory has been formulated for the first time from the analysis of representations of kinematical groups [18] and elements of the q-group have been considered, where the effects of temperature is related to a deformation in the Weyl-Heisenberg algebra [88, 86, 89]. The analysis of thermal theories via c^* algebras was carried out long ago [90, 91], resulting in the doubled structure of the Tomita-Takesaki (standard) representation that can be immediately used to construct several aspects of TFD. It is worth noticing that the structure of TFD was envisaged in a paper by Leplae, Mancini and Umezawa [92] studying superconductors; but much earlier the doubled structure was also explored by Verboven [93, 94], studying thermal oscillators.

Considering topological aspects of a thermal formalism, we can realize that the final prescription results in a scheme of compactification in time of the $T = 0$ theory. That is, the Matsubara formalism is equivalent to a path-integral calculated on $\mathbb{S}^1 \times \mathbb{R}^{D-1}$, where $\mathbb{S}^1$ is a circumference of length $\beta = 1/T$. In a generalized way the thermal field theory compactification can be extended to spatial coordinates as it is valid for finite temperature. These ideas have been developed for the Matsubara formalism [95, 96] as well as for TFD and applied to the Casimir effect considering the electromagnetic and fermion fields within a constrained geometry [97, 98], to the $\lambda\phi^4$ model as the Ginsburg-Landau theory of superconductors [99, 100], and to the Gross-Neveu model at $T = 0$ [101–103].

In this chapter the main ideas of TFD are introduced, following initially along the historical developments. Later, we present a derivation of the theory based on general arguments of symmetry. This provides not only a symmetry basis for TFD, but also for statistical mechanics, since we can derive the Liouville-von Neumann equation. This procedure points to the way to explore representations of group theory to derive properties of thermal (relativistic and non relativistic) physics. The central aspect is then to present the formalism of statistical physics as a closed theoretical framework, starting from symmetry.

5.1 Thermal Hilbert space

For a system in thermal equilibrium, the ensemble average of an operator A is given by

$$\langle A \rangle = \frac{1}{Z(\beta)} \mathrm{Tr}(e^{-\beta H} A). \tag{5.1}$$

Then assuming that $H|n\rangle = E_n|n\rangle$ with $\langle n|m\rangle = \delta_{nm}$,we write

$$\langle A\rangle = \frac{1}{Z(\beta)}\sum_n e^{-\beta E_n}\langle n|A|n\rangle.$$

We are looking for a state $|0(\beta)\rangle$ such that [71, 73]

$$\begin{aligned}\langle A\rangle &\equiv \langle 0(\beta)|A|0(\beta)\rangle \\ &= \frac{1}{Z(\beta)}\sum_n e^{-\beta E_n}\langle n|A|n\rangle. \end{aligned} \tag{5.2}$$

Let us initially investigate whether $|0(\beta)\rangle$ may be a vector in the Hilbert space; i.e.

$$|0(\beta)\rangle = \sum_n |n\rangle\langle n|0(\beta)\rangle = \sum_n g_n(\beta)|n\rangle.$$

This implies that $\langle 0(\beta)|A|0(\beta)\rangle = \sum_{nm} g_n^*(\beta)g_m(\beta)\langle n|A|m\rangle$, and the requirement given by Eq. (5.2) imposes the following condition on the coefficients $g_m(\beta)$ and $g_n^*(\beta)$,

$$g_n^*(\beta)g_m(\beta) = \frac{1}{Z(\beta)}e^{-\beta E_n}\delta_{nm}.$$

But we know that such a relation cannot be satisfied by c-numbers. Therefore $|0(\beta)\rangle$ cannot be an element of the original Hilbert space. The above condition is like an orthogonality condition, thus suggesting that $g_m(\beta)$ should be an element of a vector space. The simplest way to achieve this is by introducing a doubling of the Hilbert space. Let us do this, resulting in a tensor product of spaces, such that a vector of the basis is given by $|n,\widetilde{m}\rangle = |n\rangle\otimes|\widetilde{m}\rangle$. In the present case, taking $g_m(\beta) = f_m(\beta)|\widetilde{m}\rangle$, we write

$$|0(\beta)\rangle = \sum_n f_n(\beta)|n,\tilde{n}\rangle,$$

such that

$$\begin{aligned}\langle 0(\beta)|A|0(\beta)\rangle &= \sum_{n,m} f_n^*(\beta)f_m(\beta)\langle n,\tilde{n}|A|m,\widetilde{m}\rangle \\ &= \sum_n f_n^*(\beta)f_n(\beta)\langle n|A|n\rangle,\end{aligned}$$

where we have assumed that the operator A acts only on non-tilde vectors, i.e.

$$\langle n,\tilde{n}|A|m,\widetilde{m}\rangle = \langle n|\otimes\langle\tilde{n}|A|m\rangle\otimes|\widetilde{m}\rangle = \langle n|A|m\rangle\langle\tilde{n}|\widetilde{m}\rangle = A_{nm}\delta_{nm}.$$

The tilde in a vector $|m,\widetilde{m}\rangle$ indicates that $|\widetilde{m}\rangle$ is the replica of $|m\rangle$, with m and $\widetilde{m}$ standing for the same number: $m = \widetilde{m}$. This is why we have written $\langle\tilde{n}|\widetilde{m}\rangle = \delta_{nm}$, without reference to the tilde in the δ_{mn}. In a vector like $|m,\tilde{n}\rangle$, the tilde emphasizes the element of the tilde-Hilbert space only. In order to reproduce the thermal average, now we have $f_n^*(\beta)f_n(\beta) = Z^{-1}(\beta)\,e^{-\beta E_n}$, which has the solution $f_n(\beta) = Z^{-1/2}(\beta)\,e^{-\beta E_n/2}$. Therefore, the thermal state can be written as

$$|0(\beta)\rangle = \frac{1}{\sqrt{Z(\beta)}}\sum_n e^{-\beta E_n/2}|n,\tilde{n}\rangle.$$

The vector $|0(\beta)\rangle$ is then a pure state, defined in this doubled Hilbert space, equivalent to a mixed state describing the thermal equilibrium of a system as far as the averages are concerned.

Doubling is not a characteristic of TFD only, but rather an ingredient present in all thermal theories. In terms of the density matrix, the doubling is present when we write $\rho(t)$ as a projector, that is, $\rho \simeq |\psi\rangle\langle\psi|$, and the Liouville-von Neumann equation is written in the form

$$i\partial_t \rho(t) = \widehat{H}\rho(t). \tag{5.3}$$

The time evolution is controlled by $\widehat{H} = [H, .\,]$, the Liouvillian, which is an object associated with, but different from, the Hamiltonian operator, H. In TFD as in the density matrix formalism, this doubling, at first, looks like an artificial procedure. But this is no longer true and can be understood by exploring the fact that TFD is a thermal formalism based on a vector Hilbert space, which can be used as the carrier space for representations of Lie groups.

5.2 The meaning of the doubling: thermo-algebras

An important point now concerns with the interpretation of the doubling in the Hilbert space, necessary to introduce the thermal state $|0(\beta)\rangle$. We address this problem from the point of view of symmetry.

5.2.1 *Generators of symmetry and observables*

In order to introduce a formalism based on states $|0(\beta)\rangle$ from general assumptions, we assume that the set of kinematical variables, say $\mathcal{V}$, is a vector space of mappings in a Hilbert space denoted by $\mathcal{H}_T$. The set $\mathcal{V}$ is composed of two subspaces and is written as $\mathcal{V} = \mathcal{V}_{obs} \oplus \mathcal{V}_{gen}$, where $\mathcal{V}_{obs}$ stands for the set of kinematical observables while $\mathcal{V}_{gen}$ is the set of kinematical generators of symmetries.

Both, in quantum and classical theory, usually $\mathcal{V}_{obs}$ and $\mathcal{V}_{gen}$ are identical with each other and with $\mathcal{V}$. Let us discuss this point a little bit more. Often, to each generator of symmetry there exists a corresponding observable and both are described by the same algebraic element. For instance, consider the generator of rotations $L_3 = ix_1\partial/\partial x_2 - ix_2\partial/\partial x_1$ and the generator of space translation $P_1 = -i\,\partial/\partial x_1$. As we know, L_3 and P_1 are also considered as physical observables, an angular momentum and a linear momentum components, respectively. The effect of an infinitesimal rotation α around the x_3-axis on the observable momentum P_1 is

$$\begin{aligned}\exp(i\alpha L_3)P_1 \exp(i\alpha L_3) &\simeq (1 + i\alpha L_3)P_1(1 - i\alpha L_3)\\ &= P_1 + i\alpha[L_3, P_1].\end{aligned}$$

The commutator, expressing the effect of how much P_1 has changed, is given by

$$[L_3, P_1] = L_3P_1 - P_1L_3 = iP_2.$$

Proceeding similarly with other components, we write in general,

$$[L_i, P_j] = i\epsilon_{ijk}P_k.$$

This expression shows that $P = (P_1, P_2, P_3)$ is transformed as a vector by a rotation. In other words, the generator L_i changes P_j through the commutator operation giving rise to another observable, $i\epsilon_{ijk}P_k$. In this operation L_i has to be thought as a simple generator of symmetry, not as an observable. The same type of interpretation is valid when we consider

$$[L_i, L_j] = i\epsilon_{ijk}L_k, \tag{5.4}$$

the Lie algebra of the rotation group. In this case, the same object, the vector $L = (L_1, L_2, L_3)$, is used with two different meanings: L_i in the commutator is the generator of an infinitesimal rotation over the physical observable L_j, resulting of course in another physical quantity, $i\epsilon_{ijk}L_k$.

It has to be emphasized that, although the one-to-one correspondence among observables and generators of symmetry is based on physical grounds, there exists no *a priori* dynamical or kinematical imposition to consider a generator of symmetry and the corresponding observable as being described by the same mathematical quantity. Actually we are free to assume a more general situation; and we have already observed this separation in the Liouville-von Neumann equation written in the form of Eq. (5.3). There we have two different objects associated with the time evolution: H, the Hamiltonian, that describes the observable energy of a system, and $\widehat{H}$, the Liouvillian, the generator of time evolution.

Here we consider the same one-to-one correspondence among generators and observables, but exploring the case in which $\mathcal{V}_{obs}$ and $\mathcal{V}_{gen}$ are different from each other. That is, $\mathcal{V}_{obs}$ and $\mathcal{V}_{gen}$ correspond to different mappings in $\mathcal{H}_T$. To emphasize these aspects, we denote an arbitrary element of $\mathcal{V}_{obs}$ by A and by $\widehat{A}$ the corresponding element in $\mathcal{V}_{gen}$. Now we analyze the consequences of such separability condition for an arbitrary symmetry group.

5.2.2 *Doubled Lie algebra*

Let us denote by $\ell = \{a_i, i = 1, \cdots, s\}$ the set of generators that span a Lie algebra over $\mathbb{R}$, the real field. In the set ℓ there exists a product, $(\cdot, \cdot)$, called the Lie product, given by

$$(a_i, a_j) = C_{ij}^k a_k,$$

where the sum over repeated indices is assumed. The c-numbers C_{ij}^k are the structure constants, which characterize the nature of the symmetry group associated with ℓ,. The Lie product satisfies the condition of antisymmetry,

$$(a_i, a_j) = -(a_j, a_i),$$

and the Jacoby identity,

$$(a_i, (a_j, a_k)) + (a_k, (a_i, a_j)) + (a_j, (a_k, a_i)) = 0.$$

A well-known example is the Lie algebra of the rotation group given in Eq. (5.4) where the Lie product is a commutator.

Taking $\mathcal{H}_T$ as the carrier space for representations of ℓ, we write

$$[\widehat{A}_i, \widehat{A}_j] = iC_{ij}^k \widehat{A}_k, \tag{5.5}$$

where $\widehat{A}_i \in \mathcal{V}_{gen}$. The imaginary i in Eq. (5.5) is to characterize that we are treating a unitary representation. Although Eq. (5.5) provides a representation for ℓ, operators of type A have to be taken into consideration in a representation in the full Hilbert space $\mathcal{H}_T$, otherwise the representations will be restricted to the set of hat operators, $\mathcal{V}_{gen}$; resulting in the usual unitary representation. Therefore we have additional commutation relations among A and $\widehat{A}$ operators, and among the operators of type A. Let us then write

$$[\widehat{A}_i, A_j] = iD_{ij}^k A_k, \tag{5.6}$$

$$[A_i, A_j] = iE_{ij}^k A_k, \tag{5.7}$$

where D_{ij}^k and E_{ij}^k are constants to be fixed with the following reasoning. Observe that Eqs. (5.5)–(5.7) describe a Lie algebra, to be denoted by ℓ_T, which is the definition of a semidirect product of two subalgebras, $\mathcal{V}_{gen}$ and $\mathcal{V}_{obs}$, characterized by the fact that $\mathcal{V}_{obs}$ is an invariant subalgebra. The motive for that is a physical imposition. Since non-hat operators describe kinematical observables, Eq. (5.6) is interpreted as the infinitesimal action of a symmetry generated by $\widehat{A}_i$ on the observable A_j, resulting in another observable given by $iD_{ij}^k A_k$. This is found from the relation

$$e^{i\alpha\widehat{A}_i} A_j e^{-i\alpha\widehat{A}_i} = A_j(\alpha).$$

Considering $\alpha \ll 1$, we write

$$A_j(\alpha) = A_j + \alpha \left(\frac{\partial A_j(\alpha)}{\partial \alpha} \right)_{\alpha=0}$$

and

$$e^{i\alpha\widehat{A}_i} A_j e^{-i\alpha\widehat{A}_i} \simeq A_j + i\alpha[\widehat{A}_i, A_j].$$

Thus, taking $\alpha \to 0$, we have

$$[\widehat{A}_i, A_j] = -i\frac{\partial A_j(\alpha)}{\partial \alpha}.$$

The important thing in this relation is that

$$\frac{\partial A_j(\alpha)}{\partial \alpha}$$

is another observable specified by the commutation relation. On the other hand, the content of Eq. (5.7) is the nature of commutativity among observables. Before going further, we give an example.

Let $\ell = \{a_i = s_i, i = 1, 2, 3\}$ be the Lie algebra of the group $SU(2)$, such that

$$[l_i, l_j] = i\epsilon_{ijk} l_k.$$

A representation of $su(2)_T$ is given by

$$[S_i, S_j] = i\epsilon_{ijk} S_k, \tag{5.8}$$

$$[S_i, s_j] = i\epsilon_{ijk} s_k, \tag{5.9}$$

$$[s_i, s_j] = i\epsilon_{ijk} s_k, \tag{5.10}$$

where S_i (equivalent to a hat operator) describe a rotation, while s_j (equivalent to a non-hat operator) is the observable of spin. The fact that spin transforms as a vector under rotations is represented by Eq. (5.9). The components of spin do not commute with one another, according to Eq. (5.10), as a consequence of the measurement imposition. In this case we have $C_{ij}^k = D_{ij}^k = E_{ij}^k = \epsilon_{ijk}$.

With the example above, we find that symmetries can also be used to define the results of commutation relations among observables, and as such we assume that in Eqs. (5.5)–(5.7) $C_{ij}^k = D_{ij}^k = E_{ij}^k$. Gathering these comments, we write

$$[\widehat{A}_i, \widehat{A}_j] = iC_{ij}^k \widehat{A}_k, \tag{5.11}$$

$$[\widehat{A}_i, A_j] = iC_{ij}^k A_k, \tag{5.12}$$

$$[A_i, A_j] = iC_{ij}^k A_k. \tag{5.13}$$

These relations define the Lie algebra in the thermal Hilbert space $\mathcal{H}_T$. This representation will be called *thermo Lie algebra* [87]. Notice that this procedure opens the possibility to explore the notion of Hilbert space in the context of classical physics, if we consider $E_{ij}^k = 0$ in Eq. (5.7) [104]. Such a classical formalism will be developed in the last Part of this book.

5.2.3 *Tilde conjugation rules*

Some properties of ℓ_T can be derived. Defining the variable

$$\widetilde{A} = A - \widehat{A}, \tag{5.14}$$

we show that Eqs. (5.11)–(5.13) are written as

$$[A_i, A_j] = iC_{ij}^k A_k, \tag{5.15}$$

$$[\widetilde{A}_i, \widetilde{A}_j] = -iC_{ij}^k \widetilde{A}_k, \tag{5.16}$$

$$[A_i, \widetilde{A}_j] = 0 \tag{5.17}$$

This result shows that a doubling of degrees of freedom has been introduced, in the form of a direct product. This is a consequence of the algebraic separability between mappings in $\mathcal{H}_T$ describing the generators of symmetry and those of the observables.

Such a doubling can be considered as a mapping in $\mathcal{V} = \mathcal{V}_{obs} \oplus \mathcal{V}_{gen}$, say J :

$\mathcal{V} \to \mathcal{V}$, denoted by $JAJ = \widetilde{A}$, fulfilling the following conditions

$$(A_i A_j)\tilde{} = \widetilde{A}_i \widetilde{A}_j, \tag{5.18}$$

$$(cA_i + A_j)\tilde{} = c^* \widetilde{A}_i + \widetilde{A}_j, \tag{5.19}$$

$$(A_i^\dagger)\tilde{} = (\widetilde{A}_i)^\dagger, \tag{5.20}$$

$$(\widetilde{A}_i)\tilde{} = A_i. \tag{5.21}$$

$$[A_i, \widetilde{A}_j] = 0. \tag{5.22}$$

These properties, called *tilde conjugation rules*, are introduced as a consequence of Eqs. (5.15)–(5.17). For instance, comparing Eq. (5.15), written as

$$A_i A_j - A_j A_i = i C_{ij}^k A_k,$$

and Eq. (5.16), written as

$$\widetilde{A}_i \widetilde{A}_j - \widetilde{A}_j \widetilde{A}_i = -i C_{ij}^k \widetilde{A}_k,$$

we find $(A_i A_j)\tilde{} = \widetilde{A}_i \widetilde{A}_j$. The other relations follow from such comparisons.

5.3 Tilde and non-tilde operators

In this section we analyze, with examples, representations for the tilde and non-tilde operators. We consider the Hilbert space $\mathcal{H}$, as a Fock space with a basis vector denoted by

$$|m\rangle = \frac{1}{\sqrt{m!}} (a^\dagger)^m |0\rangle,$$

where $|0\rangle$ is the vacuum state and $a^\dagger$ is a boson creation operator fulfilling the algebra $[a, a^\dagger] = 1$, with the other commutation relations being zero. We consider then the thermal Hilbert space as a direct product $\mathcal{H}_T = \mathcal{H} \otimes \widetilde{\mathcal{H}}$. The meaning of the tilde space, $\widetilde{\mathcal{H}}$, has to be specified by the tilde conjugation rules regarding the representation space. An arbitrary basis vector in $\mathcal{H}_T$ is obtained by first taking the tilde conjugation of $\mathcal{H}$, that is $J\mathcal{H} = \widetilde{\mathcal{H}}$. For a vector $|m\rangle$ in $\mathcal{H}$ we have

$$J|m\rangle = J \frac{1}{\sqrt{m!}} (a^\dagger)^m |0\rangle = \frac{1}{\sqrt{m!}} (\tilde{a}^\dagger)^m J|0\rangle,$$

where the results $J^2 = 1$ and $J a^\dagger J = \tilde{a}^\dagger$ are used. We have to define the following conjugation $J|0\rangle = |0\rangle\tilde{}$. The simplest choice is

$$J|0\rangle = |\tilde{0}\rangle. \tag{5.23}$$

Therefore, we have $J|m\rangle = |\widetilde{m}\rangle$ and a basis vector in $\mathcal{H}_T$ is given by

$$|m, \tilde{n}\rangle = \frac{1}{\sqrt{m!}\sqrt{n!}} (a^\dagger)^m (\tilde{a}^\dagger)^n |0, \tilde{0}\rangle,$$

where $|m, \tilde{n}\rangle = |m\rangle \otimes |\tilde{n}\rangle$ and, in particular, $|0, \tilde{0}\rangle = |0\rangle \otimes |\tilde{0}\rangle$. Using this, we obtain

$$J|m, \tilde{n}\rangle = |n, \widetilde{m}\rangle.$$

Given an operator A in $\mathcal{H}$, then we can construct a corresponding non-tilde operator, say $\mathcal{A}$, in $\mathcal{H}_T$ by defining its action on a vector $|m,\tilde{n}\rangle$, as

$$\mathcal{A}|m,\tilde{n}\rangle = (A|m\rangle)\otimes|\tilde{n}\rangle.$$

In the same way, given $\widetilde{A}$ in $\widetilde{\mathcal{H}}$ we have $\widetilde{\mathcal{A}}$ in $\mathcal{H}_T$, such that

$$\widetilde{\mathcal{A}}|m,\tilde{n}\rangle = |m\rangle\otimes\widetilde{A}|\tilde{n}\rangle.$$

Using the completeness relation $1=\sum_{r,s}|r,\tilde{s}\rangle\langle\tilde{s},r|$, we have

$$\begin{aligned}\mathcal{A}|m,\tilde{n}\rangle &= \sum_{r,s,t,u}|r,\tilde{s}\rangle\langle\tilde{s},r|\mathcal{A}|t,\tilde{u}\rangle\langle\tilde{u},t|m,\tilde{n}\rangle\\ &= \sum_{r,s}\langle\tilde{s},r|\mathcal{A}|m,\tilde{n}\rangle|r,\tilde{s}\rangle\\ &= \sum_{r}A_{r,m}|r,\tilde{n}\rangle = (A|m\rangle)|\tilde{n}\rangle, \end{aligned}\tag{5.24}$$

where $A_{rm}=\langle r|A|m\rangle$. We get the tilde of $\mathcal{A}$ taking the tilde conjugation of Eq. (5.24), resulting in

$$\widetilde{\mathcal{A}}|m,\tilde{n}\rangle\tilde{} = \widetilde{\mathcal{A}}|n,\widetilde{m}\rangle = \sum_{r}A^{*}_{rm}|n,\tilde{r}\rangle,$$

where we have used $(A_{rm})\tilde{}=A^{*}_{rm}$, since A_{rm} is a c-number, and $|m,\tilde{n}\rangle\tilde{}=|n,\widetilde{m}\rangle$. On the other hand we have

$$\begin{aligned}\widetilde{\mathcal{A}}|n,\widetilde{m}\rangle &= \sum_{r,s,t,u}|r,\tilde{s}\rangle\langle\tilde{s},r|\widetilde{\mathcal{A}}|t,\tilde{u}\rangle\langle\tilde{u},t|n,\widetilde{m}\rangle\\ &= \sum_{r,s}\langle\tilde{s},r|\widetilde{\mathcal{A}}|n,\widetilde{m}\rangle|r,\tilde{s}\rangle = \sum_{s}\langle\tilde{s}|\widetilde{A}|\widetilde{m}\rangle|n,\tilde{s}\rangle.\end{aligned}$$

Then we obtain

$$\langle\tilde{s}|\widetilde{A}|\widetilde{m}\rangle = A^{*}_{sm} = (A^{T\dagger})_{sm} \ = (A^{\dagger})_{ms},\tag{5.25}$$

where $A^{T\dagger}$ is the transpose (T) and the Hermitian conjugate ($\dagger$) of A.

Writing

$$\langle\tilde{s},r|\mathcal{A}|m,\tilde{n}\rangle = \mathcal{A}_{\tilde{s}rm\tilde{n}} = \mathcal{A}_{rmsn},$$

we have

$$\mathcal{A}_{rmsn} = A_{rm}\delta_{ns}.\tag{5.26}$$

For the tilde operator we define

$$\langle\tilde{s}r|\widetilde{\mathcal{A}}|m\tilde{n}\rangle = \widetilde{\mathcal{A}}_{\tilde{s}rm\tilde{n}} = \widetilde{\mathcal{A}}_{snrm},$$

resulting in

$$\widetilde{\mathcal{A}}_{snrm} = \delta_{rm}(A^{\dagger})_{ns}\tag{5.27}$$

From Eqs. (5.26) and (5.27), we can write

$$\mathcal{A} = A\otimes 1 \ \text{ and } \ \widetilde{\mathcal{A}} = 1\otimes A^{\dagger}\,.$$

For example, consider the Pauli matrices:

$$s_1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad s_2 = \frac{i}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad s_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.28}$$

satisfying the Lie algebra

$$[s_i, s_j]_- = i\epsilon_{ij}^k s_k. \tag{5.29}$$

The representation for the corresponding operators $\mathcal{A} = \mathcal{S}$ and $\widetilde{\mathcal{A}} = \widetilde{\mathcal{S}}$, can be obtained using the Hermitian Pauli matrices; we have $\mathcal{S}_j \equiv s_j \otimes 1$ and $\widetilde{\mathcal{S}}_j \equiv 1 \otimes s_j$ with $i = 1, 2, 3$, that is

$$\mathcal{S}_1 = \frac{1}{2}\begin{pmatrix} 0&1&0&0 \\ 1&0&0&0 \\ 0&0&0&1 \\ 0&0&1&0 \end{pmatrix}, \quad \mathcal{S}_2 = \frac{1}{2}\begin{pmatrix} 0&-i&0&0 \\ i&0&0&0 \\ 0&0&0&-i \\ 0&0&i&0 \end{pmatrix},$$

$$\mathcal{S}_3 = \frac{1}{2}\begin{pmatrix} 1&0&0&0 \\ 0&-1&0&0 \\ 0&0&1&0 \\ 0&0&0&-1 \end{pmatrix}, \quad \widetilde{\mathcal{S}}_1 = \frac{1}{2}\begin{pmatrix} 0&0&1&0 \\ 0&0&0&1 \\ 1&0&0&0 \\ 0&1&0&0 \end{pmatrix},$$

$$\widetilde{\mathcal{S}}_2 = \frac{1}{2}\begin{pmatrix} 0&0&-i&0 \\ 0&0&0&-i \\ i&0&0&0 \\ 0&i&0&0 \end{pmatrix}, \quad \widetilde{\mathcal{S}}_3 = \frac{1}{2}\begin{pmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&-1&0 \\ 0&0&0&-1 \end{pmatrix}.$$

These matrices satisfy the algebra given by

$$[\mathcal{S}_i, S_j] = i\epsilon_{ijk}\mathcal{S}_k,$$
$$[\widetilde{\mathcal{S}}_i, \widetilde{\mathcal{S}}_j] = -i\epsilon_{ijk}\widetilde{\mathcal{S}}_k$$
$$[\mathcal{S}_i, \widetilde{\mathcal{S}}_j] = 0.$$

We construct another representation for $\mathcal{A} = \mathcal{S}$ and $\widetilde{\mathcal{A}} = \widetilde{\mathcal{S}}$ using Eq. (5.25), that is $\langle \tilde{s}|\widetilde{A}|\widetilde{m}\rangle = A^*_{sm}$, with an embedding in the higher dimensional space $\mathcal{H}_T$. In the case of the Pauli matrices, we have

$$\mathcal{S}_1 = \frac{1}{2}\begin{pmatrix} 0&1&0&0 \\ 1&0&0&0 \\ 0&0&1&0 \\ 0&0&0&1 \end{pmatrix}, \quad \mathcal{S}_2 = \frac{1}{2}\begin{pmatrix} 0&-i&0&0 \\ i&0&0&0 \\ 0&0&1&0 \\ 0&0&0&1 \end{pmatrix},$$

$$\mathcal{S}_3 = \frac{1}{2}\begin{pmatrix} 1&0&0&0 \\ 0&-1&0&0 \\ 0&0&1&0 \\ 0&0&0&1 \end{pmatrix}, \quad \widetilde{\mathcal{S}}_1 = \frac{1}{2}\begin{pmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&0&1 \\ 0&0&1&0 \end{pmatrix},$$

$$\widetilde{\mathcal{S}}_2 = \frac{1}{2}\begin{pmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&0&i \\ 0&0&-i&0 \end{pmatrix}, \quad \widetilde{\mathcal{S}}_3 = \frac{1}{2}\begin{pmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&1&0 \\ 0&0&0&-1 \end{pmatrix}.$$

A useful result for the tilde and non-tilde operators is derived by considering the vector

$$|1\rangle = \sum_m |m, \widetilde{m}\rangle \tag{5.30}$$

Then we have, from Eq. (5.24), for the non-tilde operator

$$\mathcal{A}|1\rangle = \sum_m \mathcal{A}|m, \widetilde{m}\rangle = \sum_{m,r} A_{rm}|r, \widetilde{m}\rangle; \tag{5.31}$$

and for the tilde operator

$$\widetilde{\mathcal{A}}|1\rangle = \sum_m \widetilde{\mathcal{A}}|m, \widetilde{m}\rangle = \sum_{m,r} \widetilde{\mathcal{A}}_{rm}|m, \tilde{r}\rangle. \tag{5.32}$$

Taking the tilde conjugation of Eq. (5.31) we have

$$\widetilde{\mathcal{A}}_{rm} = A^*_{rm} = \langle r|A^{T\dagger}|m\rangle = \langle m|A^\dagger|r\rangle.$$

Inserting this result into Eq. (5.32) we obtain

$$\widetilde{\mathcal{A}}|1\rangle = \sum_m (A^\dagger|m\rangle)|\widetilde{m}\rangle. \tag{5.33}$$

Taking $\mathcal{A} = \mathcal{B}\mathcal{C}$, such that $A = BC$, then we have

$$\widetilde{\mathcal{B}}\widetilde{\mathcal{C}}|1\rangle = (BC)^\dagger|1\rangle = C^\dagger B^\dagger|1\rangle. \tag{5.34}$$

5.4 Liouville-von Neumann equation

Let us analyze the effect of time transformations of an arbitrary observable $\mathcal{A}(t)$, generated by $\widehat{H}$,

$$\mathcal{A}(t) = e^{it\widehat{\mathcal{H}}}\mathcal{A}(0)e^{-it\widehat{\mathcal{H}}}. \tag{5.35}$$

Taking the derivative of Eq. (5.35) with respect to time, we get

$$i\partial_t\mathcal{A}(t) = [\mathcal{A}(t), \widehat{\mathcal{H}}]. \tag{5.36}$$

Assume that the state of a system is given by a vector $|\psi(t_o)\rangle \in \mathcal{H}_T$ and the average of an observable $A(t)$ in a state $|\psi(0)\rangle$ is given by

$$\langle\mathcal{A}\rangle = \langle\psi(0)|\mathcal{A}(t)|\psi(0)\rangle,$$

with $\langle\psi(0)|\psi(0)\rangle = 1$. Then from Eq. (5.35) we write $\langle\mathcal{A}\rangle = \langle\psi(t)|\mathcal{A}(0)|\psi(t)\rangle$, where $|\psi(t)\rangle$ satisfies the equation

$$i\partial_t|\psi(t)\rangle = \widehat{\mathcal{H}}|\psi(t)\rangle. \tag{5.37}$$

Despite the appearance, this equation is not the Schrödinger equation in quantum mechanics due to $\mathcal{H}_T$, that provides reducible representations. However, Eq. (5.36) is in a Heisenberg picture and Eq. (5.37) is in a Schrödinger picture.

In this section, we use a representation for $|\psi(t)\rangle$ from $|1\rangle$, in the following way. Consider a time-dependent operator $F(t)$ acting in $\mathcal{H}$. In the space $\mathcal{H}_T$ we have a vector $|F(t)\rangle$ defined by the association $F(t) \to |F(t)\rangle$, with

$$F(t)|1\rangle \equiv |F(t)\rangle.$$

Let us verify the scalar product in $\mathcal{H}_T$, with the vector constructed in this way. Consider another vector $|G(t)\rangle = G(t)|1\rangle$; then we have

$$\langle G|F\rangle = \sum_{m,n} \langle \tilde{n}, n|G^\dagger F|m, \widetilde{m}\rangle \tag{5.38}$$

$$= \sum_{m} \langle m|G^\dagger F|m\rangle = \mathrm{Tr}(G^\dagger F) \tag{5.39}$$

As far as a state of a quantum system is concerned, we take $|\psi(t)\rangle$ in Eq. (5.37) to be $|\psi(t)\rangle \equiv |F(t)\rangle$. If $|\psi(t)\rangle$ is a normalized state, then $\mathrm{Tr}(F^\dagger F) = 1$. It is then convenient to represent $F(t)$ as the square root of another operator, writing, $F(t) = \rho^{1/2}(t)$. In this case

$$|\psi(t)\rangle = |\rho^{1/2}(t)\rangle = \rho^{1/2}(t)|1\rangle.$$

Since

$$\widehat{\mathcal{H}} = \mathcal{H} - \widetilde{\mathcal{H}} = H \otimes 1 - 1 \otimes H^\dagger = H \otimes 1 - 1 \otimes H,$$

we have

$$\begin{aligned}
\widehat{\mathcal{H}}|\psi(t)\rangle &= \widehat{\mathcal{H}}\rho^{1/2}(t)|1\rangle = (\mathcal{H} - \widetilde{\mathcal{H}})\rho^{1/2}(t)|1\rangle \\
&= H\rho^{1/2}(t)|1\rangle - \widetilde{H}\rho^{1/2}(t)|1\rangle \\
&= [H\rho^{1/2}(t) - \rho^{1/2}(t)\widetilde{H}]|1\rangle \\
&= [H\rho^{1/2}(t) - \rho^{1/2}(t)H^\dagger]|1\rangle = [H, \rho^{1/2}(t)]|1\rangle;
\end{aligned}$$

thus we find

$$i\partial_t|\psi(t)\rangle = i\partial_t\rho^{1/2}(t)|1\rangle = [H, \rho^{1/2}(t)]|1\rangle.$$

This leads to

$$i\partial_t\rho^{1/2}(t) = [H, \rho^{1/2}(t)].$$

We can find the time evolution for $\rho(t) = \rho^{1/2\dagger}(t)\rho^{1/2}(t)$, by calculating $i\partial_t\rho(t)$. The result is

$$i\partial_t\rho(t) = [H, \rho(t)],$$

the original Liouville-von Neumann equation, since $\rho(t)$, a Hermitian operator with $\mathrm{Tr}\rho = 1$, can be interpreted as the density matrix.

Let us take $\rho^{1/2}$ diagonal in the basis $|n, \widetilde{m}\rangle$, such that the state $|\psi(t)\rangle$ is expanded as

$$|\psi(t)\rangle = \sum_n \rho_n^{1/2}(t)|n, \tilde{n}\rangle. \tag{5.40}$$

Hence, the average of an observable A is

$$\begin{aligned}\langle A\rangle &= \langle\psi(t)|A|\psi(t)\rangle \\ &= \sum_{n,m}\rho_m^{*1/2}(t)\rho_n^{1/2}(t)\langle m,\widetilde{m}|A|n,\tilde{n}\rangle \\ &= \sum_n \rho_n(t)\langle n|A|n\rangle = \mathrm{Tr}(\rho A).\end{aligned}$$

Then the canonical average can be derived. For that let us write

$$\rho_n^{1/2} = \frac{e^{-\beta E_n/2}}{\sqrt{Z(\beta)}},$$

resulting in the canonical ensemble if we calculate $\rho = \rho^{\dagger 1/2}\rho^{1/2}$. Beyond that, from Eq. (5.40) the state $|0(\beta)\rangle$, defining the equilibrium average, is

$$|0(\beta)\rangle = \frac{1}{\sqrt{Z(\beta)}}\sum_n e^{-\beta E_n/2}|n,\tilde{n}\rangle.$$

In short, considering general aspects of symmetries, the Liouville-von Neumann equation is derived, but with an additional ingredient: Eq. (5.37) is an amplitude density matrix equation, such that $|\psi\rangle = \rho^{1/2}|1\rangle$ is associated with the square root of the density matrix. In this sense, the theory of Lie groups, so often used in the case of $T = 0$ theories, is useful for thermal physics through the doubled representation, or the thermo-algebra. This makes statistical mechanics a self-contained theoretical structure starting from group theory, for with Liouville-von Neumann equation, we introduce the entropy in the standard way and follow with the proper connection with thermodynamics. The self-contained elements are reflected in the fact that no mention to the Schrödinger equation or even the notion of ensemble has been necessary to develop the statistical mechanics. Some algebraic aspects that we have derived in this chapter were earlier found but implicitly presented in the axiomatic structure of quantum statistical mechanics based on c^*-algebra. Actually the concept of thermo Lie group discussed here is a way to bring part of the c^*-algebra formalism to the language of Lie groups [85, 86].

5.5 Physical implications of thermo-algebras

In this chapter, the fundamental result has been the notion of thermo-algebra, i.e. the scheme of representations of Lie algebras, based on the fact that the dynamical variables of symmetry are composed of two classes of operators. One set describes the observables, and others are generators of symmetry. Although there is a one-to-one association among these sets, they are described by different mathematical objects, each one with its proper physical interpretation. The known example in statistical physics of this separability is the Liouvillian, describing the evolution of the system in Liouville-von Neumann equation, and the Hamiltonian.

From this dichotomy arises a duplication in the original Hilbert space. Here these elements are related to the language of group theory, and we explore this fact in depth in following chapters. However, some aspects can be emphasized and anticipated .

First, it is worth making an additional comment regarding tilde operators. According to Eq. (5.14), a tilde operator is introduced by the difference among generators of symmetry and observables. On the other hand, in the literature, tilde operators, when used to define generators of time evolution, are referred to as heat-bath variables; and this is the case for some specific examples [104]. If the tilde operators, however, are not interpreted in a consistent way, their use would be considered somewhat artificial, and for this reason such variables have been, at times, designated as ghost variables. But this artificiality is removed, since the content of doubling degrees of freedom in thermal theories is related to symmetries as we have seen. Beyond that, once there is a connection between the Matsubara formalism and real-time approaches, with the proper interpretation of the doubling, we understand better the real meaning of working with an imaginary time formalism.

We observe that the role played by tilde variables is to give rise to physical states described by density matrices, in the sense that we have: $|m, \widetilde{m}\rangle \rightarrow |m\rangle\langle m|$. The meaning of the thermal states introduced from this duplication is interpreted in terms of this association with the density matrix states; an aspect to be discussed in Chapter 12. There are other consequences. Since we have a doubling in the degrees of freedom, we can explore linear mappings of the type given by a Bogoliubov transformation in this doubled Hilbert space. Actually, this will be the mechanism to introduce temperature, and thus the thermal phenomena can be viewed as a condensate process. Furthermore, using the KMS condition with Bogoliubov transformations, we can extend this method to describe compactification in space coordinates of a field theory in topologies such as $(\mathbb{S}^1)^d \times \mathbb{R}^{D-d}$, where d $(< D)$ is the number of compactified dimensions in a D-dimensional manifold [105, 106]. These developments will arise from representations of kinematical groups, Poincaré and Galilei, and will be applied to describe processes such as spontaneous symmetry breaking and phase transitions for compactified fields in space, at finite temperature.

In order to develop the ideas of symmetry, we initiate our discussion by considering a simple system with boson and fermion oscillators. Bogoliubov transformations and the doubled Hilbert space are introduced. This gives us a clear idea about the nature of TFD in such a system and, thus, prepares us for considering the problem of fields in TFD.

Chapter 6

Thermal Oscillators: Bosons and Fermions

The algebraic approach is applied to bosonic and fermionic oscillators. This provides new elements for the formalism which will be useful for the study of thermal fields. In particular the process of thermalization will be implemented via a Bogoliubov transformation in a doublet notation.

6.1 Boson oscillators

A boson oscillator is described by a Hamiltonian (we use $\hbar = 1$),

$$H = wa^\dagger a,$$

neglecting the zero-point energy. The creation and destruction operators, $a^\dagger$ and a respectively, satisfy the algebra

$$[a, a^\dagger] = 1\,; \quad [a, a] = [a^\dagger, a^\dagger] = 0. \tag{6.1}$$

The eigenvalues and eigenstates of H are specified by

$$H|n\rangle = nw|n\rangle,$$

where the vacuum state $|0\rangle$ is such that

$$a|0\rangle = 0 \tag{6.2}$$

$$(a^\dagger)^n|0\rangle = \sqrt{n!}\,|n\rangle, \tag{6.3}$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle. \tag{6.4}$$

These states are orthonormal, i.e. $\langle m|n\rangle = \delta_{mn}$, and the number operator, $N = a^\dagger a$, is such that

$$N|n\rangle = n|n\rangle.$$

The eigenvalues of N, the integers $n = 0, 1, 2, \ldots$, determine the energy levels of the oscillator, nw. Since $a^\dagger$ and a describe bosons, $|n\rangle$ is a state with n bosons.

6.1.1 *Thermal vacuum*

To double degrees of freedom, tilde operators $\tilde{a}^\dagger$ and $\tilde{a}$ are introduced. Applying the tilde conjugation rule to the algebra given in Eq. (6.1) we obtain

$$(aa^\dagger - a^\dagger a)^\sim = \tilde{1} = 1,$$

$$[\tilde{a}, \tilde{a}^\dagger] = 1\,, \qquad [\tilde{a}, \tilde{a}] = [\tilde{a}^\dagger, \tilde{a}^\dagger] = 0, \tag{6.5}$$

and with similar relations as in Eqs. (6.2)–(6.4). The generator of time translations $\widehat{H}$ is given by

$$\widehat{H} = H - \widetilde{H} = w(a^\dagger a - \tilde{a}^\dagger \tilde{a}),$$

and the thermal state $|0(\beta)\rangle$ is

$$\begin{aligned} |0(\beta)\rangle &= \frac{1}{\sqrt{Z(\beta)}} \sum_n e^{-n\beta w/2} |n, \tilde{n}\rangle \\ &= \frac{1}{\sqrt{Z(\beta)}} \sum_n e^{-n\beta w/2} \frac{1}{(n!)^{1/2}} \frac{1}{(\tilde{n}!)^{1/2}} (a^\dagger)^n (\tilde{a}^\dagger)^n |0, \tilde{0}\rangle. \end{aligned} \tag{6.6}$$

It follows that

$$\begin{aligned} \langle 0(\beta)|0(\beta)\rangle &= \frac{1}{Z(\beta)} \sum_{n,m} \langle m, \widetilde{m}| e^{-\beta w(n+m)/2} |n, \tilde{n}\rangle \\ &= \frac{1}{Z(\beta)} \sum_{n,m} e^{-\beta w(n+m)/2} \delta_{nm} \delta_{mn} \\ &= \frac{1}{Z(\beta)} \sum_n e^{-\beta w n}. \end{aligned}$$

Using $\langle 0(\beta)|0(\beta)\rangle = 1$ and the geometric series expansion $1/(1-x) = \sum_n x^n$, we find

$$Z(\beta) = \frac{1}{1 - e^{-\beta w}}. \tag{6.7}$$

Observe that in these calculations the tilde in the state $|n, \tilde{n}\rangle$ is just to indicate the vector on which a tilde operator acts, but n and $\tilde{n}$ are the same number as in the sum. Finally, from Eq. (6.6) we have

$$|0(\beta)\rangle = \sqrt{1 - e^{-\beta w}} \sum_n \frac{e^{-n\beta w/2}}{n!} (a^\dagger)^n (\tilde{a}^\dagger)^n |0, \tilde{0}\rangle. \tag{6.8}$$

In this way we are able to proceed with calculations in statistical mechanics using, instead of the canonical density matrix, the state $|0(\beta)\rangle$. To explore this possibility, Eq. (6.8) is written in the form $|0(\beta)\rangle = U(\beta)|0, \tilde{0}\rangle$, where $U(\beta)$ is a unitary operator.

6.1.2 *Bogoliubov transformation*

The sum in Eq. (6.8) is an exponential, that is

$$|0(\beta)\rangle = \sqrt{1-e^{-\beta w}}\exp(e^{-\beta w/2}a^\dagger\tilde{a}^\dagger)|0,\tilde{0}\rangle. \tag{6.9}$$

This result is written as an exponential function only, and as such a unitary operator, by taking into account the operator relation

$$e^{\alpha(A+B)} = e^{\tanh\alpha B}e^{\ln\cosh\alpha C}e^{\tanh\alpha A}, \tag{6.10}$$

where $C=[A,B]$. First we define

$$\cosh\theta(\beta) = \frac{1}{\sqrt{1-e^{-\beta w}}} \equiv u(\beta), \tag{6.11}$$

$$\sinh\theta(\beta) = \frac{e^{-\beta w/2}}{\sqrt{1-e^{-\beta w}}} \equiv v(\beta), \tag{6.12}$$

which is a consistent definition since

$$u^2(\beta) - v^2(\beta) = \cosh^2\theta(\beta) - \sinh^2\theta(\beta) = 1. \tag{6.13}$$

A result of these definitions is that

$$\tanh\theta(\beta) = e^{-\beta w/2}. \tag{6.14}$$

Using then Eqs. (6.11) and (6.14), Eq. (6.9) reads

$$\begin{aligned}|0(\beta)\rangle &= \cosh^{-1}\theta(\beta)e^{\tanh\theta(\beta)a^\dagger\tilde{a}^\dagger}|0,\tilde{0}\rangle \\ &= \exp\left[\tanh\theta a^\dagger\tilde{a}^\dagger\right]\exp\left[-\ln\cosh\theta(\tilde{a}\tilde{a}^\dagger + a^\dagger a)\right]\exp\left[\tanh\theta(-\tilde{a}a)\right]|0,\tilde{0}\rangle,\end{aligned} \tag{6.15}$$

where we have used the commutation relation $[\tilde{a},\tilde{a}^\dagger]=1$ and

$$e^{f(\theta)\tilde{a}^\dagger\tilde{a}}|0,\tilde{0}\rangle = e^0|0,\tilde{0}\rangle = |0,\tilde{0}\rangle,$$

where $f(\theta)$ is an arbitrary function of θ.

Considering Eq. (6.10) with

$$\begin{aligned}&A = -\tilde{a}a,\ B = a^\dagger\tilde{a}^\dagger,\\ &C = [A,B] = -\tilde{a}\tilde{a}^\dagger - a^\dagger a,\\ &\alpha = \theta = \theta(\beta),\end{aligned}$$

Eq. (6.15) reads

$$|0(\beta)\rangle = e^{-iG(\beta)}|0,\tilde{0}\rangle, \tag{6.16}$$

where

$$G(\beta) = -i\theta(\beta)(\tilde{a}a - \tilde{a}^\dagger a^\dagger). \tag{6.17}$$

Hence the unitary operator, transforming $|0,\tilde{0}\rangle$ into $|0(\beta)\rangle$, is given by

$$U(\beta) = e^{-iG(\beta)}. \tag{6.18}$$

The operator $U(\beta)$ is called a Bogoliubov transformation.

6.1.3 *Thermal operators*

Using $U(\beta)$ let us introduce the following thermal operators through the relations

$$\begin{aligned} a(\beta) &= U(\beta)aU^\dagger(\beta) \\ a^\dagger(\beta) &= U(\beta)a^\dagger U^\dagger(\beta), \\ \tilde{a}(\beta) &= U(\beta)\tilde{a}U^\dagger(\beta), \\ \tilde{a}^\dagger(\beta) &= U(\beta)\tilde{a}^\dagger U^\dagger(\beta). \end{aligned}$$

The importance of these operators lies in the fact that

$$\begin{aligned} a(\beta)|0(\beta)\rangle &= U(\beta)aU^\dagger(\beta)U(\beta)|0,\widetilde{0}\rangle \\ &= U(\beta)a|0,\tilde{0}\rangle = 0, \end{aligned}$$

and

$$\tilde{a}(\beta)|0(\beta)\rangle = 0.$$

Then $|0(\beta)\rangle$ is a vacuum for $a(\beta)$ and $\tilde{a}(\beta)$, but it is not a vacuum for a and $\tilde{a}$. In this sense, $|0(\beta)\rangle$ is a pure state for thermal operators, and a thermal state for non-thermal operators; this is why $|0(\beta)\rangle$ is called a thermal vacuum.

Since $U(\beta)$ is a unitary transformation, the algebra of the original operators a and $\tilde{a}$ is kept invariant, that is, the operators $a(\beta)$ and $\tilde{a}(\beta)$ satisfy the following commutation relations

$$[a(\beta), a^\dagger(\beta)] = 1; \quad [\tilde{a}(\beta), \tilde{a}^\dagger(\beta)] = 1, \tag{6.19}$$

with all the other commutation relations being zero.

The operator $a(\beta)$ can be written in the following form

$$a(\beta) = u(\beta)a - v(\beta)\tilde{a}^\dagger. \tag{6.20}$$

The proof is given by writing

$$a(\beta) = e^{-iG(\beta)}ae^{iG(\beta)}, \tag{6.21}$$

with the aid of the operator relation

$$\begin{aligned} e^{-iB}Ae^{iB} &= A + (-i)[B,A] + \frac{(-i)^2}{2!}[B,[B,A]] \\ &\quad + \frac{(-i)^3}{3!}[B,[B,[B,A]]] + \cdots, \end{aligned} \tag{6.22}$$

and choosing $A = a$ and $B = G$. From Eq. (6.21) we have

$$\begin{aligned} a(\beta) &= (1 + \frac{1}{2!}\theta^2(\beta) + \frac{1}{4!}\theta^4(\beta) + \cdots)a \\ &\quad - (\theta(\beta) + \frac{1}{3!}\theta^3(\beta) + \frac{1}{5!}\theta^5(\beta) + \cdots)\tilde{a}^\dagger \\ &= \cosh\theta(\beta)a - \sinh\theta(\beta)\tilde{a}^\dagger \\ &= u(\beta)a - v(\beta)\tilde{a}^\dagger. \end{aligned} \tag{6.23}$$

A similar relation is derived for $\tilde{a}^\dagger(\beta)$,

$$\tilde{a}^\dagger(\beta) = u(\beta)\tilde{a}^\dagger - v(\beta)a. \tag{6.24}$$

Such a result is proved by using

$$\tilde{a}^\dagger(\beta) = e^{-iG(\beta)}\tilde{a}^\dagger e^{iG(\beta)},$$

or simply using the tilde and the Hermitian conjugation in Eq. (6.20). Then we find, in short, the following set of consistent relations,

$$\begin{aligned}
\tilde{a}^\dagger(\beta) &= u(\beta)\tilde{a}^\dagger - v(\beta)a,\\
a^\dagger(\beta) &= u(\beta)a^\dagger - v(\beta)\tilde{a},\\
a(\beta) &= u(\beta)a - v(\beta)\tilde{a}^\dagger,\\
\tilde{a}(\beta) &= u(\beta)\tilde{a} - v(\beta)a^\dagger.
\end{aligned}$$

Non-thermal operators a and $a^\dagger$ are derived from the thermal ones by inverting these relations. For instance, multiplying Eq. (6.20) by $u(\beta)$ and Eq. (6.24) by $v(\beta)$, that is

$$\begin{aligned}
u(\beta)a(\beta) &= u^2(\beta)a - u(\beta)v(\beta)\tilde{a}^\dagger,\\
v(\beta)\tilde{a}^\dagger(\beta) &= v(\beta)u(\beta)\tilde{a}^\dagger - v^2(\beta)a,
\end{aligned}$$

summing up both of these equations and using Eq. (6.13), we get

$$a = u(\beta)a(\beta) + v(\beta)\tilde{a}^\dagger(\beta). \tag{6.25}$$

In a similar way, or simply taking the tilde or the adjoint or both conjugations of Eq. (6.25), we have

$$\tilde{a} = u(\beta)\tilde{a}(\beta) + v(\beta)a^\dagger(\beta), \tag{6.26}$$

$$a^\dagger = u(\beta)a^\dagger(\beta) + v(\beta)\tilde{a}(\beta), \tag{6.27}$$

$$\tilde{a}^\dagger = u(\beta)\tilde{a}^\dagger(\beta) + v(\beta)a(\beta). \tag{6.28}$$

Such relations are useful in practical calculations. Quite often the physical observables are written as a combination of a and $a^\dagger$. Then it is convenient to write the non-thermal operators in terms of thermal ones. Let us consider, as an example, the average of the number operator $N = a^\dagger a$. We find that

$$\begin{aligned}
n(\beta) &= \langle N\rangle = \langle 0(\beta)|a^\dagger a|0(\beta)\rangle\\
&= \langle 0(\beta)|[u(\beta)a^\dagger(\beta) + v(\beta)\tilde{a}(\beta)][u(\beta)a(\beta) + v(\beta)\tilde{a}^\dagger(\beta)]|0(\beta)\rangle\\
&= v^2(\beta) = \frac{1}{e^{\beta w} - 1},
\end{aligned} \tag{6.29}$$

where we have used $a(\beta)|0(\beta)\rangle = 0$ and $\tilde{a}(\beta)|0(\beta)\rangle = 0$. This is the boson distribution function for a system in thermal equilibrium.

Using Eq. (6.13), we show that

$$a^\dagger(\beta)a(\beta) - \tilde{a}^\dagger(\beta)\tilde{a}(\beta) = a^\dagger a - \tilde{a}^\dagger\tilde{a}. \tag{6.30}$$

Hence the operator $\widehat{H} = H - \widetilde{H}$ is β-independent and is

$$\begin{aligned}\widehat{H}(\beta) &= H(\beta) - \widetilde{H}(\beta) = \omega[a^\dagger(\beta)a(\beta) - \tilde{a}^\dagger(\beta)\tilde{a}(\beta)] \\ &= \omega[a^\dagger a - \tilde{a}^\dagger\tilde{a}] = \widehat{H}.\end{aligned}$$

The thermal Fock space is constructed from the vacuum $|0(\beta)\rangle$, and is spanned by the set of states given by

$$\{\ |0(\beta)\rangle,\ a^\dagger(\beta)|0(\beta)\rangle,\ \ \tilde{a}^\dagger(\beta)|0(\beta)\rangle,\ \dots,\ \frac{1}{\sqrt{n!}}\frac{1}{\sqrt{m!}}\left(a^\dagger(\beta)\right)^n\left(\tilde{a}^\dagger(\beta)\right)^m|0(\beta)\rangle\ \dots\}.$$

From the thermal vacuum and the thermal one-particle state, $a^\dagger(\beta)|0(\beta)\rangle$, we have

$$\begin{aligned}\widehat{H}|0(\beta)\rangle &= 0. \\ \widehat{H}a^\dagger(\beta)|0(\beta)\rangle &= \omega a^\dagger(\beta)|0(\beta)\rangle, \\ \widehat{H}\tilde{a}^\dagger(\beta)|0(\beta)\rangle &= -\omega\tilde{a}^\dagger(\beta)|0(\beta)\rangle, \\ \widehat{H}a^\dagger(\beta)\tilde{a}^\dagger(\beta)|0(\beta)\rangle &= 0.\end{aligned}$$

Let us prove the second relation above:

$$\begin{aligned}\widehat{H}a^\dagger(\beta)|0(\beta)\rangle &= \widehat{H}U(\beta)a^\dagger U^{-1}(\beta)|0(\beta)\rangle \\ &= (\omega a^\dagger a - \omega\tilde{a}^\dagger\tilde{a})U(\beta)a^\dagger U^{-1}(\beta)U(\beta)|0,\tilde{0}\rangle \\ &= \omega[a^\dagger(\beta)a(\beta) - \tilde{a}^\dagger(\beta)\tilde{a}(\beta)]U(\beta)a^\dagger|0,\tilde{0}\rangle \\ &= \omega U(\beta)(a^\dagger a - \tilde{a}^\dagger\tilde{a})U^{-1}(\beta)U(\beta)a^\dagger|0,\tilde{0}\rangle \\ &= \omega U(\beta)(a^\dagger a - \tilde{a}^\dagger\tilde{a})a^\dagger|0,\tilde{0}\rangle \\ &= \omega U(\beta)a^\dagger|0,\tilde{0}\rangle = \omega a^\dagger(\beta)|0(\beta)\rangle.\end{aligned}$$

Similar relations can be derived for states such as $\frac{1}{\sqrt{n!}}\left(a^\dagger(\beta)\right)^n|0(\beta)\rangle$.

The action of the thermal creation operator, in terms of non-thermal operators, on the thermal vacuum is obtained as follows: observe that

$$a^\dagger(\beta)|0(\beta)\rangle = [u(\beta)a^\dagger - v(\beta)\tilde{a}]|0(\beta)\rangle. \tag{6.31}$$

But using $a(\beta)|0(\beta)\rangle = [u(\beta)a - v(\beta)\tilde{a}^\dagger]|0(\beta)\rangle = 0$, we have

$$u(\beta)a|0(\beta)\rangle = v(\beta)\tilde{a}^\dagger|0(\beta)\rangle.$$

With the tilde conjugation rules it follows that

$$v(\beta)\tilde{a}|0(\beta)\rangle = \frac{v^2(\beta)}{u(\beta)}a^\dagger|0(\beta)\rangle.$$

Using this result in Eq. (6.31) we obtain

$$a^\dagger(\beta)|0(\beta)\rangle = \frac{u^2(\beta)a^\dagger - v^2(\beta)a^\dagger}{u(\beta)}|0(\beta)\rangle \tag{6.32}$$

$$= \frac{1}{u(\beta)}a^\dagger|0(\beta)\rangle. \tag{6.33}$$

This shows that the thermal one-particle state $a^\dagger(\beta)|0(\beta)\rangle$ is constructed by adding one particle in the thermal vacuum $|0(\beta)\rangle$, weighted by $u(\beta)$ in order to assure normalization. The generalization of this expression is given by

$$(a^\dagger(\beta))^n|0(\beta)\rangle = \frac{1}{u^n(\beta)}(a^\dagger)^n|0(\beta)\rangle,$$

where we have used $a^\dagger(\beta)a^\dagger = [u(\beta)a^\dagger - v(\beta)\tilde{a}]a^\dagger = a^\dagger a^\dagger(\beta)$.

6.1.4 *Matrix notation*

A condensed doublet notation is introduced by realizing that Eqs. (6.20) and (6.24) can be written as

$$\begin{pmatrix} a(\beta) \\ \tilde{a}^\dagger(\beta) \end{pmatrix} = B(\beta) \begin{pmatrix} a \\ \tilde{a}^\dagger \end{pmatrix}, \tag{6.34}$$

where

$$B(\beta) = \begin{pmatrix} u(\beta) & -v(\beta) \\ -v(\beta) & u(\beta) \end{pmatrix}. \tag{6.35}$$

We introduce a notation to be adopted from now on. Given two arbitrary (boson) operators A and $\widetilde{A}$, a doublet notation is given by

$$(A^a) = \begin{pmatrix} A^1 \\ A^2 \end{pmatrix} = \begin{pmatrix} A \\ \widetilde{A}^\dagger \end{pmatrix}, \tag{6.36}$$

with a tilde transposition given by

$$(\overline{A}^a) = (A^\dagger, -\widetilde{A}). \tag{6.37}$$

In this notation the set of commutation relations given by Eqs. (6.1), (6.5) and (6.19) reads

$$[a^a, \overline{a}^b] = \delta^{ab}; \qquad [a^a(\beta), \overline{a}^b(\beta)] = \delta^{ab}. \tag{6.38}$$

In addition, Eq. (6.34) is

$$a^a(\beta) = B(\beta)_{ab}a^b. \tag{6.39}$$

The inverse transformation is

$$B^{-1}(\beta) = \begin{pmatrix} u(\beta) & v(\beta) \\ v(\beta) & u(\beta) \end{pmatrix},$$

such that

$$a^a = \left(B^{-1}(\beta)\right)_{ab} a^b(\beta).$$

6.2 Fermion oscillators

A fermion (or Dirac) oscillator is a system defined by the Hamiltonian

$$H = wa^\dagger a,$$

where now the operators $a^\dagger$ and a satisfy the algebra

$$\{a^\dagger, a\} = 1, \quad \{a^\dagger, a^\dagger\} = \{a, a\} = 0, \tag{6.40}$$

where $\{A, B\} = AB + BA$ is the anti-commutator. The number operator is $N = a^\dagger a$, with the eigenvalue equation being given by

$$N|n\rangle = n|n\rangle.$$

Notice that we are using here the same notation as for the boson case. Using Eq. (6.40) and the fact that $\langle n|n\rangle = 1$, it can be shown that $n = 0, 1$, such that

$$\begin{aligned} a|0\rangle &= 0, \\ a|1\rangle &= |0\rangle, \\ a^\dagger|0\rangle &= |1\rangle, \\ a^\dagger|1\rangle &= 0. \end{aligned}$$

The Hilbert space is, therefore, generated by two vectors, only: $|0\rangle$ and $|1\rangle$. The energy eigenvalues are then

$$H|n\rangle = \epsilon_n|n\rangle = wn|n\rangle,$$

with $\epsilon_0 = 0$ and $\epsilon_1 = w$.

6.2.1 *Thermal vacuum*

In order to construct TFD for this system, we perform doubling of the degrees of freedom by introducing the tilde operators furnishing the algebra

$$\{\tilde{a}^\dagger, \tilde{a}\} = 1, \quad \{\tilde{a}^\dagger, \tilde{a}^\dagger\} = \{\tilde{a}, \tilde{a}\} = 0,$$

which is a direct consequence of the tilde conjugation rules.

A crucial aspect at this point is to define the relation among tilde and non-tilde variables. According to the construction presented in the previous chapter, observables and generators of symmetry have to satisfy commutations relations, and tilde and non-tilde generators of symmetry commute with each other. However, the operators $a^\dagger$ and a are neither observables nor generators of symmetry, although combination of them can act in this manner. So we are free to choose physically correct relations among tilde and non-tilde fermion variables. A consistent theory is constructed if we define

$$\{a, \tilde{a}\} = \{\tilde{a}^\dagger, a\} = \{a^\dagger, \widetilde{a}\} = \{a^\dagger, \tilde{a}^\dagger\} = 0. \tag{6.41}$$

The doubled system has a vacuum given by $|0,\tilde{0}\rangle$, from which we derive

$$|0,\tilde{1}\rangle = \tilde{a}^\dagger|0,\tilde{0}\rangle,$$
$$|1,\tilde{0}\rangle = a^\dagger|0,\tilde{0}\rangle,$$
$$|1,\tilde{1}\rangle = a^\dagger\tilde{a}^\dagger|0,\tilde{0}\rangle.$$

Therefore, the orthonormalized vectors $|0,\tilde{0}\rangle, |0,\widetilde{1}\rangle, |1,\tilde{0}\rangle$ and $|1,\tilde{1}\rangle$ form a basis which spans the doubled Hilbert space $\mathcal{H}_T$ of the fermion oscillator. Following the approach of Chapter 5, we obtain

$$\begin{aligned}|0(\beta)\rangle &= \frac{1}{\sqrt{Z(\beta)}}\textstyle\sum_n e^{-\beta\varepsilon_n/2}|n,\tilde{n}\rangle \\ &= \frac{1}{\sqrt{Z(\beta)}}(|0,\tilde{0}\rangle + e^{-\beta\varepsilon_1/2}|1,\tilde{1}\rangle) \\ &= \frac{1}{\sqrt{Z(\beta)}}(1+e^{-\beta w/2}a^\dagger\tilde{a}^\dagger)|0,\tilde{0}\rangle.\end{aligned}$$

Using the normalization of the thermal state $\langle 0(\beta)|0(\beta)\rangle = 1$, we get

$$Z(\beta) = 1 + e^{(-\beta w)},$$

resulting in

$$|0(\beta)\rangle = \frac{1}{\sqrt{1+e^{-\beta w}}}(1+e^{-\beta w/2}a^\dagger\tilde{a}^\dagger)|0,\tilde{0}\rangle. \tag{6.42}$$

From the definition of $|0(\beta)\rangle$, the average of the number operator $N = a^\dagger a$ is

$$\begin{aligned}n(\beta) = \langle N\rangle &= \langle 0(\beta)|N|0(\beta)\rangle \\ &= \frac{1}{1+e^{-\beta w}}\langle 0,\tilde{0}|(1+e^{-\beta w/2}\tilde{a}a)a^\dagger a(1+e^{-\beta w/2}a^\dagger\tilde{a}^\dagger)|0,\tilde{0}\rangle \\ &= \frac{e^{-\beta w}}{1+e^{-\beta w}}\langle 0,\tilde{0}|\tilde{a}aa^\dagger aa^\dagger\tilde{a}^\dagger|0,\tilde{0}\rangle \\ &= \frac{1}{1+e^{\beta w}}.\end{aligned}$$

This is the fermion distribution function.

6.2.2 *Bogoliubov transformation*

Following the scheme for bosons, Eq. (6.42) can be written in terms of a unitary transformation. Indeed, we define

$$u(\beta) = \cos\theta = \frac{1}{\sqrt{1+e^{-\beta w}}},$$
$$v(\beta) = \sin\theta = \frac{1}{\sqrt{1+e^{\beta w}}},$$

such that

$$u(\beta)^2 + v(\beta)^2 = \cos^2\theta + \sin^2\theta = 1,$$

and

$$|0(\beta)\rangle = (\cos\theta + \sin\theta a^\dagger \tilde{a}^\dagger)|0,\tilde{0}\rangle \tag{6.43}$$

Using the property

$$(\tilde{a}a - a^\dagger\tilde{a}^\dagger)^n|0,\widetilde{0}\rangle = (-1)^n|0,\tilde{0}\rangle,$$

and expanding $\cos\theta$ and $\sin\theta$ in Eq. (6.43), we write

$$\begin{aligned}|0(\beta)\rangle &= [1-\theta(\tilde{a}a - a^\dagger\tilde{a}^\dagger) + \frac{\theta^2}{2!}(\tilde{a}a - a^\dagger\tilde{a}^\dagger)^2 + \cdots]|0,\tilde{0}\rangle \\ &= U(\beta)|0,\tilde{0}\rangle,\end{aligned} \tag{6.44}$$

where

$$U(\beta) = e^{-iG}, \tag{6.45}$$

with

$$G = -i\theta(\tilde{a}a - a^\dagger\tilde{a}^\dagger).$$

Note that the ordering of the operators in these expressions is important since $\tilde{a}$ and a anticommute with one another. This is the main motive for choosing the definition given in Eq. (6.41).

6.2.3 *Thermal operators*

The thermal operators are introduced through the relations

$$\begin{aligned}a(\beta) &= U(\beta)aU^\dagger(\beta), \\ a^\dagger(\beta) &= U(\beta)a^\dagger U^\dagger(\beta), \\ \tilde{a}(\beta) &= U(\beta)\tilde{a}U^\dagger(\beta), \\ \tilde{a}^\dagger(\beta) &= U(\beta)\tilde{a}^\dagger U^\dagger(\beta).\end{aligned}$$

Therefore we have

$$\begin{aligned}a(\beta)|0(\beta)\rangle &= U(\beta)aU^\dagger(\beta)U(\beta)|0,\widetilde{0}\rangle \\ &= U(\beta)a|0,\tilde{0}\rangle = 0,\end{aligned}$$

and $\tilde{a}(\beta)|0(\beta)\rangle = 0$. Then $|0(\beta)\rangle$ is a vacuum for fermion operators $a(\beta)$ and $\tilde{a}(\beta)$, but it is not a vacuum for a and $\tilde{a}$.

Since $U(\beta)$ is an unitary transformation, the algebra of the original operators a and $\tilde{a}$ is kept invariant, that is, the operators $a(\beta)$ and $\tilde{a}(\beta)$ satisfy the following anticommutation relations

$$\{a(\beta), a^\dagger(\beta)\} = 1 \text{ and } \{\tilde{a}(\beta), \tilde{a}^\dagger(\beta)\} = 1, \tag{6.46}$$

with all the other anticommutation relations being zero.

Expanding the unitary operator U, thermal operators are written as,

$$a(\beta) = u(\beta)a - v(\beta)\tilde{a}^\dagger, \tag{6.47}$$
$$\tilde{a}(\beta) = u(\beta)\tilde{a} + v(\beta)a^\dagger, \tag{6.48}$$
$$a^\dagger(\beta) = u(\beta)a^\dagger - v(\beta)\tilde{a}, \tag{6.49}$$
$$\tilde{a}^\dagger(\beta) = u(\beta)\tilde{a}^\dagger + v(\beta)a, \tag{6.50}$$

Note that Eqs. (6.47) and (6.50) are not compatible with the tilde conjugation rules. For instance, taking the tilde conjugation of Eq. (6.47) we do not get Eq. (6.48). However, since $a^\dagger$ and a are not elements of a thermo-algebra, we can also assume, without contradiction or loss of generality, that

$$\tilde{\tilde{a}} = -a$$

for fermions. Now the tilde conjugation rules give a consistent result.

The Fock space is constructed from of the vacuum $|0(\beta)\rangle$, and is spanned by the set of states given by

$$\{\ |0(\beta)\rangle,\ a^\dagger(\beta)|0(\beta)\rangle,\ \tilde{a}^\dagger(\beta)|0(\beta)\rangle,\ a^\dagger(\beta)\tilde{a}^\dagger(\beta)|0(\beta)\rangle\ \}.$$

The operator $\widehat{H} = H - \widetilde{H}$ is invariant under the Bogoliubov transformation, i.e.

$$\begin{aligned}\widehat{H}(\beta) &= H(\beta) - \widetilde{H}(\beta) = \omega[a^\dagger(\beta)a(\beta) - \tilde{a}^\dagger(\beta)\tilde{a}(\beta)] \\ &= \omega[a^\dagger a - \tilde{a}^\dagger\tilde{a}] = \widehat{H}.\end{aligned}$$

From the thermal vacuum $|0(\beta)\rangle$ and the thermal one-particle state, $a^\dagger(\beta)|0(\beta)\rangle$, we have

$$\begin{aligned}\widehat{H}|0(\beta)\rangle &= 0. \\ \widehat{H}a^\dagger(\beta)|0(\beta)\rangle &= \omega a^\dagger(\beta)|0(\beta)\rangle, \\ \widehat{H}\tilde{a}^\dagger(\beta)|0(\beta)\rangle &= -\omega\tilde{a}^\dagger(\beta)|0(\beta)\rangle, \\ \widehat{H}a^\dagger(\beta)\tilde{a}^\dagger(\beta)|0(\beta)\rangle &= 0.\end{aligned}$$

It is to be noted that

$$u(\beta)a|0(\beta)\rangle = v(\beta)\tilde{a}^\dagger|0(\beta)\rangle \tag{6.51}$$

and

$$a^\dagger(\beta)|0(\beta)\rangle = \frac{u^2(\beta)a^\dagger + v^2(\beta)a^\dagger}{u(\beta)}|0(\beta)\rangle = \frac{1}{u(\beta)}a^\dagger|0(\beta)\rangle$$

6.2.4 *Matrix notation*

The matrix notation in the case of fermions is introduced from Eqs. (6.47)–(6.50) by writing

$$\begin{pmatrix} a(\beta) \\ \tilde{a}^\dagger(\beta) \end{pmatrix} = B(\beta) \begin{pmatrix} a \\ \tilde{a}^\dagger \end{pmatrix}, \tag{6.52}$$

where

$$B(\beta) = \begin{pmatrix} u(\beta) & -v(\beta) \\ v(\beta) & u(\beta) \end{pmatrix}. \tag{6.53}$$

Therefore, for fermion operators A and $\widetilde{A}$, the doublet notation is given by

$$(A^a) = \begin{pmatrix} A^1 \\ A^2 \end{pmatrix} = \begin{pmatrix} A \\ \widetilde{A}^\dagger \end{pmatrix}, \tag{6.54}$$

with the tilde transposition

$$(\overline{A}^a) = (A^\dagger, \widetilde{A}). \tag{6.55}$$

In this case, the set of anti-commutation relations reads

$$\{a^a, \overline{a}^b\} = \delta^{ab}; \quad \{a^a(\beta), \overline{a}^b(\beta)\} = \delta^{ab}. \tag{6.56}$$

The Bogoliubov transformation, Eq. (6.53), is given by

$$a^a(\beta) = B^{ab}(\beta) a^b. \tag{6.57}$$

The inverse of Eqs. (6.47)–(6.50), is given as

$$a = u(\beta)a(\beta) + v(\beta)\tilde{a}^\dagger(\beta), \tag{6.58}$$
$$\tilde{a} = u(\beta)\tilde{a}(\beta) - v(\beta)\tilde{a}^\dagger(\beta), \tag{6.59}$$
$$a^\dagger = u(\beta)a^\dagger(\beta) + v(\beta)\tilde{a}(\beta), \tag{6.60}$$
$$\tilde{a}^\dagger = u(\beta)\tilde{a}^\dagger(\beta) - v(\beta)a(\beta). \tag{6.61}$$

such that

$$\begin{pmatrix} a \\ \tilde{a}^\dagger \end{pmatrix} = B^{-1}(\beta) \begin{pmatrix} a(\beta) \\ \tilde{a}^\dagger(\beta) \end{pmatrix},$$

with

$$B^{-1}(\beta) = \begin{pmatrix} u(\beta) & v(\beta) \\ -v(\beta) & u(\beta) \end{pmatrix}.$$

Notice that, as we have already done, we are using here the same notation as in the case of bosons. The results derived in this chapter are concerned with one boson or one fermion mode. However, we can generalize this for an arbitrary number of modes. This will be important, in particular, to write the thermal propagator for a quantum field.

6.3 TFD and spin 1/2 lattices

The TFD formalism can be used for spin systems. Here we specify it to consider spin 1/2 particles.

6.3.1 *Boson representation for the SU(2) algebra*

In this subsection we consider the construction of the TFD approach for a system of particles (or sites in a lattice) of spin 1/2. At first we consider one site described by the $SU(2)$ algebra,

$$[s_i, s_j] = i\epsilon_{ijk}s_k. \tag{6.62}$$

A boson representation of the $SU(2)$ algebra [107] provides an alternative algebraic approach to study spin-1/2 systems [18, 74, 108]. Let us first introduce

$$S_\pm = (s_1 \pm is_2) \quad \text{and} \quad S_0 = s_3,$$

such that for each spin variable we have,

$$[S_0, S_\pm] = \pm S_\pm, \tag{6.63}$$

$$[S_+, S_-] = 2S_0. \tag{6.64}$$

Define then

$$\begin{aligned} S_+ &= a_1^\dagger a_2 \\ S_- &= a_2^\dagger a_1 \\ S_0 &= \frac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2), \end{aligned}$$

with a_1 and a_2 furnishing a double boson algebra, that is

$$[a_1, a_1^\dagger] = 1,, \quad [a_2, a_2^\dagger] = 1, \tag{6.65}$$

with all the other commutation relations being zero.

The number operators, $N_1 = a_1^\dagger a_1$ and $N_2 = a_2^\dagger a_2$, satisfy

$$N_1|n_1, n_2\rangle = n_1|n_1, n_2\rangle, \;\; N_2|n_1, n_2\rangle = n_2|n_1, n_2\rangle,$$

where

$$|n_1, n_2\rangle = \frac{1}{(n_1!n_2!)^{1/2}}(a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}|0, 0\rangle.$$

Other useful results are

$$S_+|n_1, n_2\rangle = \sqrt{n_2(n_1+1)}\,|n_1+1, n_2-1\rangle, \tag{6.66}$$

$$S_-|n_1, n_2\rangle = \sqrt{n_1(n_2+1)}\,|n_1-1, n_2+1\rangle, \tag{6.67}$$

$$S_0|n_1, n_2\rangle = \frac{1}{2}(n_1 - n_2)|n_1, n_2\rangle. \tag{6.68}$$

The connection with the original $SU(2)$ algebra emerges if it is assumed that

$$n_1 = s + m, \;\; n_2 = s - m;$$

where s and m are related to the usual results:

$$\begin{aligned} \mathbf{s}^2|s, m\rangle &= s(s+1)|s, m\rangle, \\ s_3|s, m\rangle &= m|s, m\rangle, \end{aligned}$$

and s and s_3 are respectively the total and the z-component of spin. In the case of spin 1/2, we need to consider $s = 1/2$ and $m = 1/2$ and $-1/2$. In terms of the two bosonic spectra we have $n_1 = 0, 1$ and $n_2 = 0, 1$. As a consequence, the action of S_+ and S_- on such states is

$$S_+|s, m\rangle = S_+|n_1, n_2\rangle, \tag{6.69}$$
$$S_-|s, m\rangle = S_-|n_1, n_2\rangle, \tag{6.70}$$

such that,

$$n_1 = 0, n_2 = 1 \;\Rightarrow\; m = -1/2$$
$$n_1 = 1, n_2 = 0 \;\Rightarrow\; m = 1/2,$$

i.e.

$$S_+|1/2, -1/2\rangle \equiv S_+|n_1 = 0, n_2 = 1\rangle = |1, 0\rangle, \tag{6.71}$$
$$S_+|1/2, 1/2\rangle \equiv S_+|n_1 = 1, n_2 = 0\rangle = 0, \tag{6.72}$$
$$S_-|1/2, -1/2\rangle \equiv S_-|n_1 = 0, n_2 = 1\rangle = 0, \tag{6.73}$$
$$S_-|1/2, 1/2\rangle = S_-|n_1 = 1, n_2 = 0\rangle = |0, 1\rangle, \tag{6.74}$$

It is to be noted that

$$S_-|n_1, n_2\rangle = |n_1 = 0, n_2 = 1\rangle = 0, \tag{6.75}$$

that is, the state $|n_1 = 0, n_2 = 1\rangle = |0_a\rangle$ is the vacuum state for S_-. Now we are in a position to develop TFD for an N spin-1/2 system.

6.3.2 *Thermo-SU(2) algebra*

Using the tilde conjugations rules we proceed to the doubling of the $su(2)$ algebra, resulting in

$$[S_0, S_\pm] = \pm S_\pm, \tag{6.76}$$
$$[S_+, S_-] = 2S_0, \tag{6.77}$$
$$[\widetilde{S}_0, \widetilde{S}_\pm] = \pm \widetilde{S}_\pm, \tag{6.78}$$
$$[\widetilde{S}_+, \widetilde{S}_-] = 2\widetilde{S}_0. \tag{6.79}$$

There exists a doubling of the bosonic representation of this algebra; and so we consider this auxiliary bosonic system as our primary system.

A thermal Bogoliubov transformation is introduced by

$$U(\beta) = e^{-iG(\theta(\beta))},$$

such that generators $G(\theta(\beta)) = G(\theta)$ furnish an $su(2)$ algebra, in agreement with the usual TFD formulation for bosons. The two vacua of the doubled spin vacuum $|0, \tilde{0}\rangle$ is given by $|0, \tilde{0}\rangle = |0, 1\rangle \otimes |\tilde{0}, \tilde{1}\rangle$. Now we have to find an explicit expression for $U(\beta)$.

The unitary operator $U(\beta)$ is assumed to be a canonical transformation for the algebra describing the physical system, such that the TFD thermal operators are now given by

$$\begin{aligned}
S_+(\beta) &= U(\beta)S_+U^{-1}(\beta),\\
S_-(\beta) &= U(\beta)S_-U^{-1}(\beta),\\
\widetilde{S}_+(\beta) &= U(\beta)\widetilde{S}_+U^{-1}(\beta),\\
\widetilde{S}_-(\beta) &= U(\beta)\widetilde{S}_-U^{-1}(\beta).\\
S_0(\beta) &= U(\beta)S_0U^{-1}(\beta),\\
\widetilde{S}_0(\beta) &= U(\beta)\widetilde{S}_0U^{-1}(\beta).
\end{aligned}$$

It is easy to show that the thermal operators $S_+(\beta), S_-(\beta), \widetilde{S}_+(\beta), \widetilde{S}_-(\beta), S_0(\beta)$ and $\widetilde{S}_0(\beta)$ provide a representation for the $su(2)_T$ algebra, given by Eq. (6.76) to (6.79).

The thermal operators satisfy the condition below of destroying the thermal vacuum,

$$S_-(\beta)|0(\beta)\rangle = 0 \quad \text{and} \quad \widetilde{S}_-(\beta)|0(\beta)\rangle = 0,$$

where the thermal vacuum $|0(\beta)\rangle$ is defined by

$$|0(\beta)\rangle = U(\beta)|0,\tilde{0}\rangle = U(\beta)(|0,1\rangle\otimes|\tilde{0},\tilde{1}\rangle);$$

satisfying the normalization condition

$$\langle 0(\beta)|0(\beta)\rangle = 1.$$

The thermal average of an observable, say A, is specified by

$$\langle A\rangle = \langle 0(\beta)|A|0(\beta)\rangle.$$

From these recipes, we infer an explicit definition of $U(\beta)$ for the N-spin system; that is, we write

$$\begin{aligned}
U(\beta) &= \exp\left[\sum_{r=1}^{N}\theta_r(\beta)(\tilde{a}^\dagger_{r,1}a^\dagger_{r,1}a_{r,2}\tilde{a}_{r,2} - a^\dagger_{r,2}\tilde{a}^\dagger_{r,2}a_{r,1}\tilde{a}_{r,1})\right]\\
&= \exp\left[\sum_{r=1}^{N}\theta_r(\beta)(S_{+,r}\widetilde{S}_{+,r} - S_{-,r}\widetilde{S}_{-,r})\right].
\end{aligned}$$

Using the following properties

$$\begin{aligned}
(\widetilde{S}_-S_- - \widetilde{S}^\dagger_+S^\dagger_+)^{2n}|0,\tilde{0}\rangle &= (-1)^n|0,\tilde{0}\rangle,\\
(\widetilde{S}_-S_- - \widetilde{S}^\dagger_+S^\dagger_+)^{2n+1}|0,\tilde{0}\rangle &= (-1)^{n+1}|0,\tilde{0}\rangle,\ \ n=0,1,2,\cdots,
\end{aligned}$$

derived from Eqs. (6.71)–(6.74), it leads to

$$|0(\beta)\rangle = U(\beta)|0,\tilde{0}\rangle = \prod_{i=1}^{N}(\cos\theta + \sin\theta\widetilde{S}^\dagger_{+,i}S^\dagger_{+,i})|0,\widetilde{0}\rangle.$$

As an example, consider a non-interacting N-particle spin-1/2 system in an external magnetic field h described by the Hamiltonian

$$H_0 = \mu h \sum_{r=1}^{N} s_{3,r}$$

where μ is the magnetic moment. Since we are taking the spin system as a bosonic system, we assume that

$$\cosh\theta = \frac{1}{\sqrt{1-e^{-\beta\omega}}},$$
$$\sinh\theta = \frac{e^{-\beta\omega}}{\sqrt{1-e^{-\beta\omega}}},$$

where $\omega = \frac{1}{2}\mu h$. Hence we derive the usual result for the magnetization density

$$m = \langle 0(\beta)|s_3|0(\beta)\rangle = \frac{1}{2}\tanh(\frac{1}{2}\beta\mu h).$$

This simple illustration shows how to use such an algebraic approach to treat a spin system. Here, we do not intend to go much further. However, it should be of interest to point out that we can use this boson formulation to introduce the Green functions and diagrammatic approaches to treat spins 1/2 systems. For instance, consider the average $\langle S_+S_-\rangle = \langle 0(\beta)|S_+S_-|0(\beta)\rangle$. Using $S_+ = a_1^\dagger a_2$ and $S_- = a_2^\dagger a_1$, we write

$$\langle S_+S_-\rangle = \langle 0(\beta)|a_1^\dagger a_2 a_2^\dagger a_1|0(\beta)\rangle.$$

Then we can proceed with the definition of a time-ordered product and the thermal propagator as is usual for boson systems, and write

$$\begin{aligned}\langle S_+S_-\rangle &= \lim_{t\to t'}\langle S_+(t)S_-(t')\rangle \\ &= \lim_{t\to t'}\langle 0(\beta)|T[a_1^\dagger(t)a_2(t)a_2^\dagger(t')a_1(t')]|0(\beta)\rangle \\ &= \lim_{t\to t'}\langle 0(\beta)|T[a_1^\dagger(t)a_1(t')a_2(t)a_2^\dagger(t')]|0(\beta)\rangle,\end{aligned}$$

where T is the time-ordering operator.

Here we have analyzed the case with one mode. It can be extended to the multi-mode case and to the field theory. And in Chapters 12 and 13 we will consider thermalized states of a boson oscillator and physical implications will become clear.

Chapter 7

Thermal Poincaré and Galilei Groups

The importance of symmetry groups for non-thermal field theories is a fact without question, and this aspect has already been emphasized in Chapter 4. In Chapter 5, using the notion of thermoalgebra, we presented a derivation of thermal theories based on general arguments of symmetry, opening the possibility to bring to the realm of thermal systems the representation theory for Lie symmetries. This provides not only a strong basis for the thermal quantum field theory, but also for statistical mechanics, since we can derive the Liouville-von Neumann equation. In the present chapter we develop representations of the Poincaré and Galilei groups, taking the notion of thermoalgebra as the key concept [87]. We begin reviewing some aspects of the Poincaré group, and then we proceed with the derivation of relativistic density matrices. Tilde and non-tilde Lagrangians are then derived preparing the way to study the introduction of temperature associated with a quantum field via a Bogoliubov transformation. The Galilei group results from a contraction of the Poincaré group. The representations of this group are studied at the end of the chapter.

7.1 The Poincaré group

The Poincaré group or the inhomogeneous Lorentz group, is the Lorentz group plus translations in the Minkowski space; the general transformation is written as

$$x'^{\mu} = \Lambda^{\mu}{}_{\nu} x^{\nu} + a^{\mu},$$

with $\det \Lambda = 1$. The generators of the symmetry are

$$M^{\mu\nu} = i(x^{\mu}\partial^{\nu} - x^{\nu}\partial^{\mu}), \quad P_{\mu} = i\partial_{\mu}.$$

These relations are checked by observing that for the Lorentz group we have

$$S(\Lambda)f(x) = \exp(-i\omega_{\mu\nu}M^{\mu\nu})f(x) = f(x^{\mu} + \omega^{\mu}{}_{\nu}x^{\nu})$$

and for the translations,

$$S(\Lambda)f(x) = \exp(-ia^{\mu}P_{\mu})f(x) = f(x^{\mu} + a^{\nu}).$$

This defines a representation of the Poincaré group [109, 110], which is used to find all its algebraic properties. The Lie algebra for generators of symmetry is

$$[M_{\mu\nu}, M_{\sigma\rho}] = -i(g_{\mu\rho}M_{\nu\sigma} - g_{\nu\rho}M_{\mu\sigma} + g_{\mu\sigma}M_{\rho\nu} - g_{\nu\sigma}M_{\rho\mu}),$$
$$[M_{\mu\nu}, P_{\sigma}] = i(g_{\nu\sigma}P_{\mu} - g_{\sigma\mu}P_{\nu}),$$

with all the other commutation relations being zero. This is the Poincaré-Lie algebra, denoted by $\mathfrak{p}$.

The invariants of this algebra are derived from the Pauli-Lubanski matrices defined by $w_\mu = \frac{1}{2}\varepsilon_{\mu\nu\rho\sigma}M^{\nu\sigma}P^{\rho}$, where $\varepsilon_{\mu\nu\rho\sigma}$ is the Levi-Civita symbol. The invariants are $w^2 = w_\mu w^\mu$ and $P^2 = P_\mu P^\mu$. An invariant is a multiple of the identity operator, thus each value is a characteristic of the representation. A simple representation of this algebra is constructed by taking $\omega = 0$ and $P^2 = k^2 I$, where I is the identity operator and k is a c-number. Interpreting P as the momentum, the relation $P^2 = k^2 I$ means the mass shell condition, and $k \equiv m$. Considering the Hilbert space defined by Lorentz-scalar functions, as the space carrying representations of the group, that is, where the generators are defined to act as operators, then we have $P^2\phi(x) = m^2\phi(x)$. The explicit representation for P^2 as a unitary operator, using $P_\mu = -i\partial_\mu$, leads to the Klein-Gordon equation,

$$(\Box + m^2)\phi(x) = 0.$$

The general form of the invariant w^2 is

$$w^2 = -m^2 s(s+1)$$

where s is the spin value. When we take $w^2 = 0$, then $s = 0$, i.e. a scalar field. Such an equation describes massive spin-zero particles. For $\omega^2 \neq 0$ it can be shown [12] that only integral and half-integral spins are possible.

7.2 Relativistic density matrices

The thermo-algebra associated to the Poincaré group [87], denoted by $\mathfrak{p}_T$, is

$$[M_{\mu\nu}, P_{\sigma}] = i(g_{\nu\sigma}P_{\mu} - g_{\sigma\mu}P_{\nu}), \tag{7.1}$$
$$[P_{\mu}, P_{\nu}] = 0, \tag{7.2}$$
$$[M_{\mu\nu}, M_{\sigma\rho}] = -i(g_{\mu\rho}M_{\nu\sigma} - g_{\nu\rho}M_{\mu\sigma} + g_{\mu\sigma}M_{\rho\nu} - g_{\nu\sigma}M_{\rho\mu}), \tag{7.3}$$
$$[\widehat{M}_{\mu\nu}, P_{\sigma}] = [M_{\mu\nu}, \widehat{P}_{\sigma}] = i(g_{\nu\sigma}P_{\mu} - g_{\sigma\mu}P_{\nu}), \tag{7.4}$$
$$[\widehat{P}_{\mu}, P_{\nu}] = 0, \tag{7.5}$$
$$[M_{\mu\nu}, \widehat{M}_{\sigma\rho}] = -i(g_{\mu\rho}M_{\nu\sigma} - g_{\nu\rho}M_{\mu\sigma} + g_{\mu\sigma}M_{\rho\nu} - g_{\nu\sigma}M_{\rho\mu}), \tag{7.6}$$
$$[\widehat{M}_{\mu\nu}, \widehat{P}_{\sigma}] = i(g_{\nu\sigma}\widehat{P}_{\mu} - g_{\sigma\mu}\widehat{P}_{\nu}), \tag{7.7}$$
$$[\widehat{P}_{\mu}, \widehat{P}_{\nu}] = 0, \tag{7.8}$$
$$[\widehat{M}_{\mu\nu}, \widehat{M}_{\sigma\rho}] = -i(g_{\mu\rho}\widehat{M}_{\nu\sigma} - g_{\nu\rho}\widehat{M}_{\mu\sigma} + g_{\mu\sigma}\widehat{M}_{\rho\nu} - g_{\nu\sigma}\widehat{M}_{\rho\mu}), \tag{7.9}$$

where $\widehat{M}_{\mu\nu}$ stands for the generator of rotations and $\widehat{P}_\mu$ for translations in the Minkowski space. This algebra is written in a short notation by

$$\begin{array}{ll}
[\mathbf{M},\mathbf{P}] = i\mathbf{P}, & [\widehat{\mathbf{M}},\mathbf{M}] = i\mathbf{M} \\
[\mathbf{P},\mathbf{P}] = 0, & [\widehat{\mathbf{M}},\widehat{\mathbf{P}}] = i\widehat{\mathbf{P}}, \\
[\mathbf{M},\mathbf{M}] = i\mathbf{M}, & [\widehat{\mathbf{M}},\widehat{\mathbf{M}}] = i\widehat{\mathbf{M}}. \\
[\widehat{\mathbf{M}},\mathbf{P}] = i\mathbf{P}, & [\widehat{\mathbf{P}},\widehat{\mathbf{P}}] = 0, \\
[\widehat{\mathbf{P}},\mathbf{P}]=0. &
\end{array}$$

The invariants of $\mathfrak{p}_T$ are

$$w^2 = w_\mu w^\mu, \tag{7.10}$$

$$P^2 = P_\mu P^\mu = m^2, \tag{7.11}$$

$$\widehat{w^2} = 2\widehat{w}_\mu w^\mu - \widehat{w}_\mu \widehat{w}^\mu, \tag{7.12}$$

$$\widehat{P^2} = 2\widehat{P}_\mu P^\mu - \widehat{P}_\mu \widehat{P}^\mu; \tag{7.13}$$

where

$$\widehat{w}_\mu = \frac{1}{2}\varepsilon_{\mu\nu\rho\sigma}\widehat{M}^{\ \nu\sigma}P^\rho + \frac{1}{2}\varepsilon_{\mu\nu\rho\sigma}M^{\nu\sigma}\widehat{P}^\rho - \frac{1}{2}\varepsilon_{\mu\nu\rho\sigma}\widehat{M}^{\ \nu\sigma}\widehat{P}^\rho.$$

The vector

$$\overline{w}_\mu = \frac{1}{2}\varepsilon_{\mu\nu\rho\sigma}\widehat{M}^{\ \nu\sigma}\widehat{P}^\rho$$

is used to define the scalar $\overline{w}^2 = \overline{w}_\mu \overline{w}^\mu$, which is not an invariant of $\mathfrak{p}_T$ but rather that of the subalgebra of the hat operators, Eqs. (7.7)-(7.9). Using the definition of the hat variables, it is established that

$$\begin{aligned}
\widehat{w^2} &= (w_\mu w^\mu)\widehat{\ } \\
&= w_\mu w^\mu - (w_\mu w^\mu)\widetilde{\ } \\
&= w_\mu w^\mu - \widetilde{w}_\mu \widetilde{w}^\mu,
\end{aligned} \tag{7.14}$$

and

$$\widehat{P^2} = P_\mu P^\mu - \widetilde{P}_\mu \widetilde{P}^\mu. \tag{7.15}$$

Representations for $\mathfrak{p}_T$ are built from the Casimir invariants, $\widehat{w^2}$ and $\widehat{P^2}$. From the definition of tilde variables, $\widetilde{\mathbf{P}} = \mathbf{P} - \widehat{\mathbf{P}}$ and $\widetilde{\mathbf{M}} = \mathbf{M} - \widehat{\mathbf{M}}$, non-null commutation relations for the algebra $\mathfrak{p}_T$ are

$$\begin{aligned}
[\mathbf{M},\mathbf{P}] &= i\mathbf{P}, \\
[\mathbf{M},\mathbf{M}] &= i\mathbf{M}, \\
[\widetilde{\mathbf{M}},\widetilde{\mathbf{P}}] &= -i\widetilde{\mathbf{P}}, \\
[\widetilde{\mathbf{M}},\widetilde{\mathbf{M}}] &= -i\widetilde{\mathbf{M}}.
\end{aligned}$$

This is the direct sum of two algebras. Therefore there will be only two invariants $\widetilde{m}$ and m. By definition of the tilde operation, with m being real, we have $\widetilde{m} = m$.

7.2.1 *Bosons*

Using the Hilbert space for TFD (Chapter 5), the invariants $P_\mu P^\mu$ and $\widetilde{P}_\mu \widetilde{P}^\mu$, are

$$[(P^2 - m^2) \otimes 1]|\phi(t)\rangle = 0, \tag{7.16}$$

and

$$[1 \otimes (P^2 - m^2)]|\phi(t)\rangle = 0,$$

where $|\phi(t)\rangle$ is chosen as

$$|\phi(t)\rangle = \rho(\phi) \otimes 1|I\rangle, \tag{7.17}$$

with $|I\rangle = \sum_n |n, \widetilde{n}\rangle$ and $\rho(\phi) = |\phi\rangle\langle\phi|$. This defines the TFD representation for the states $|\phi\rangle$.

Two equations are associated with the two invariants $P^2 \equiv -\Box$ and $\widehat{P^2} \equiv -\widehat{\Box}$. For the observable P^2, we have

$$(P^2 - m^2)|\phi\rangle = (P^2 - m^2)\rho(\phi) \otimes 1|I\rangle = 0, \tag{7.18}$$

resulting in

$$(P^2 - m^2)|\phi\rangle\langle\phi| = 0,$$

or

$$(P^2 - m^2)|\phi\rangle = 0.$$

Using the $|x\rangle$ basis, $\langle x|\phi\rangle = \phi(x)$

$$\langle x|(P^2 - m^2)|\phi\rangle = \int d^4x' \left[\langle x|P^2\, x'\rangle\langle x'|\phi\rangle - m^2\langle x|x'\rangle\langle x'|\phi\rangle\right],$$

we get the Klein-Gordon equation,

$$(\Box^2 + m^2)\phi(x) = 0.$$

The physical content here is that the observable (the non-hat variable) satisfies the mass-shell condition.

For the generator $\widehat{P^2}$ we have

$$\begin{aligned}\widehat{P^2}|\phi\rangle &= -(\Box \otimes 1 - 1 \otimes \Box)|\phi\rangle \\ &= -(\Box\rho(\phi) - \rho(\phi)\Box) \otimes 1|I\rangle = 0,\end{aligned} \tag{7.19}$$

then the Liouville-von Neumann equation for $\rho(\phi)$ follows,

$$[\Box, \rho(\phi)] = 0. \tag{7.20}$$

The content of the Liouville-von Neumann equation is realized by multiplying Eq. (7.20) by $|\phi\rangle$, resulting in

$$(\Box|\phi\rangle\langle\phi| - |\phi\rangle\langle\phi|\Box)|\phi\rangle = (\Box|\phi\rangle\langle\phi|\phi\rangle - |\phi\rangle\langle\phi|\Box|\phi\rangle = 0.$$

Since $\langle\phi|\Box|\phi\rangle = -m^2$ and $\langle\phi|\phi\rangle = 1$, we derive the Klein-Gordon equation for $|\phi\rangle$. Using, on the other hand, the bra vector, $\langle\phi|$, the Klein-Gordon equation in the dual Hilbert space is obtained from Eq. (7.20),

$$\langle\phi|(\Box|\phi\rangle\langle\phi| - |\phi\rangle\langle\phi|\Box) = \langle\phi|(m^2 + \Box) = 0.$$

This result shows that Eq. (7.20) is equivalent to a density matrix equation for the Klein-Gordon field $\phi(x)$.

7.2.2 *Fermions*

In order to construct a spinor density-matrix, we introduce the invariant equation

$$(\alpha^\mu P_\mu)\widehat{\ }|\Psi\rangle = 0, \tag{7.21}$$

such that,

$$(\alpha^\mu P_\mu)\widehat{\ }(\alpha^\mu P_\mu)\widehat{\ } = \widehat{P^2}. \tag{7.22}$$

With the condition given by Eq. (7.19), a generic solution is found to be

$$\alpha^\mu = \sigma\gamma^\mu, \tag{7.23}$$

where γ^μ are Dirac matrices, and σ is some non-null Lorentz invariant to be specified. A trivial choice is $\sigma = 1$. Then we find $(\gamma^\mu P_\mu)\widehat{\ }\ \ |\Psi\rangle = 0$, or

$$(\gamma^\mu P_\mu)|\Psi\rangle \otimes \langle\bar{\Psi}| - |\Psi\rangle \otimes \langle\bar{\Psi}|(\gamma^\mu P_\mu)^\dagger = 0. \tag{7.24}$$

where now $|\Psi\rangle$ is a 16-component spinor, and $|\psi\rangle(\langle\bar{\psi}|)$ is the 4-component (dual) Dirac spinor.

Multiplying the right hand side of Eq. (7.24) by $|\Psi\rangle$, it results in $(\gamma^\mu P_\mu - m)\ |\Psi\rangle = 0$, the Dirac equation. Now, multiplying the left hand side of Eq. (7.24) by $\langle\bar{\Psi}|$ it results in $\langle\bar{\Psi}|(P_\mu\gamma^\mu - m) = 0$, the conjugate Dirac equation. In this sense, in fact, Eq. (7.24) is a density matrix equation for the Dirac field.

Looking ahead for solutions, we note that Eq. (7.24) is invariant under the unitary transformation [18]

$$\widehat{(\gamma^\mu P_\mu)'}\ = U\ \widehat{(\gamma^\mu P_\mu)}\ \ U^{-1}, \tag{7.25}$$

and

$$|\Psi\rangle' = U|\Psi\rangle. \tag{7.26}$$

Then Eq. (7.24) reads

$$\widehat{(\gamma^\mu P_\mu)'}\ |\Psi\rangle' = 0. \tag{7.27}$$

On the other hand, if $[U, (\gamma^\mu P_\mu)\widehat{\ }\ ] = 0$ then $|\Psi\rangle'$ given in Eq. (7.26) is a solution of Eq. (7.24). In this case, an example is provided by $U = U(y^\mu \widehat{P}_\mu)$ written in the form

$$U = U(y\widehat{P}) = \exp[-iy\widehat{P}], \tag{7.28}$$

where y is the transformation parameter. Accordingly, Eq. (7.26) reads

$$|\Psi\rangle' \to \exp(-iyP)|\phi\rangle \otimes \langle\bar{\phi}|\exp(iyP^\dagger).$$

The gauge invariance can be considered if we write

$$P_\mu \quad \to \quad -iD_\mu = p_\mu + gA_\mu,$$

where D_μ is the usual covariant derivative. Then

$$|\Psi\rangle' \to \exp(-yD)|\phi\rangle \otimes \langle\bar{\phi}|\exp(yD^\dagger). \tag{7.30}$$

where $\otimes$ involves, in a general situation, spin and color indices in non-abelian gauge theory. This function is a solution of the density matrix equation, which is derived from Eq. (7.24), but rather considering the gauge field, that is

$$[(\gamma^\mu D_\mu) \otimes 1 - 1 \otimes (\gamma^\mu D_\mu)]|\phi\rangle \otimes \langle\bar{\phi}| = 0. \tag{7.31}$$

If we use the definition given by Eq. (7.17), then we write $\langle x, x'|\Psi\rangle = \Psi(x, x')$, such that Eq. (7.30) is

$$\Psi(x, y) = \exp\left[-yD(x)\right]\ \phi(x) \otimes \bar{\phi}(x)\ \exp\left[yD(x)^\dagger\right]. \tag{7.32}$$

which is the generalized Heinz density operator [111]. Thus this result shows how to derive the Heinz's approach for the spinorial field from a first-principle method based on the group representation theory of thermo-algebra. The analysis for the scalar field follows the same lines; and the approach can be generalized for higher spin fields, taking advantage of the standard methods to derive arbitrary-spin density-matrix equations.

7.3 The Galilei group

The Galilei group is defined by the set of transformations [112],

$$\mathbf{x}' = R\mathbf{x} + \mathbf{v}t + \mathbf{a}, \tag{7.33}$$

$$t' = t + b, \tag{7.34}$$

taking a point of the Newtonian space and time $(\mathbf{x}, t)$ to another point given by $(\mathbf{x}', t')$, where $\mathbf{x} =(x^1, x^2, x^3)$ stands for the coordinates of Euclidian space; t stands for the time; R describes the rotations; $\mathbf{v} =(v^1, v^2, v^3)$ is a velocity describing the Galilei boost, the change from one inertial frame to another; $\mathbf{a}$ and b are space and time translations, respectively. Denote the transformations given in Eqs. (7.33) and (7.34) by the operation G,

$$(\mathbf{x}', t') = G(\mathbf{x}, t), \tag{7.35}$$

with G specified by

$$G = [b, \mathbf{a}, \mathbf{v}, R]. \tag{7.36}$$

The transformations G form a group. To prove it, consider $G_1 = [b_1, \mathbf{a}_1, \mathbf{v}_1, R_1]$ and $G_2 = [b_2, \mathbf{a}_2, \mathbf{v}_2, R_2]$, then

$$G_2 \circ G_1 = [b, \mathbf{a}, \mathbf{v}, R], . \tag{7.37}$$

with

$$\begin{aligned} b &= b_2 + b_1, \\ \mathbf{a} &= \mathbf{a}_2 + R_2\mathbf{a}_1 + b_1\mathbf{v}_2, \\ \mathbf{v} &= \mathbf{v}_2 + R_2\mathbf{v}_1, \\ R &= R_2R_1. \end{aligned}$$

The operation $G_2 \circ G_1$, to be denoted simply by $G_2 G_1$, is a closed product equipping the set $\mathbb{G}$ of all transformations with a group structure. Indeed, the composition operation defined in Eq. (7.37) is associative; also there is an identity transformation,

$$E = (0, 0, 0, 1); \tag{7.38}$$

and, for each transformation $G = (b, \mathbf{a}, \mathbf{v}, R)$ there is an inverse G^{-1}, such that $G^{-1}G = GG^{-1} = E$, with G^{-1} given by

$$G^{-1} = \left(-b, -R^{-1}\left(\mathbf{a} - b\mathbf{v}\right), -R^{-1}\mathbf{v}, R^{-1}\right). \tag{7.39}$$

The set of transformations $\mathbb{G}$ is called the *Galilei Group*; it is the kinematical symmetry group of the non-relativistic physics.

The Galilei group $\mathbb{G}$ is specified by ten parameters: three for spatial rotations given by the three Euler angles, for instance defining the matrix R; three for Galilei boosts ($\mathbf{v}$); three for space translations ($\mathbf{a}$); and finally one parameter b for the time translation. The defining representations of $\mathbb{G}$ in the space $\mathbb{R}^3 \times \mathbb{T}$ (with $\mathbb{T} \sim \mathbb{R}$) are given by Eqs. (7.33) and (7.34).

The basic subgroups of $\mathbb{G}$ are $\mathcal{T} = \{(b, 0, 0, 1)\}$ time translations; $\mathcal{S} = \{(0, \mathbf{a}, 0, 1)\}$ space translations; $\mathcal{V} = \{(0, 0, \mathbf{v}, 1)\}$ boosts; $\mathcal{R} = \{(0, 0, 0, R)\}$ rotations. The subgroup $\mathcal{T} \times \mathcal{S}$ is an invariant abelian subgroup and $\mathbb{G}/(\mathcal{T} \times \mathcal{S})$ is isomorphic to $\mathcal{V} \times \mathcal{R}$, the homogeneous Galilei group.

Let us now derive the Lie algebra of $\mathbb{G}$, which will be denoted by $\mathfrak{g}$, using the space of analytical scalar functions of $(\mathbf{x}, t)$. We have

$$S(G) f(\mathbf{x}, t) = S(b, \mathbf{a}, \mathbf{v}, R) f(\mathbf{x}, t) = f(\mathbf{x}', t'). \tag{7.40}$$

For finite unitary representations,

$$S(b, \mathbf{a}, \mathbf{v}, R) = U(b, \mathbf{a}, \mathbf{v}, R) = e^{ibH} e^{i\mathbf{a}\cdot\mathbf{p}} e^{i\mathbf{v}\cdot\mathbf{k}} e^{i\theta\cdot\mathbf{J}}, \tag{7.41}$$

are such that the generators of the Galilei group are given by

$$H = i\frac{\partial}{\partial t} \text{ is the generator of } \mathcal{T}; \tag{7.42}$$

$$\mathbf{P} = -i\nabla \text{ is the generator of } \mathcal{S}; \tag{7.43}$$

$$\mathbf{J} = -i\mathbf{r} \times \nabla \text{ is the generator of } \mathcal{R}; \tag{7.44}$$

$$\mathbf{K} = it\nabla \text{ is the generator of } \mathcal{V}. \tag{7.45}$$

The commutation relations among these generators define the Lie algebra $\mathfrak{g}$,

$$[J_i, J_j] = i\varepsilon_{ijk} J_k, \tag{7.46}$$

$$[J_i, K_j] = i\varepsilon_{ijk} K_k, \tag{7.47}$$

$$[J_i, P_j] = i\varepsilon_{ijk} P_k, \tag{7.48}$$

$$[K_i, H] = -P_i, \tag{7.49}$$

where ϵ_{ijk} is the skew-symmetric pseudo-tensor , and $i, j, k = 1, 2, 3$. All the other commutation relations are null.

7.4 Galilean density matrices

To construct the thermo-algebra of the Galilei group, we distinguish the dynamical variables between generators of symmetry and observables. The commutation relations for the generators of the Galilei symmetries are [113]

$$[\widehat{J}_i, \widehat{J}_j] = i\epsilon_{ijk}\widehat{J}_k, \tag{7.50}$$

$$[\widehat{J}_i, \widehat{P}_j] = i\epsilon_{ijk}\widehat{P}_k, \tag{7.51}$$

$$[\widehat{J}_i, \widehat{K}_j] = i\epsilon_{ijk}\widehat{K}_k, \tag{7.52}$$

$$[\widehat{H}, \widehat{K}_j] = i\widehat{P}_j, \tag{7.53}$$

$$[\widehat{K}_i, \widehat{P}_j] = 0, \tag{7.54}$$

where $\widehat{\mathbf{J}} = (\widehat{J}_1, \widehat{J}_2, \widehat{J}_3)$ stand for the generators of rotation, $\widehat{\mathbf{P}} = (\widehat{P}_1, \widehat{P}_2, \widehat{P}_3)$ for the generators of spatial translation, $\widehat{\mathbf{K}} = (\widehat{K}_1, \widehat{K}_2, \widehat{K}_3)$ for the Galilei boosts, and $\widehat{H}$ for the time translation.

The subalgebra of the generators of the Galilei symmetry, Eqs. (7.50)–(7.54), describes faithful representations of the Galilei group. Usually, the projective, not faithful, representation, in which

$$[\widehat{K}_i, \widehat{P}_j] = \text{constant} \neq 0,$$

is used to derive physical representations, where the constant is the central charge describing mass. This is not the case here. The physical representation will be determined by the nature of the invariant subalgebra involving the observables, $J_i, P_i, K_i, H,\ \ i = 1, 2, 3$. That is, we postulate the existence of the following observables: the angular momentum, $\mathbf{J}$, the linear momentum, $\mathbf{P}$; the energy, H; and a position operator, $\mathbf{Q}$, which can be introduced via the Galilei boost, considering that an observable

$$K_i = mQ_i + f(\mathbf{P}) \tag{7.55}$$

is associated, by construction, with the generator of boosts, $\widehat{K}_i$, and m is a constant.

Here we are looking for unitary operators describing quantum systems, then as another postulate, we assume that the three components of the observable angular momentum do not commute with each other. So we have

$$[J_i, J_j] = i\epsilon_{ijk}J_k. \tag{7.56}$$

The other non-null relations for the observables arise then by consistency,

$$[J_i, P_j] = i\epsilon_{ijk}P_k, \tag{7.57}$$

$$[J_i, K_j] = i\epsilon_{ijk}K_k, \tag{7.58}$$

$$[H, K_j] = iP_j, \tag{7.59}$$

$$[K_j, P_k] = im\delta_{jk}. \tag{7.60}$$

The relations among generators of symmetry and observables are represented by the following commutations relations

$$[J_i, \widehat{J}_j] = [\widehat{J}_i, J_j] = i\epsilon_{ijk} J_k, \tag{7.61}$$

$$[J_i, \widehat{P}_j] = [\widehat{J}_i, P_j] = i\epsilon_{ijk} P_k, \tag{7.62}$$

$$[J_i, \widehat{K}_j] = [\widehat{J}_i, K_j] = i\epsilon_{ijk} K_k, \tag{7.63}$$

$$[H, \widehat{K}_j] = [\widehat{H}, K_j] = iP_j, \tag{7.64}$$

$$[K_i, \widehat{P}_j] = [\widehat{K}_i, P_j] = im\delta_{ij}. \tag{7.65}$$

Therefore, the observable angular momentum, $\mathbf{J}$, transforms as a vector, a rotation generated by $\widehat{\mathbf{J}}$, as indicated in Eq. (7.61). The other relations, Eqs. (7.62)–(7.65), can be interpreted in a similar way by considering the corresponding transformations.

The set of commutation relations given by Eqs. (7.50)–(7.65) is, then, a thermal Galilei Lie algebra, $\mathfrak{g}_T$. In this case, for some values of the structure constants, we have the situation in which $C_{ijk} \neq D_{ijk} = E_{ijk}$.

The interpretation of each observable is obtained from transformation rules. For instance, consider the observables Q and P under a boost transformations, that is,

$$U(\widehat{K})\ Q\ U^{-1}(\widehat{K}) = Q + vt\mathbf{1} \tag{7.66}$$

and

$$U(\widehat{K})\ P\ U^{-1}(\widehat{K}) = P + mv\mathbf{1} \tag{7.67}$$

where

$$U(\widehat{K}) = \exp(-imv\widehat{K}).$$

Therefore, under the boost the operators Q and P transform the position and momentum, respectively; and so are candidates to describe observables, if m is the mass. In addition we have, due to Eq. (7.60) with $m \neq 0$ only, $[Q_i, P_j] = i\delta_{ij}$. This corresponds to the Heisenberg uncertainty relations and for the sake of consistency $J_i = \epsilon_{ijk} Q_j P_k + S_i$ with S_i being an operator commuting with all the operators in the algebra. In this way, Eqs. (7.56)–(7.60) furnish a compatible set of algebraic relations among the basic observables with J_i being used to describe the angular momentum. If $m = 0$, along these lines of reasoning, we do not derive physical representations, since Eq. (7.60), in this case, is incompatible with Eqs. (7.56)–(7.59). In other words, rigorously we cannot find a representation for particles with zero mass in the non-relativistic context. This discussion would be different in the realm of a Fock space representation, important to many-body systems.

Another important aspect is that $\mathfrak{g}_T$ is a reducible algebra, in the sense that, we can rewrite it in terms of the tilde and nontilde operators. That is,

$$\widetilde{A} = A - \widehat{A}.$$

Then we find that $\mathfrak{g}_T$ is the direct product of two unfaithful representations of the Galilei group, i.e.

$$[J_i, J_j] = i\epsilon_{ijk}J_k, \quad [\widetilde{J}_i, \widetilde{J}_j] = -i\epsilon_{ijk}\widetilde{J}_k. \tag{7.68}$$

$$[J_i, P_j] = i\epsilon_{ijk}P_k, \quad [\widetilde{J}_i, \widetilde{P}_j] = -i\epsilon_{ijk}\widetilde{P}_k, \tag{7.69}$$

$$[J_i, K_j] = i\epsilon_{ijk}K_k, \quad [\widetilde{J}_i, \widetilde{K}_j] = -i\epsilon_{ijk}\widetilde{K}_k, \tag{7.70}$$

$$[H, K_j] = iP_j, \quad [\widetilde{H}, \widetilde{K}_j] = -i\widetilde{P}_j, \tag{7.71}$$

$$[K_j, P_k] = im\delta_{jk}, \quad [\widetilde{K}_j, \widetilde{P}_k] = -im\delta_{jk}, \tag{7.72}$$

and the other commutation relations among tilde and nontilde variables are null. Notice that, in the case of classical systems, the commutation relations given by Eqs. (7.56)–(7.60) are null, representing abelian observables. In that case $\mathfrak{g}_T$ is no longer a reducible representation, in the sense that we cannot derive Eqs. (7.68)–(7.72).

The invariants of g_T are

$$I_1 = \frac{P^2}{2m} - H\,,$$

$$I_2 = \left(J - \frac{1}{m}K \times P\right)^2\,,$$

$$I_3 = \widehat{I}_1 = \left(\frac{P^2}{2m}\right)^{\wedge} - \widehat{H}\,,$$

$$I_4 = \widehat{I}_2 = \left[\left(J - \frac{1}{m}K \times P\right)^2\right]^{\wedge}.$$

These invariants are used to specify representations. Their meaning is: I_1 defines the conservation of energy and I_2 the spin. The operators I_3 and I_4 are invariants associated with I_1 and I_2, respectively.

The invariant I_3 is associated with the so-called Liouvillian in the density matrix formalism. From the thermal Galilei-Lie algebra, $\widehat{H}$ is the generator of time translation, such that the time evolution of an arbitrary dynamical variable is specified by $\overline{A}(t) = e^{it\widehat{H}}\ \overline{A}\,(0)\ e^{-it\widehat{H}}$, where $\overline{A}$ stands for $\widehat{A}$ or A operator. Hence the time evolution equation for $\overline{A}(t)$, is,

$$i\partial_t \overline{A}(t) = [\overline{A}(t), H],$$

which corresponds to the Heisenberg equation.

In the Schrödinger picture, as seen in Chapter 5,

$$i\partial_t\,|\psi(t)\rangle = \widehat{H}\,|\psi(t)\rangle. \tag{7.73}$$

where we have assumed a representation with $I_2 = 0$, i.e., there is no spin. Considering the state of the system, $|\psi(t)\rangle$, written as

$$\begin{aligned} |\psi(t)\rangle &= |\rho^{1/2}(t)\cdot 1\rangle, \\ &= |\rho^{1/2}(t)\rangle|1\rangle \\ &\equiv \rho^{1/2}(t)|1\rangle, \end{aligned} \tag{7.74}$$

where $|1\rangle = \sum_n |n, \widetilde{n}\rangle$, we derive

$$i\partial_t \rho(t) = [H, \rho(t)] = L\rho(t)$$

the Liouville-von Neumann equation, where $L = \widehat{H} = [H, \cdot]$ is the Liouvillian. In order to include a spin index, we have to consider representations $I_2 \neq 0$. The main result of this section is to show that the Liouville-von Neumann equation is derived directly from the group theory.

Observe that in terms of the tilde and non-tilde operators, we find two Schrödinger equations,

$$\begin{aligned} i\partial_t \psi(\mathbf{x}, t) &= H\psi(\mathbf{x}, t), \\ -i\partial_t \widetilde{\psi}(\mathbf{x}, t) &= \widetilde{H}\widetilde{\psi}(\mathbf{x}, t). \end{aligned}$$

7.5 Lagrangians

In this section we write the Lagrangians for the Klein-Gordon and Dirac fields using the thermal representations. This will be used to construct the thermal field theory, in the next two chapters. For the case of bosons, using the invariant $\widehat{P^2} = P_\mu P^\mu - \widetilde{P}_\mu \widetilde{P}^\mu$, it stands for the hat-Hamiltonian of the theory. Then there is a Lagrangian associated with it. For the Klein-Gordon field we have the set of equations

$$\begin{aligned} (\Box^2 + m^2)\phi(x) &= 0, \\ (\Box^2 + m^2)\widetilde{\phi}(x) &= 0, \end{aligned}$$

which are derived from the Lagrangian density,

$$\widehat{\mathcal{L}} = \mathcal{L} - \widetilde{\mathcal{L}} = \frac{1}{2}\partial_\alpha \phi \partial^\alpha \phi - \frac{1}{2}m^2\phi^2 - \frac{1}{2}\partial_\alpha \widetilde{\phi}\partial^\alpha \widetilde{\phi} + \frac{1}{2}m^2\widetilde{\phi}^2. \tag{7.75}$$

For the Dirac field we have

$$\begin{aligned} \widehat{\mathcal{L}} = &\frac{1}{2}\overline{\psi}(x)\gamma \cdot i\overleftrightarrow{\partial}\psi(x) - m\overline{\psi}(x)\psi(x) \\ &+ \frac{1}{2}\widetilde{\overline{\psi}}(x)\gamma^* \cdot i\overleftrightarrow{\partial}\widetilde{\psi}(x) + m\widetilde{\overline{\psi}}(x)\widetilde{\psi}(x). \end{aligned}$$

The γ-matrices in these equations are taken in the representation with $\widetilde{\gamma} = (\gamma^T)^\dagger = \gamma^*$, as in Chapter 4. Both representations for the tilde matrices are compatible with the algebra of the γ-matrices, that is, $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$ or $\{\gamma^{*\mu}, \gamma^{*\nu}\} = 2g^{\mu\nu}$. This doubled structure points us to explore Bogoliubov transformations in these representations. This is analyzed in the next chapter.

Chapter 8

Thermal Propagator

We introduce now temperature effects in a quantum field theory. We consider a field in the space $\mathcal{H}_T$, with the modes thermalized via the Bogoliubov transformation. The main goal is to write the thermal free field propagator, following in parallel with the $T = 0$ theories. First we derive the imaginary-time propagator for boson and fermion fields, and in what follows, the so called real-time propagator. Interacting fields at finite temperature are considered with a path integral formalism [105, 114, 115].

8.1 Thermal Klein-Gordon field

The Lagrangian density of the Klein-Gordon scalar field with an external source is written in the thermal representation as

$$\begin{aligned}\widehat{\mathcal{L}} &= \mathcal{L}-\widetilde{\mathcal{L}} \\ &= \frac{1}{2}\partial_\alpha\phi\partial^\alpha\phi - \frac{1}{2}m^2\phi^2 + J\phi - \frac{1}{2}\partial_\alpha\widetilde{\phi}\partial^\alpha\widetilde{\phi} + \frac{1}{2}m^2\widetilde{\phi}^2 - \widetilde{J}\widetilde{\phi}.\end{aligned}$$

In order to introduce the Hamiltonian formalism, we define the canonical momentum density by

$$\begin{aligned}\pi(x) &= \frac{\partial\mathcal{L}(\phi,\partial\phi)}{\partial\dot{\phi}}, \\ \widetilde{\pi}(x) &= \frac{\partial\widetilde{\mathcal{L}}(\widetilde{\phi},\partial\widetilde{\phi})}{\partial\dot{\widetilde{\phi}}}\end{aligned}$$

The Hamiltonian is defined by

$$\widehat{H} = \int \widehat{\mathcal{H}}\, d^3x = \int [\mathcal{H}(\phi,\pi) - \widetilde{\mathcal{H}}(\widetilde{\phi},\widetilde{\pi})]\, d^3x, \tag{8.1}$$

where the Hamiltonian density is

$$\widehat{\mathcal{H}} = \frac{1}{2}\pi^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{1}{2}m^2\phi^2 - J\phi - \frac{1}{2}\widetilde{\pi}^2 - \frac{1}{2}(\nabla\widetilde{\phi})^2 - \frac{1}{2}m^2\widetilde{\phi}^2 + \widetilde{J}\widetilde{\phi}).$$

A quantum field theory is introduced by requiring that the equal-time commutation relations are fulfilled,

$$[\phi(t,\mathbf{x}),\pi(t,\mathbf{y})] = i\delta(\mathbf{x}-\mathbf{y}), \tag{8.2}$$

$$[\phi(t,\mathbf{x}),\phi(t,\mathbf{y})] = [\pi(t,\mathbf{x}),\pi(t,\mathbf{y})] = 0, \tag{8.3}$$

$$[\widetilde{\phi}(t,\mathbf{x}),\widetilde{\pi}(t,\mathbf{y})] = -i\delta(\mathbf{x}-\mathbf{y}), \tag{8.4}$$

$$[\widetilde{\phi}(t,\mathbf{x}),\phi(t,\mathbf{y})] = [\pi(t,\mathbf{x}),\pi(t,\mathbf{y})] = 0 \tag{8.5}$$

The fields ϕ and π are operators defined to act on a Hilbert space $\mathcal{H}_T$. We use the Bogoliubov transformation to introduce thermal operators. In this case there are infinite modes and so a Bogoliubov transformation is defined for each mode, i.e.

$$\phi(x;\beta) = \int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k}\,[a(k;\beta)e^{-ikx} + a^\dagger(k;\beta)e^{ikx}]$$

and

$$\widetilde{\phi}(x;\beta) = \int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k}\,[\tilde{a}(k;\beta)e^{ikx} + \tilde{a}^\dagger(k;\beta)e^{-ikx}],$$

where $a(k;\beta)$ ($\tilde{a}(k;\beta)$) and $a^\dagger(k;\beta)$ ($\tilde{a}^\dagger(k;\beta)$) are thermal (tilde) annihilation and creation operators respectively. For the momenta, $\pi(x;\beta)$ and $\widetilde{\pi}(x;\beta)$, we have

$$\pi(x;\beta)=\dot{\phi}(x;\beta) = \int \frac{d^3k}{(2\pi)^3}(-i)\,\frac{1}{2}[a(k;\beta)e^{-ikx} - a^\dagger(k;\beta)e^{ikx}]$$

and

$$\widetilde{\pi}(x;\beta)=\dot{\widetilde{\phi}}(x;\beta) = \int \frac{d^3k}{(2\pi)^3}\,\frac{i}{2}[\tilde{a}(k;\beta)e^{ikx} - \tilde{a}^\dagger(k;\beta)e^{-ikx}],$$

where we have used the tilde conjugation rules to write $\widetilde{\phi}(x;\beta)$ and $\widetilde{\pi}(x;\beta)$ from $\phi(x;\beta)$ and $\pi(x;\beta)$, respectively.

The algebra given by Eqs. (8.2)–(8.5) is still valid for the operators $\phi(x;\beta)$, $\widetilde{\phi}(x;\beta), \pi(x;\beta)$ and $\widetilde{\pi}(x;\beta)$. Then the commutation relations for the thermal modes read

$$[a(k;\beta), a^\dagger(k';\beta)] = (2\pi)^3 2k_0\delta(\mathbf{k}-\mathbf{k}'), \tag{8.6}$$

$$[\tilde{a}(k;\beta), \tilde{a}^\dagger(k';\beta)] = (2\pi)^3 2k_0\delta(\mathbf{k}-\mathbf{k}'), \tag{8.7}$$

with all the other commutation relations being zero. The general Bogoliubov transformation applied to all modes is written in the form

$$\begin{aligned} U(\beta) &= \exp\left\{\sum_k \theta_k(\beta)[a^\dagger(k)\tilde{a}^\dagger(k) - a(k)\tilde{a}(k)]\right\} \\ &= \prod_k U(k,\beta), \end{aligned} \tag{8.8}$$

where

$$U(k,\beta) = \exp\{\theta_k(\beta)[a^\dagger(k)\tilde{a}^\dagger(k) - a(k)\tilde{a}(k)]\},$$

with θ_k defined by $\cosh\theta_k = v(k,\beta)$, in the continuum limit. However in this limit the unitary nature of the Bogoliubov transformation is lost, a property that gives rise to non-equivalent vacua in the theory [116, 117]. Despite the loss of unitarity, the Bogoliubov transformation is still canonical, in the sense that, the algebraic structure of the theory is preserved [72].

The Hilbert space is constructed from the thermal vacuum, $|0(\beta)\rangle = U(\beta)|0,\tilde{0}\rangle$, where

$$|0,\tilde{0}\rangle = \bigotimes_k |0,\tilde{0}\rangle_k$$

and $|0,\tilde{0}\rangle_k$ is the vacuum for the mode k. The thermal vacuum is such that

$$a(k;\beta)|0(\beta)\rangle = \tilde{a}(k;\beta)|0(\beta)\rangle = 0$$

and $\langle 0(\beta)|0(\beta)\rangle = 1$. The basis vectors are given in the form

$$[a^\dagger(k_1;\beta)]^{n_1}\cdots[a^\dagger(k_N;\beta)]^{n_N}[\tilde{a}^\dagger(k_1;\beta)]^{m_1}\cdots[\tilde{a}^\dagger(k_M;\beta)]^{m_M}|0(\beta)\rangle,$$

where $n_i, m_i \in \mathbb{N}$ and k_i refers to an arbitrary mode.

The thermal and non-thermal operators are related by

$$\begin{aligned} a(k;\beta) &= U(\beta)a(k)U^{-1}(\beta) = U(k,\beta)a(k)U^{-1}(k,\beta) \\ &= u(k,\beta)a(k) - v(k,\beta)\tilde{a}^\dagger(k), \end{aligned} \tag{8.9}$$

where

$$v(k,\beta) = \frac{1}{\sqrt{\exp(\beta\omega_k)-1}}$$

and $u^2(k,\beta) - v^2(k,\beta) = 1$. The inverse is

$$a(k) = u(k,\beta)a(k;\beta) + v(k,\beta)\tilde{a}^\dagger(k;\beta). \tag{8.10}$$

The other operators, $a^\dagger(k)$, $\tilde{a}(k)$ and $\tilde{a}^\dagger(k)$ are derived by using the Hermitian and the tilde conjugation rules.

The thermal average of an observable, A, has already been defined as $\langle A\rangle = \langle 0(\beta)|A|0(\beta)\rangle$. Let us calculate the thermal propagator, using the thermal vacuum. The thermal Feymann propagator for the real scalar field is then defined by

$$G_0(x-y,\beta) = -i\langle 0(\beta)|T[\phi(x)\phi(y)]|0(\beta)\rangle, \tag{8.11}$$

or

$$iG_0(x-y,\beta) = \theta(x^0-y^0)g(x-y,\beta) + \theta(y^0-x^0)g(y-x,\beta), \tag{8.12}$$

with $\theta(x)$ being the step function, such that $\theta(x) = 1$, for $x > 1$, $\theta(x) = 0$, for $x < 1$, and $g(x-y;\beta) = \langle 0(\beta)|\phi(x)\phi(y)|0(\beta)\rangle$. Explicitly, we have

$$\begin{aligned} g(x-y,\beta) = \langle 0(\beta)|\int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k}\,[a(k)e^{-ikx} + a^\dagger(p)e^{ikx}] \\ \times \int \frac{d^3p}{(2\pi)^3}\frac{1}{2\omega_p}\,[a(p)e^{-ipy} + a^\dagger(p)e^{ipy}]|0(\beta)\rangle. \end{aligned}$$

Separating the terms, $g(x-y,\beta)$ reads

$$\begin{aligned} g(x-y,\beta) = \int \frac{d^3p}{(2\pi)^3}\frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_p}\frac{1}{2\omega_k} \\ \times[\langle 0(\beta)|a^\dagger(k)a^\dagger(p)|0(\beta)\rangle e^{i(kx+py)} \\ +\langle 0(\beta)|a(k)a^\dagger(p)|0(\beta)\rangle e^{-i(kx-py)} \\ +\langle 0(\beta)|a^\dagger(k)a(p)|0(\beta)\rangle e^{i(kx-py)} \\ +\langle 0(\beta)|a(k)a(p)|0(\beta)\rangle e^{-i(kx+py)}]. \end{aligned} \tag{8.13}$$

Using Eq. (8.10), and the equivalent expressions for $a^\dagger$, $\tilde{a}$ and $\tilde{a}^\dagger$ each of them written in terms of the thermal operators, each term in the integrand is calculated. The first one is

$$\begin{aligned} \langle 0(\beta)|a^\dagger(k)a^\dagger(p)|0(\beta)\rangle = \langle 0(\beta)|[u(k,\beta)a^\dagger(k;\beta)+v(k,\beta)\tilde{a}(k;\beta)] \\ \times[u(p,\beta)a^\dagger(p;\beta)+v(p,\beta)\tilde{a}(p;\beta)]|0(\beta)\rangle \end{aligned}$$

resulting in

$$\langle 0(\beta)|a^\dagger(k)a^\dagger(p)|0(\beta)\rangle = 0.$$

The second term in Eq. (8.10) is

$$\begin{aligned} \langle 0(\beta)|a(k)a^\dagger(p)|0(\beta)\rangle &= \langle 0(\beta)|[u(k,\beta)a(k;\beta)+v(k,\beta)\tilde{a}^\dagger(k;\beta)] \\ &\quad\times[u(p,\beta)a^\dagger(p;\beta)+v(p,\beta)\tilde{a}(p;\beta)]|0(\beta)\rangle \\ &= u(k,\beta)u(p,\beta)\langle 0(\beta)|a(k;\beta)a^\dagger(p;\beta)|0(\beta)\rangle \\ &= u(k,\beta)u(p,\beta)\langle 0(\beta)|a^\dagger(p;\beta)a(k;\beta)+[a(k;\beta),a^\dagger(p;\beta)]|0(\beta)\rangle \\ &= u(k,\beta)u(p,\beta)\langle 0(\beta)|a^\dagger(p;\beta)a(k;\beta)+(2\pi)^3 2k_0\delta(\mathbf{k}-\mathbf{p})|0(\beta) \\ &= u(k,\beta)u(p,\beta)(2\pi)^3 2k_0\delta(\mathbf{k}-\mathbf{p}) \end{aligned}$$

where we have used Eq. (8.6). The same procedure is used for the other terms to get

$$\begin{aligned} \langle 0(\beta)|a^\dagger(k)a(p)|0(\beta)\rangle &= v(k,\beta)v(p,\beta)\delta(\mathbf{k}-\mathbf{p}), \\ \langle 0(\beta)|a^\dagger(k)a^\dagger(p)|0(\beta)\rangle &= 0. \end{aligned}$$

Substituting these results in Eq. (8.13), it leads to

$$g(x-y,\beta) = \int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k}[u^2(k,\beta)e^{-ik(x-y)}+v^2(k,\beta)e^{ik(x-y)}].$$

Then Eq. (8.12) reads

$$\begin{aligned} iG_0(x-y,\beta) = \theta(x^0-y^0)\int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k}[u^2(k,\beta)e^{-ik(x-y)}+v^2(k,\beta)e^{ik(x-y)}] \\ +\theta(y^0-x^0)\int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k}[u^2(k,\beta)e^{-ik(y-x)}+v^2(k,\beta)e^{ik(y-x)}]. \end{aligned}$$

As $u^2(k,\beta) - v^2(k,\beta) = 1$, then

$$\begin{aligned} iG_0(x-y,\beta) &= \theta(x^0-y^0)\int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k}[(v^2(k,\beta)+1)e^{-ik(x-y)} + v^2(k,\beta)e^{ik(x-y)}] \\ &\quad +\theta(y^0-x^0)\int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k}[(v^2(k,\beta)+1)e^{-ik(y-x)} \\ &\quad +v^2(k,\beta)e^{ik(y-x)}] \\ &= \int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k}\left[\theta(x^0-y^0)e^{-ik(x-y)} + \theta(y^0-x^0)e^{-ik(y-x)}\right] \\ &\quad + \int \frac{d^3k}{(2\pi)^3}v^2(k,\beta)\frac{1}{2\omega_k}[\theta(x^0-y^0)e^{-ik(x-y)} + \theta(y^0-x^0)e^{-ik(y-x)}] \\ &\quad + \int \frac{d^3k}{(2\pi)^3}v^2(k,\beta)\frac{1}{2\omega_k}[\theta(x^0-y^0)e^{ik(x-y)} + \theta(y^0-x^0)e^{ik(y-x)}]. \end{aligned}$$

Using the Fourier representation of $\theta(x)$, we obtain

$$G_0(x-y,\beta) = \int \frac{d^4k}{(2\pi)^4}e^{-ik(x-y)}G_0(k,\beta), \tag{8.14}$$

where

$$G_0(k,\beta) = G_0(k) + v^2(k,\beta)[G_0(k) - G_0^*(k)]. \tag{8.15}$$

Since

$$\begin{aligned} G_0(k) - G_0^*(k) &= \frac{-1}{k^2-m^2+i\varepsilon} + \frac{1}{k^2-m^2-i\varepsilon} \\ &= 2\pi i\delta(k^2-m^2), \end{aligned}$$

we have

$$G_0(k,\beta) = G_0(k) + 2\pi i n(k;\beta)\delta(k^2-m^2), \tag{8.16}$$

where $n(k;\beta) = v^2(k,\beta)$ is the boson distribution function for the mode k.

Using the definition of the TFD propagator, Eq. (8.11), in the Heisenberg picture, we have

$$\begin{aligned} G_0(x-y,\beta) &= -i\langle 0(\beta)|T[\phi(\mathbf{x},t)\phi(\mathbf{y},t)]|0(\beta)\rangle \\ &= -i\mathrm{Tr}\{\frac{1}{Z}e^{-\beta H}T[\phi(\mathbf{x},t)\phi(\mathbf{y},t)]\} \\ &= -i\mathrm{Tr}\{\frac{1}{Z}e^{-\beta H}T[\phi(x)\phi(y-i\beta n_0)]\} \\ &= -i\langle 0(\beta)|T[\phi(x)\phi(y-i\beta n_0)]|0(\beta)\rangle \\ &= G_0(x-y-i\beta n_0,\beta), \end{aligned} \tag{8.17}$$

where $n_0 = (n_0^\mu) = (1,0,0,0)$. This means that the propagator is a periodic function with a period β in the imaginary-time axis, with frequencies

$$w_n = \frac{2\pi n}{\beta},$$

which are called Matsubara frequencies. Therefore, we can also write $G_0(x-y,\beta)$ as

$$G_0(x-y,\beta) = \frac{-1}{i\beta}\sum_n \int d^3p \frac{e^{-ik_n\cdot x}}{k_n^2 - m^2 + i\varepsilon}, \tag{8.18}$$

where $k_n = (k_n^0, \mathbf{k})$. The connection between these two representations of the thermal free propagator, Eqs. (8.14)–(8.16) and Eq. (8.18), will be discussed in detail in Chapter 15. The propagator $G_0(x-y,\beta)$ given in Eq. (8.18) is one of the main results of the method first proposed by Matsubara, using the Wick rotation from real to imaginary time. This method is called *the imaginary time formalism* [43].

In Chapter 3, it is shown that the partition function is a generating function Z_{ab} but with $a = b$, and a Wick rotation. We introduce here the partition function as a generating functional for $G_0(x-y,\beta)$, generalizing the previous results. Using the generating functional defined in Chapter 3 for the scalar field, we write

$$Z_0[\beta, J] = N\int D\phi \ \exp\left\{\int_0^\beta d\tau \int d^3x \left[\frac{1}{2}\phi(\Box_\tau + m^2)\phi - J\phi\right]\right\}, \tag{8.19}$$

where $\tau = it$, such that

$$\Box + m^2 = -\partial_\tau^2 - \nabla^2 + m^2$$

and the the field ϕ satisfies the periodicity condition $\phi(0) = \phi(\beta)$. The effect of finite temperature is taken into account by implementing a Wick rotation of the real axis, limiting the imaginary time in a range from 0 to β and to perform the functional integration with the field satisfying periodic boundary conditions. Performing the ϕ integration we get,

$$Z_0[\beta, J] = N\exp\left[\frac{i}{2}\int_0^\beta J(x)(\Box + m^2)^{-1}J(y)d^4x\right][\det(\Box + m^2)]^{1/2}, \tag{8.20}$$

where we are using the notation $\int_0^\beta d\tau \int d^3x = \int_0^\beta d^4x$ and

$$[\det(\Box + m^2)]^{1/2} = \int D\phi \ \exp\left\{-\int_0^\beta d^4x[\frac{1}{2}\phi(\Box + m^2)\phi]\right\} \equiv Z_0[\beta]. \tag{8.21}$$

The kernel of the operator $(\Box + m^2)^{-1}$ is the propagator $G_0(x-y,\beta)$ given in Eq. (8.11), since $G_0(x-y,\beta)$ is a solution of

$$(\Box + m^2)G_0(x-y,\beta) = -\delta(\tau_x - \tau_y)\delta(\mathbf{x}-\mathbf{y}).$$

This solution is unique since the boundary condition given in Eq. (8.17) is satisfied. This shows that $Z_0[\beta, J]$ is the generating functional of $G_0(x-y,\beta)$.

For an arbitrary operator A we have $\ln(\det A) = \mathrm{Tr}(\ln A)$ and so we write

$$\ln Z_0[\beta] = \frac{1}{2}\ln[\det(\Box + m^2)] = \frac{1}{2}\mathrm{Tr}\ln(\Box + m^2).$$

In the Fourier representation we have

$$\ln Z_0[\beta] = \frac{1}{2}\frac{2\pi}{\beta}\sum_{n=-\infty}^{\infty}\int\frac{d^3k}{(2\pi)^3}\ln(\omega_n^2+\omega_k^2+m^2)].$$

This leads to the result for the scalar field free energy, given by $F(\beta) = -\frac{1}{\beta}\ln Z_0(\beta)$.

As a final observation it is worth mentioning that the propagator $G_0(x-y,\beta)$ can also be written in the form

$$G_0(x-y,\beta) = -i\langle 0,\tilde{0}|T[\phi(x,\beta)\phi(y,\beta)]|0,\tilde{0}\rangle.$$

To prove this, observe that in $|0(\beta)\rangle = U(\beta)|0,\tilde{0}\rangle$, the Bogoliubov transformation $U(\beta)$ is given by Eq. (8.8), involving all the modes, and that $a(k;\beta)$ is defined in Eq. (8.9) involving only one mode k.

8.2 Thermal Dirac field

The hat Lagrangian density of the Dirac field with an external source in the thermal representations is written as

$$\begin{aligned}\widehat{\mathcal{L}} = {} & \frac{1}{2}\overline{\psi}(x)[\gamma\cdot i\overleftrightarrow{\partial} - m]\psi(x) + \overline{\eta}(x)\psi(x) + \overline{\psi}(x)\eta(x)\\ & -\frac{1}{2}\widetilde{\overline{\psi}}(x)[-\gamma^*\cdot i\overleftrightarrow{\partial} - m]\widetilde{\psi}(x) + \widetilde{\overline{\eta}}(x)\widetilde{\psi}(x) + \widetilde{\overline{\psi}}(x)\widetilde{\eta}(x),\end{aligned}$$

where $\gamma^* = (\gamma^T)^\dagger$. In order to introduce the Hamiltonian formalism for the thermal quantum field theory, we define the canonical momentum density in terms of the hat Lagrangian density by

$$\begin{aligned}\pi(x) &= \frac{\partial\mathcal{L}(\psi,\partial\psi)}{\partial\dot{\psi}} = i\psi^\dagger(x),\\ \widetilde{\pi}(x) &= \frac{\partial\widetilde{\mathcal{L}}(\widetilde{\psi},\partial\widetilde{\psi})}{\partial\dot{\widetilde{\psi}}} = -i\widetilde{\psi}^\dagger(x).\end{aligned}$$

The Hamiltonian is defined by,

$$\widehat{H} = \int\widehat{\mathcal{H}}\,d^3x = \int[\widehat{\pi}(x)\dot{\widehat{\psi}}(x) - \widehat{\mathcal{L}}]\,d^3x.$$

Each operator is mapped into a thermal operator by a Bogoliubov transformation. The anti-commutation relations are given by

$$\begin{aligned}\{\psi(\mathbf{x},t;\beta),\pi(\mathbf{y},t;\beta)\} &= i\delta(\mathbf{x}-\mathbf{y}),\\ \{\psi(\mathbf{x},t;\beta),\psi(\mathbf{y},t;\beta)\} &= \{\pi(\mathbf{x},t;\beta),\pi(\mathbf{y},t;\beta)\} = 0,\\ \{\widetilde{\psi}(\mathbf{x},t;\beta),\widetilde{\pi}(\mathbf{y},t;\beta)\} &= -i\delta(\mathbf{x}-\mathbf{y}),\\ \{\widetilde{\psi}(\mathbf{x},t;\beta),\psi(\mathbf{y},t;\beta)]\} &= \{\pi(\mathbf{x},t;\beta),\pi(\mathbf{y},t;\beta)\} = 0.\end{aligned}$$

The fields are expanded in modes, k, by

$$\psi(x,\beta) = \int \frac{d^3k}{(2\pi)^3}\frac{m}{\omega_k}\sum_{\alpha=1}^{2}[b_\alpha(k,\beta)u^{(\alpha)}(k)e^{-ikx} + d_\alpha^\dagger(k,\beta)v^{(\alpha)}(k)e^{ikx}],$$

$$\overline{\psi}(x) = \int \frac{d^3k}{(2\pi)^3}\frac{m}{\omega_k}\sum_{\alpha=1}^{2}[b_\alpha^\dagger(k,\beta)\bar{u}^{(\alpha)}(k)e^{ikx} + d_\alpha(k,\beta)\bar{v}^{(\alpha)}(k)e^{-ikx}],$$

$$\widetilde{\psi}(x,\beta) = \int \frac{d^3k}{(2\pi)^3}\frac{m}{\omega_k}\sum_{\alpha=1}^{2}[\tilde{b}_\alpha(k,\beta)u^{*(\alpha)}(k)e^{ikx} + \tilde{d}_\alpha^\dagger(k,\beta)v^{*(\alpha)}(k)e^{-ikx}],$$

$$\widetilde{\overline{\psi}}(x) = \int \frac{d^3k}{(2\pi)^3}\frac{m}{\omega_k}\sum_{\alpha=1}^{2}[\tilde{b}_\alpha^\dagger(k,\beta)\bar{u}^{*(\alpha)}(k)e^{-ikx} + \tilde{d}_\alpha(k,\beta)\bar{v}^{*(\alpha)}(k)e^{ikx}].$$

The anti-commutation relations for the creation ($b_\alpha^\dagger$ and $d_\alpha^\dagger$), annihilation (b_α and d_α) and the corresponding tilde operators are

$$\{b_\alpha(k,\beta),b_\gamma^\dagger(k',\beta)\} = \{d_\alpha(k,\beta),d_\gamma^\dagger(k',\beta)\} = (2\pi)^3\frac{k_0}{m}\delta(\mathbf{k}-\mathbf{k}')\delta_{\alpha\gamma},$$

$$\{\tilde{b}_\alpha(k,\beta),\tilde{b}_\gamma^\dagger(k',\beta)\} = \{\tilde{d}_\alpha(k,\beta),\tilde{d}_\gamma^\dagger(k',\beta)\} = (2\pi)^3\frac{k_0}{m}\delta(\mathbf{k}-\mathbf{k}')\delta_{\alpha\gamma},$$

with all the other anti-commutation relations being zero.

The Bogoliubov transformation is

$$\begin{aligned} U(\beta) &= \exp\left\{\sum_k\{\theta_{b,k}[b^\dagger(k)\tilde{b}^\dagger(k) - b(k)\tilde{b}(k)] + \theta_{d,k}[d^\dagger(k)\tilde{d}^\dagger(k) - d(k)\tilde{d}(k)]\}\right\} \\ &= \prod_k U_b(k,\beta)U_d(k,\beta), \end{aligned}$$

where

$$\begin{aligned} U_b(k,\beta) &= \exp\{\theta_{b,k}[b^\dagger(k)\tilde{b}^\dagger(k) - b(k)\tilde{b}(k)]\}, \\ U_d(k,\beta) &= \exp\{\theta_{d,k}[d^\dagger(k)\tilde{d}^\dagger(k) - d(k)\tilde{d}(k)]\} \end{aligned}$$

with $\theta_{b,k}$ defined by $\cos\theta_{b,k} = v_b(k,\beta)$, and $\theta_{d,k}$ defined by $\cos\theta_{d,k} = v_d(k,\beta)$, where

$$\begin{aligned} v_b^2(k,\beta) &= \frac{1}{e^{\beta(w_k-\mu_b)}+1}, \\ v_d^2(k,\beta) &= \frac{1}{e^{\beta(w_k+\mu_d)}+1}, \end{aligned}$$

with $\mu_{b,d}$ being the chemical potentials, $v_d^2(k,\beta) + u_d^2(k,\beta) = 1$ and $v_b^2(k,\beta) + u_b^2(k,\beta) = 1$. Here $v_b^2(k,\beta)$ and $v_d^2(k,\beta)$ give the distribution functions of particles and anti-particles, respectively.

The Hilbert space is constructed from the thermal vacuum, $|0(\beta)\rangle = U(\beta)|0,\tilde{0}\rangle$, where

$$|0,\tilde{0}\rangle = \bigotimes_k |0,\tilde{0}\rangle_k$$

and $|0,\tilde{0}\rangle_k$ is the vacuum for the mode k considering particles and anti-particles. The thermal vacuum is such that

$$b(k;\beta)|0(\beta)\rangle = \tilde{b}(k;\beta)|0(\beta)\rangle = 0,$$
$$d(k;\beta)|0(\beta)\rangle = \tilde{d}(k;\beta)|0(\beta)\rangle = 0,$$

and $\langle 0(\beta)|0(\beta)\rangle = 1$. Basis vectors are given in the form

$$[b^\dagger(k_1;\beta)]^{n_1}\cdots[d^\dagger(k_M;\beta)]^{n_M}[\tilde{b}^\dagger(k_1;\beta)]^{m_1}\cdots[\tilde{d}^\dagger(k_N;\beta)]^{m_N}|0(\beta)\rangle,$$

where now $n_i, m_i = 0, 1$.

Thermal and non-thermal fermion operators are related by

$$\begin{aligned} b(k;\beta) &= U(\beta)b(k)U^{-1}(\beta) = U(k,\beta)b(k)U^{-1}(k,\beta) \\ &= u_b(k,\beta)b(k) - v_b(k,\beta)\tilde{b}^\dagger(k), \\ d(k;\beta) &= U(\beta)d(k)U^{-1}(\beta) = U(k,\beta)d(k)U^{-1}(k,\beta) \\ &= u_b(k,\beta)d(k) - v_b(k,\beta)\tilde{d}^\dagger(k); \end{aligned}$$

The inverse formulas are written as

$$b(k) = u_b(k,\beta)b(k,\beta) + v_b(k,\beta)\tilde{b}^\dagger(k,\beta),$$
$$d(k) = u_b(k,\beta)b(k,\beta) + v_b(k,\beta)\tilde{b}^\dagger(k,\beta).$$

Observe that each operator b or d carries a spin index. This is understood to be in the mode k.

The thermal Feynman propagator for the Dirac field is defined by

$$S_0(x-y,\beta) = -i\langle 0(\beta)|T[\psi(x)\overline{\psi}(y)]|0(\beta)\rangle, \tag{8.22}$$

such that

$$iS_0(x-y,\beta) = \theta(x^0-y^0)S(x-y,\beta) - \theta(y^0-x^0)\overline{S}(y-x,\beta), \tag{8.23}$$

with $S(x-y,\beta) = \langle 0(\beta)|\psi(x)\overline{\psi}(y)|0(\beta)\rangle$ and $\overline{S}(x-y,\beta) = \langle 0(\beta)|\overline{\psi}(y)\psi(x)|0(\beta)\rangle$.

Let us calculate $S_{ij}(x-y,\beta) = \langle 0(\beta)|\psi_i(x)\overline{\psi}_j(y)|0(\beta)\rangle$, i.e.

$$\begin{aligned} S_{ij}(x-y,\beta) = &\int \frac{d^3p}{(2\pi)^3}\frac{d^3k}{(2\pi)^3}\frac{m}{\omega_p}\frac{m}{\omega_k}\sum_\alpha\sum_{\alpha'} \\ &\times[\langle 0(\beta)|u^2(k,\beta)b_{\alpha k}(\beta)b^\dagger_{\alpha' p}(\beta)u^\alpha_{k,i}\bar{u}^{\alpha'}_{p,j}\ e^{-ikx}e^{ipy}|0(\beta)\rangle] \\ &+\langle 0(\beta)|v^2(k,\beta)\tilde{d}_{\alpha k}(\beta)\tilde{d}^\dagger_{\alpha' p}(\beta)v^\alpha_{k,i}\bar{v}^{\alpha'}_{p,j}e^{ikx}e^{-ipy}|0(\beta)\rangle \\ = &\int \frac{d^3k}{(2\pi)^3}\frac{m}{\omega_p}\sum_\alpha \\ &\times[u^2(k,\beta)u^\alpha_{k,i}\bar{u}^\alpha_{k,j}\ e^{-ik(x-y)} + v^2(k,\beta)v^\alpha_{k,i}\bar{v}^\alpha_{k,j}\ e^{ik(x-y)}]. \end{aligned}$$

Using the projection operators,

$$\sum_{\alpha=1}^{2} u_i^{(\alpha)}(k)\bar{u}_j^{(\alpha)}(k) = \frac{1}{2m}(\gamma\cdot k + m)_{ij},$$
$$\sum_{\alpha=1}^{2} v_i^{(\alpha)}(k)\bar{v}_j^{(\alpha)}(k) = \frac{1}{2m}(\gamma\cdot k - m)_{ij},$$

we obtain

$$S_{ij}(x-y,\beta) = \int \frac{d^3k}{(2\pi)^3}\frac{1}{2\omega_k}[(1-v^2(k,\beta))(i\gamma\cdot\partial+m)_{ij}e^{-ik(x-y)} -v^2(k,\beta))(i\gamma\cdot\partial+m)_{ij}e^{ik(x-y)}].$$

Suppressing the matrix indices we have

$$S(x-y,\beta) = (i\gamma\cdot\partial+m)\int\frac{d^3k}{(2\pi)^3} \times[\frac{e^{-ik(x-y)}}{2\omega_k} - \frac{v^2(k,\beta)}{2\omega_k}(e^{-ik(x-y)} - e^{ik(x-y)})]. \tag{8.24}$$

For the term $\overline{S}(x-y,\beta)$ we get

$$\overline{S}(x-y,\beta) = (i\gamma\cdot\partial+m)\int\frac{d^3k}{(2\pi)^3} \times[-\frac{e^{ik(x-y)}}{2\omega_k} + \frac{v^2(k,\beta)}{2\omega_k}(e^{-ik(x-y)} + e^{ik(x-y)})]. \tag{8.25}$$

Using Eqs. (8.24) and (8.25) in Eq. (8.23) we obtain

$$S_0(x-y,\beta) = (i\gamma\cdot\partial+m)G_0(x-y,\beta).$$

8.3 Doubled notation for bosons

In this section we analyze the two-by-two propagator in TFD which accounts also for the tilde fields. This analysis will give us the possibility to introduce a thermal path integral in real time. In chapter 6, we have defined

$$(A^a) = \begin{pmatrix} A(\beta) \\ \widetilde{A}^\dagger(\beta)\end{pmatrix}, \quad (A^{a\dagger}) = \left(A^\dagger(\beta), -\widetilde{A}(\beta)\right). \tag{8.26}$$

Then the algebraic rules for the thermal boson operators are written as $[a^a(\beta), a^{b\dagger}(\beta)] = \delta^{ab}$; $a,b = 1,2$; and all other commutation relations being zero. The Bogoliubov transformation, Eq. (6.35), is therefore written as a 2×2 matrix,

$$B = \begin{pmatrix} u\ (\beta) & -v(\beta) \\ -v(\beta) & u(\beta)\end{pmatrix}, \tag{8.27}$$

such that for Eq. (8.10) we write

$$a^a = (\mathcal{B}^{-1})^{ab}a^b(\beta) \quad \text{and} \quad a^{a\dagger} = a^{b\dagger}(\beta)\,\mathcal{B}^{ba}.$$

In the doubled notation, the Lagrangian density is

$$\widehat{\mathcal{L}} = \frac{1}{2}\,\partial_\mu\Phi^\dagger(x)\,\partial^\mu\Phi(x) - \frac{m^2}{2}\,\Phi^\dagger(x)\Phi(x),$$

where

$$\Phi(x) = \begin{pmatrix}\phi(x)\\ \widetilde{\phi}(x)\end{pmatrix}, \quad \Phi^\dagger(x) = \left(\phi(x),\ -\widetilde{\phi}(x)\right).$$

The thermal Green function is given by

$$\begin{aligned} iG(x-y;\beta)^{ab} &= \langle 0,\tilde{0}|T[\phi(x;\beta)^a\phi(y;\beta)^b|0,\tilde{0}\rangle \\ &= \frac{1}{(2\pi)^4}\int d^4k\, G(k;\beta)^{ab}e^{ik(x-y)}, \end{aligned} \tag{8.28}$$

where $G(k;\beta)^{ab} = \mathcal{B}^{-1}(k_0)G_0(k)^{ab}\mathcal{B}(k_0)$, with

$$G_0(k)^{ab} = \begin{pmatrix} \frac{1}{k^2-m^2+i\epsilon} & 0 \\ 0 & \frac{-1}{k^2-m^2-i\epsilon} \end{pmatrix}. \tag{8.29}$$

Using the definition of $\mathcal{B}(k_0)$ given in Eq. (8.27), the components of $G(k;\beta)^{ab}$ read

$$\begin{aligned} G(k;\beta)^{11} &= \frac{1}{k^2-m^2+i\epsilon} - 2\pi i\, n(k_0)\,\delta(k^2-m^2), \\ G(k;\beta)^{22} &= \frac{-1}{k^2-m^2-i\epsilon} - 2\pi i\, n(k_0)\,\delta(k^2-m^2), \\ G(k;\beta)^{12} &= G(k;\beta)^{21} = -2\pi i\,[n(k_0)+n^2(k_0)]^{1/2}\,\delta(k^2-m^2), \end{aligned}$$

where $n(k_0) = v_k^2(\beta)$. The propagator $G(k;\beta)^{11}$ is the same as in the Matsubara method; and the two-by-two Green function in Eq. (8.28) is similar to the propagator in the Schwinger-Keldysh approach [72].

8.4 Generating functional for bosons

For a system of free bosons, we consider, up to normalization factors, the following generating functional

$$\begin{aligned} Z_0 &\simeq \int D\phi D\widetilde{\phi} e^{i\mathcal{S}} \\ &= \int D\phi D\widetilde{\phi}\exp[i\int dx(L-\widetilde{L})] \\ &= \int D\phi D\widetilde{\phi}\exp\{-i\int dx[\frac{1}{2}\phi(\Box+m^2)\phi - J\phi - \frac{1}{2}\widetilde{\phi}(\Box+m^2)\widetilde{\phi} + \widetilde{J}\widetilde{\phi}]\}. \end{aligned}$$

Such a functional can then be written as

$$\begin{aligned} Z_0 \simeq \exp\{\frac{i}{2}\int dxdy\, J(x)(\Box+m^2-i\varepsilon)^{-1}J(y) \\ +\widetilde{J}(x)(-1)(\Box+m^2+i\varepsilon)^{-1}\widetilde{J}(y)]\} \end{aligned} \tag{8.30}$$

The Feynman propagators for the non-tilde and tilde variables are then given as, $(\Box+m^2+i\varepsilon)G_0(x) = -\delta(x)$ and $(-1)(\Box+m^2-i\varepsilon)\widetilde{G}_0(x) = -\delta(x)$, such that

$$\widetilde{G}_0(x) = -G_0^*(x).$$

Using these results in Eq. (8.30) we find the normalized functional

$$Z_0[\mathbf{J}^T,\mathbf{J}] = \exp\left[\frac{i}{2}\int dxdy\,\mathbf{J}^T(x)\mathbf{G}_0(x-y)\mathbf{J}(y)\right] \tag{8.31}$$

where

$$\mathbf{J}(x) = \begin{pmatrix} J_1(x) \\ J_2(x) \end{pmatrix}; \quad \mathbf{J}^T(x) = (J_1(x), J_2(x))$$

with $J_1(x) = J(x), J_2(x) = \widetilde{J}(x)$ and

$$\mathbf{G}_0(x) = (G_0^{ab}(x)) = \begin{pmatrix} G_0(x) & 0 \\ 0 & -G_0^*(x) \end{pmatrix},$$

with the Fourier transform given by Eq. (8.29). From Z we have

$$\mathbf{G}_0(x-y) = i\frac{\delta^2 Z_0[\mathbf{J}^T, \mathbf{J}]}{\delta \mathbf{J}(y)\delta \mathbf{J}^T(x)}\bigg|_{J=J^T=0},$$

where the short notation we have used is such that, for instance,

$$G_0^{ab}(x) = i\frac{\delta^2 Z_0[\mathbf{J}^T, \mathbf{J}]}{\delta J_a(x)\delta J_b(y)}\bigg|_{J=J^T=0}.$$

In order to introduce the effect of temperature in this doubled quantum field theory, we transform $Z_0[\mathbf{J}^T, \mathbf{J}]$ using a Bogoliubov transformation. Then we reach

$$Z_0[\mathbf{J}^T, \mathbf{J};\beta] = \exp\left[\frac{i}{2}\int dxdy\, \mathbf{J}^T(x)\mathbf{G}_0(x-y;\beta)\mathbf{J}(y)\right],$$

where $\mathbf{G}_0(x-y;\beta) = (G_0^{ab}(x-y;\beta))$ and

$$\mathbf{G}_0^{ab}(x-y;\beta) = i\frac{\delta^2 Z[\mathbf{J}^T, \mathbf{J}, \beta]}{\delta J_a(x)\delta J_b(y)}|_{J=J^T=0},$$

reproducing the results from the canonical formalism.

In order to treat interactions, we consider the Lagrangian density

$$\widehat{L} = \frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) - \frac{m^2}{2}\phi^2 + L_{int}(\phi) - \frac{1}{2}\partial_\mu\widetilde{\phi}(x)\partial^\mu\widetilde{\phi}(x) + \frac{m^2}{2}\widetilde{\phi}(x)^2 - \widetilde{L}_{int}(\phi).$$

In this case, using the doubling formalism, the functional $Z[\mathbf{J}^T, \mathbf{J}]$ obeys the following equation

$$(\Box + m^2)\frac{\delta Z[\mathbf{J}^T, \mathbf{J}]}{i\delta \mathbf{J}(x)} + \widehat{L}_{int}\left(\frac{1}{i}\frac{\delta}{\delta \mathbf{J}}; \frac{1}{i}\frac{\delta}{\delta \mathbf{J}^T}\right) Z[\mathbf{J}^T, \mathbf{J}] = \mathbf{J}(x) Z[\mathbf{J}^T, \mathbf{J}]$$

with the solution

$$Z[\mathbf{J}^T, \mathbf{J}] = N\exp\left[i\int dx \widehat{L}_{int}\left(\frac{1}{i}\frac{\delta}{\delta \mathbf{J}}; \frac{1}{i}\frac{\delta}{\delta \mathbf{J}^T}\right)\right] Z_0[\mathbf{J}^T, \mathbf{J}],$$

where

$$\widehat{L}_{int}\left(\frac{1}{2}\frac{\delta}{\delta \mathbf{J}}\right) = L_{int}\left(\frac{1}{2}\frac{\delta}{\delta J}\right) - \widetilde{L}_{int}\left(\frac{1}{2}\frac{\delta}{\delta \widetilde{J}}\right).$$

To introduce a temperature dependent functional, we map

$$U(\beta) : Z[\mathbf{J}^T, \mathbf{J}] \to Z[\mathbf{J}^T, \mathbf{J};\beta],$$

by mapping

$$U(\beta) : Z_0[\mathbf{J}^T, \mathbf{J}] \to Z_0[\mathbf{J}^T, \mathbf{J};\beta],$$

as before, resulting in

$$Z[\mathbf{J}^T, \mathbf{J}, \beta] = \frac{\exp\left[i\int dx \widehat{L}_{int}\left(\frac{1}{i}\frac{\delta}{\delta \mathbf{J}}; \frac{1}{i}\frac{\delta}{\delta \mathbf{J}^T}\right)\right] Z_0[\mathbf{J}^T, \mathbf{J}; \beta]}{\exp\left[i\int dx \widehat{L}_{int}\left(\frac{1}{i}\frac{\delta}{\delta \mathbf{J}}; \frac{1}{i}\frac{\delta}{\delta \mathbf{J}^T}\right)\right] Z_0[\mathbf{J}^T, \mathbf{J}; \beta]|_{\mathbf{J}=\mathbf{J}^T=0}}.$$

For $\beta \to \infty$, we recover the zero temperature results.

8.5 Generating functional for fermions

The Lagrangian density for fermions with an external source, is

$$\widehat{\mathcal{L}} = i\overline{\psi}\gamma^{\mu}\partial_{\mu}\psi - m\overline{\psi}\psi + i\widetilde{\overline{\psi}}\gamma^{*\mu}\partial_{\mu}\widetilde{\psi} + m\widetilde{\overline{\psi}}\ \widetilde{\psi} + \overline{\psi}\eta + \overline{\eta}\psi - \widetilde{\overline{\psi}}\widetilde{\eta} - \widetilde{\overline{\eta}}\widetilde{\psi}.$$

The functional

$$Z_0 \simeq \int D\psi D\overline{\psi} D\widetilde{\psi} D\widetilde{\overline{\psi}} e^{i\mathcal{S}}$$

in a normalized form reduces to

$$Z_0[\eta,\overline{\eta},\widetilde{\eta},\widetilde{\overline{\eta}}] = \exp\{-i\int dxdy[\overline{\eta}(x)S(x-y)\eta(x) + \widetilde{\overline{\eta}}(x)\widetilde{S}(x-y)\widetilde{\eta}(x)]\},$$

where $\eta, \overline{\eta}, \widetilde{\eta}$ and $\widetilde{\overline{\eta}}$ are Grassmann variables, and

$$\begin{aligned} S^{-1} &= \ i\gamma^{\mu}\partial_{\mu} - m, \\ \widetilde{S}^{-1} &= \ i\gamma^{*\mu}\partial_{\mu} + m. \end{aligned}$$

Since

$$S^{-1}S = \delta(x), \quad \widetilde{S}^{-1}\widetilde{S} = \delta(x),$$

then S and $\widetilde{S}$ are given respectively by

$$\begin{aligned} S &= (i\gamma\cdot\partial + m)G_0, \\ \widetilde{S} &= (i\gamma^{*}\cdot\partial - m)G_0^{*}, \end{aligned}$$

such that $\widetilde{S} = -S^{*}$. In a matrix notation we have

$$Z_0[\eta,\overline{\eta}] = \exp\{-i\int dxdy[\overline{\eta}(x)\mathbf{S}(x-y)\eta(x)]\},$$

where

$$\overline{\eta} = \left(\overline{\eta}, \widetilde{\overline{\eta}}\right), \quad \eta = \begin{pmatrix} \eta \\ \widetilde{\eta} \end{pmatrix}$$

with $\overline{\eta}_1 = \overline{\eta}, \overline{\eta}_2 = \widetilde{\overline{\eta}}, \eta_1 = \eta, \eta_2 = \widetilde{\eta}$ and

$$\mathbf{S} = \begin{pmatrix} S_0 & 0 \\ 0 & \widetilde{S}_0 \end{pmatrix}$$

This functional provides correct expressions for the propagator components according to the canonical formalism, that is

$$\mathbf{S}(x-y) = i\frac{\delta^2}{\delta\overline{\eta}\delta\eta} Z_0[\eta,\overline{\eta}]|_{\eta=\overline{\eta}=0}.$$

The temperature dependent functional is obtained by using

$$U(\beta) : \mathbf{S}(x-y) \to \mathbf{S}(x-y,\beta),$$

as in the case of bosons, resulting in the thermal propagator. For interacting fields, we obtain

$$Z[\overline{\eta},\eta,\beta] = \frac{\exp\left[i\int dx\widehat{L}_{int}\left(\frac{1}{i}\frac{\delta}{\delta\overline{\eta}};\frac{1}{i}\frac{\delta}{\delta\eta}\right)\right] Z_0[\overline{\eta},\eta;\beta]}{\exp\left[i\int dx\widehat{L}_{int}\left(\frac{1}{i}\frac{\delta}{\delta\overline{\eta}};\frac{1}{i}\frac{\delta}{\delta\eta}\right)\right] Z_0[\overline{\eta},\eta;\beta]|_{\overline{\eta}=\eta=0}}.$$

This leads to the full interacting propagator in TFD.

8.6 Thermal gauge fields

Consider the case of gauge fields such as QCD as presented in Chapter 4. The thermal generating functional and the thermal propagator for each sector of the QCD theory can now be written for TFD. The free fermion sector has been already discussed in the last section. Let us focus on the Gauge and the Faddeev-Popov terms.

For the gauge field we have

$$\mathbf{Z}_0^{G(A,B)}[\mathbf{J}^T,\mathbf{J};\beta] = \exp\{\frac{i}{2}\int dxdy[\mathbf{J}^{T\mu}(x)\mathbf{D}_{0\mu\nu}^{(A,B)}(x-y;\beta)\mathbf{J}^{\nu}(y)\},$$

where (A,B) stands for the gauge group indices and

$$\mathbf{D}_0^{(A,B)\mu\nu}(x;\beta) = \frac{1}{(2\pi)^4}\int d^4k e^{-ikx}\mathbf{D}_0^{(A,B)\mu\nu}(k;\beta)$$

with

$$\mathbf{D}_0^{(A,B)\mu\nu}(k;\beta) = \delta^{AB}\begin{pmatrix} D_0^{11,\mu\nu}(k;\beta) & D_0^{12,\mu\nu}(k;\beta) \\ D_0^{21,\mu\nu}(k;\beta) & D_0^{22,\mu\nu}(k;\beta)\end{pmatrix},$$

such that

$$D_0^{11,\mu\nu}(k;\beta) = D_0^{\mu\nu}(k;\beta) - 2\pi i v^2(k,\beta)d^{\mu\nu}(k)\delta(k), \tag{8.32}$$

$$D_0^{12,\mu\nu}(k;\beta) = D_0^{21,\mu\nu}(k;\beta) = -2\pi i v(k,\beta)u(k,\beta)d^{\mu\nu}(k)\delta(k), \tag{8.33}$$

$$D_0^{22,\mu\nu}(k;\beta) = -D_0^{\mu\nu\ *}(k;\beta) - 2\pi i v^2(k,\beta)d^{\mu\nu}(k)\delta(k), \tag{8.34}$$

with

$$D_0^{\mu\nu}(k;\beta) = d^{\mu\nu}(k)\frac{-1}{k^2+i\varepsilon},$$

where

$$d^{\mu\nu}(k) = g^{\mu\nu} - (1-\alpha)\frac{p^\mu p^\nu}{p^2}.$$

For the Fadeev-Popov fields we have

$$\mathbf{Z}_0^{FP(A,B)}[\overline{\xi},\xi;\beta] = \exp\{\frac{i}{2}\int dxdy[\overline{\xi}^T(x)\mathbf{D}_0^{(A,B)}(x-y;\beta)\xi(y),$$

where $\overline{\xi}$ and ξ are Grassmann variables and $\mathbf{D}_0^{(A,B)}(x-y;\beta)$ is the finite temperature propagator for the scalar field. In terms of the $(1,1)$-(TFD physical) component, we have for the perturbative expression

$$Z[J,\overline{\xi},\xi,\overline{\eta},\eta,\beta] = \mathcal{N}\exp\left[i\int dx\widehat{L}_{int}\left(\frac{1}{i}\frac{\delta}{\delta J},\frac{1}{i}\frac{\delta}{\delta\overline{\xi}},\frac{1}{i}\frac{\delta}{\delta\xi},\frac{1}{i}\frac{\delta}{\delta\overline{\eta}},\frac{1}{i}\frac{\delta}{\delta\eta}\right)\right]$$
$$\times Z_0[J,\overline{\xi},\xi,\overline{\eta},\eta,\beta],$$

where

$$\mathcal{N}^{-1} = \exp\left[i\int dx\widehat{L}_{int}\left(\frac{1}{i}\frac{\delta}{\delta J},\frac{1}{i}\frac{\delta}{\delta\overline{\xi}},\frac{1}{i}\frac{\delta}{\delta\xi},\frac{1}{i}\frac{\delta}{\delta\overline{\eta}},\frac{1}{i}\frac{\delta}{\delta\eta}\right)\right]$$
$$\times Z_0[J,\overline{\xi},\xi,\overline{\eta},\eta,\beta]|_{J,\overline{\xi},\xi,\overline{\eta},\eta=0}.$$

As an example, the contribution to the 3-gluon coupling to the first order is given by

$$D^{A_1A_2A_3}_{\alpha_1\alpha_1\alpha_1}(x_1x_2x_3;\beta) = (-i)^2\frac{\delta^3}{\delta J_1\delta J_2\delta J_3}\int d^4x\mathcal{L}_I^{3G}(\frac{1}{i}\frac{\delta}{\delta J^{A\mu}})Z_0^G[J;\beta]|_{J=0},$$

where $J_i = J^{A_i\mu_i}$, $i = 1,2,3$. We obtain for the physical propagator (1,1-TFD component)

$$\begin{aligned}
D^{A_1A_2A_3}_{\alpha_1\alpha_2\alpha_3}(x_1x_2x_3) = gc^{ABC}&\int d^4x\{\partial_\mu D^{AA_1}_{\nu\mu_1}(x-x_1;\beta) - \partial_\nu D^{AA_1}_{\mu\mu_1}(x-x_1;\beta)\}\\
&\times D^{BA_2\mu}_{\mu_2}(x-x_2;\beta)\ D^{CA_3\nu}_{\mu_3}(x-x_3;\beta)\\
&+gc^{ABC}\int d^4x\{\partial_\mu D^{AA_2}_{\nu\mu_2}(x-x_2;\beta) - \partial_\nu D^{AA_2}_{\mu\mu_2}(x-x_2;\beta)\}\\
&\times D^{BA_3\mu}_{\mu_3}(x-x_3;\beta)\ D^{CA_1\nu}_{\mu_1}(x-x_1;\beta)\\
&+gc^{ABC}\int d^4x\{\partial_\mu D^{AA_3}_{\nu\mu_3}(x-x_3;\beta) - \partial_\nu D^{AA_3}_{\mu\mu_3}(x-x_3;\beta)\}\\
&\times D^{BA_1\mu}_{\mu_1}(x-x_1;\beta)D^{CA_2\nu}_{\mu_2}(x-x_2;\beta).
\end{aligned}$$

It is worth emphasizing that the doubling is a natural structure of the thermal formalism, and we have taken advantage of this fact to introduce the thermalization procedure through a Bogoliubov transformation in the generating functional. However, in calculations treating equilibrium, we have to use just the (1,1)-component of the generating functional, and also for the Green function. Using the (1,1)-functional component, the interaction emerges from the term involving powers of the functional derivatives with respect to the sources, for instance $(\partial/i\partial J)^m$; thus the effect of temperature does not change the interaction terms. As a consequence, the Feynman rules are the same as the ones for $T = 0$ theory, except that we have to use the thermal propagator. This propagator, as that given in Eq. (8.34), can be mapped in the Matsubara propagator, written in term of the Matsubara frequencies, using the analytical procedure presented by Dolan and Jackiw [60]. This aspect is treated in detail in Chapter 15.

Chapter 9

Scattering Process at Finite Temperature

The finite temperature quantum field theory has been used to define response functions in many-body systems [73, 118]. As for zero temperature field theory, the self-energy Σ and the polarization (Π) parts are defined and then the response function is obtained to an arbitrary level of accuracy. This has been applied to the case of magnetic systems, superconducting magnetic systems and just about any other case of a many-body system. TFD has provided results that are valid at any time, t, and finite temperature, T. However, the question of applying TFD to microscopic processes like decay rates, reactions and transition amplitudes has been considered only recently [119]. Use of the imaginary time method [43], a multiple scattering expansion of the self-energy has been attempted. It has been used to calculate the finite temperature response function. Retarded Green's functions have been used to calculate the forward scattering amplitude at two loops. The closed-time path method [120] has been employed to calculate the decay rates and scattering amplitudes [121, 122]. It is important to emphasize that the imaginary time approach is particularly useful for processes in equilibrium. The closed-time path method may be used for both equilibrium and nonequilibrium processes. Over the years these two methods have been used extensively for both many-body systems and for quantum field theory. However, the method using TFD will be considered here in order to provide a general procedure to calculate decay rates, transition amplitudes and reaction rates for particles at finite temperature.

It is worth indicating that such aspects are useful in many diverse areas of physics. In the interior of stars, the particles form a gas at finite temperature. In colliding heavy ion beams at collider facilities such as Relativistic Heavy Ion Collider (RHIC) and at Large Hadron Collider (LHC) the collisions lead to a gas of baryons, nucleons and mesons, or a quark-gluon plasma (QGP). The latter is formed if the temperature of the baryon gas is raised close to 200 MeV, a temperature just above the critical temperature to deconfine the quarks and gluons. The reaction rates of these particles will be affected by the temperature of the interacting particles. This entails a knowledge of reaction rates, decays and transition amplitudes at finite temperature. All of this requires a formalism to calculate such processes.

It should be stressed that a better understanding of dense nuclear matter and

hot QGP would help us to get a better understanding of the early universe. It is important to mention that both in hot QGP and in early universe, the system is strongly time-dependent (i.e. the systems are not in equilibrium). This would require a development of treating many-body systems in a nonequilibrium state. This would lead to the development of mechanisms that lead to a phase transition. Such a study constitutes a distinct subject. However, it should be mentioned that both closed-time path method and TFD are, in principle, capable of handling such nonequilibrium processes leading to phase transitions. Both methods still require further developments. Possible procedures are discussed in the last part of this book.

9.1 Scattering matrix in TFD

In order to calculate quantities such as decay rates, reaction rates and transition amplitudes at finite temperature the Feynman method is adopted. This method is described very well by Dyson [123] when he compares the approach of Schwinger, Tomonaga and Feynman to solve the problem of quantum electrodynamics (see Chapter 4). In the Feynman approach [23], $F_1(x_1), F_2(x_2), \ldots, F_n(x_n)$ are operators defined at points $x_1, x_2, \ldots, x_n$, respectively. The expression

$$T[F_1(x_1)F_2(x_2)...F_n(x_n)]$$

denotes a product of these operators, taken in the order, reading from right to left, in which the surfaces $\sigma(x_1), \sigma(x_2), \ldots, \sigma(x_n)$ occur ordered in time. This defines the time ordering operator T. In practical cases $F_i(x_i)$ and $F_j(x_j)$ will commute if x_i and x_j are located outside the light cone. In such a case, the product depends only on $x_1, x_2, \ldots, x_n$ time ordering. Now, consider an integral

$$I_n = \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{+\infty} dx_n \, T(H^{\ell}(x_0)H_I(x_1)\cdots H_I(x_n)),$$

where $H_I(x_i)$ is the interaction Hamiltonian and $H^{\ell}(x_0)$ is an arbitrary operator. The integral is a symmetrical function of $x_i, \ldots, x_n$. The value of the integral is exactly equal to $n!$ times the integral obtained by restricting the integral such that the surface $\sigma(x_i)$ occurs after $\sigma(x_{i+1})$ for each i. Now the restricted integral may be split into $(n+1)$ parts, the jth part being an integral with $\sigma(x_0)$ lies between $\sigma(x_{j-1})$ and $\sigma(x_j)$. Then we have

$$\begin{aligned} I_n = n! \sum_{j=1}^{N} \int_{-\infty}^{\sigma(x_0)} dx_j ... \int_{-\infty}^{\sigma(x_{n-1})} dx_n \\ \times \int_{\sigma(x_0)}^{\infty} dx_{j-1} ... \int_{\sigma 1 n_0}^{\infty} H_I(x_1)...H_I(x_{j-1})H^{\ell}(x_0)H_I(x_j)...H_I(x_n). \end{aligned}$$

We finally get

$$\begin{aligned} H_F(x_0) &= \sum_{n=0}^{\infty}(-i)^n \frac{1}{n!} I_n \\ &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dx_1 ... \int_{-\infty}^{+\infty} dx_n \\ &\quad \times T[H^{\ell}(x_0) H_I(x_1) ... H_I(x_n)]. \end{aligned}$$

With the choice of $H^{\ell}(x_0) = 1$, we have

$$\begin{aligned} H_F &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dx_1 ... \int_{-\infty}^{+\infty} dx_n \\ &\quad \times T[H_I(x_{n_1}) ... H_I(x_{n_n})]. \end{aligned} \tag{9.1}$$

By taking matrix elements of this operator between appropriate states, various amplitudes and decay rates are obtained not only at zero temperature but also at finite temperature. The states need to be defined appropriately. It should be noticed that the operator H_F, as defined by Feynman, is the same as the S-matrix defined by using asymptotic scattering states. However it is important to point out that at finite temperature there are no well-defined asymptotic states. This necessitated the use of the Feynman method to write down such an operator.

Now we can proceed to calculate individual processes at finite temperature. It is possible to find Cutkosky rules [124] for getting imaginary parts of Feynman diagrams. We calculate the imaginary parts by using the above expression explicitly as well as using the Cutkosky rules.

Symbolically Eq. (9.1), as an S-matrix, is written as

$$\begin{aligned} S &= \sum_{n=0}^{\infty} S^n \\ &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int dx_1 dx_2 ... dx_n T[H_I(x_1) H_I(x_2) ... H_I(x_n)]. \end{aligned} \tag{9.2}$$

Considering the doubling and the tilde-conjugation rules, the S-matrix for TFD is

$$\begin{aligned} \widehat{S} &= \sum_{n=0}^{\infty} \widehat{S}^n \\ &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int dn_1 dx_2 ... dx_n T[\widehat{H}_I(x_1) \widehat{H}_I(x_2) ... \widehat{H}_I(x_n)], \end{aligned} \tag{9.3}$$

where $\widehat{H}_I = H_I(x) - \widetilde{H}_I(x)$. In particular at the tree level

$$\hat{S} = 1 - i \int d^4x [H_I(x) - \widetilde{H}_I(x)]. \tag{9.4}$$

In order to calculate amplitudes, expressions for $H_I(x)$ and $\widetilde{H}_I(x)$ have to be introduced, explicitly. Then Wick theorem is used, as in the zero temperature field

theory, to obtain all the contributions in any order of perturbation theory. To find the temperature dependence, the Bogoliubov transformations of boson and fermion, creation and annihilation, operators have to be used. These operations bring the temperature dependent factors in the matrix elements of the 2×2 Green functions. The cross-section and decay rates depend on the matrix elements, with the phase space remaining unaffected by the finite temperature.

9.2 Reaction rates

Consider a process

$$p_1 + p_2 + ... + p_r \rightarrow p_1' + p_2' + ... + p_r'.$$

The amplitude at $T = 0$ for this process is obtained by the usual Feynman rules by taking

$$\langle f| S |i\rangle = \sum_{n=0}^{\infty} \langle f| S^n |i\rangle ,$$

where $|i\rangle = a^\dagger_{p_1} a^\dagger_{p_2} ... a^\dagger_{p_r} |0\rangle$ and $|f\rangle = a^\dagger_{p_1'} a^\dagger_{p_2'} ... a^\dagger_{p_r'} |0\rangle$ with $|0\rangle$ being the vacuum state, such that $a_p |0\rangle = 0$. For $T \neq 0$, similar procedure may be used. The amplitude for the process is given as

$$\langle f| \widehat{S} |i\rangle = \sum_{n=0}^{\infty} \langle f| \widehat{S}^n |i\rangle ,$$

where

$$|i\rangle = a^\dagger_{p_1}(\beta) a^\dagger_{p_2}(\beta) ... a^\dagger_{p_r}(\beta) |0(\beta)\rangle ,$$
$$|f\rangle = a^\dagger_{p_1'}(\beta) a^\dagger_{p_2'}(\beta) ... a^\dagger_{p_r'}(\beta) |0(\beta)\rangle ,$$

we use the same notation for $|i\rangle$ and $|f\rangle$, since there is no risk of confusion. The state $|0(\beta)\rangle$ is the thermal vacuum. The phase-space factors are the same in both cases. The differential cross-section for the process

$$p_1 + p_2 \rightarrow p_1' + p_2' + ... + p_r'$$

is given as

$$d\sigma = (2\pi)^4 \delta^4(p_1' + p_2' + p_3' + ... + p_r' - p_1 - p_2) \times \frac{1}{4E_1 E_2 v_{rel}} \prod_j (2m_j) \prod_{j=1}^{r} \frac{d^3 p_j'}{(2\pi)^3 2E_j'} |M_{fi}|^2 , \tag{9.5}$$

where $E_j = \sqrt{m_j^2 + \mathbf{p}_j^2}$ and v_{rel} is the relative velocity of the two initial particles with momenta $\mathbf{p}_1$ and $\mathbf{p}_2$. The amplitude M_{fi} is related to the S-matrix element by

$$\langle f| \hat{S} |i\rangle = i (2\pi)^4 M_{fi} \prod_{ext} \left(\frac{M}{VE} \right)^{\frac{1}{2}} \prod_{ext} \left[\frac{m}{Vw} \right]^{\frac{1}{2}} \delta^4(p_f - p_i). \tag{9.6}$$

Here p_f and p_i are the total 4-momenta in the final and initial state; the product extends over all the external fermions and bosons, with $E(M)$ and $w(m)$ being the energy (mass) of fermions and bosons respectively, and V is the volume.

9.3 Decay of particles and generalized Cutkosky rules

It is well-known that at $T = 0$, the decay rates can be calculated by evaluating appropriate Feynman amplitudes. These can also be obtained by evaluating the discontinuities of the self-energy of the decaying particles (Cutkosky rules [124]). These rules have been generalized to finite temperature by Kobes and Semenoff [125]. Here we will use both methods, Feynman amplitudes and generalized Cutkosky rules, to calculate the decay rates. This would validate the use of Feynman diagrams to find decay rates and scattering amplitudes at finite temperature. We analyze the decay rate: $\sigma \to \pi\pi$.

Considering σ and π boson fields, the interaction Lagrangian is

$$\mathcal{L}_I = \lambda\sigma\pi\,\pi, \tag{9.7}$$

that leads to the TFD-interaction Lagrangian

$$\widehat{\mathcal{L}}_I = \mathcal{L}_I - \widetilde{\mathcal{L}}_I = \lambda\sigma\pi\,\pi - \lambda\widetilde{\sigma}\widetilde{\pi}\widetilde{\pi}. \tag{9.8}$$

The initial and final states at finite temperature are, respectively,

$$|i\rangle = a_k^\dagger(\beta)\,|0(\beta)\rangle\,,$$

and

$$|f\rangle = b_{k_1}^\dagger(\beta)b_{k_2}^\dagger(\beta)\,|0(\beta)\rangle\,,$$

where $a_k^\dagger(\beta)$ and $b_k^\dagger(\beta)$ are creation operators at finite temperature for the σ- and π- particles with momenta k. (The association of states like $|i\rangle$ and $|f\rangle$ with the density matrix is discussed in Chapter 12.) At the tree level, the transition matrix element is

$$\begin{aligned}\langle f|\,\widehat{S}\,|i\rangle = i\lambda\int dx\,\langle 0(\beta)|\,b_{k_2}(\beta)b_{k_1}(\beta)\\ \times[\sigma(x)\pi(x)\pi(x) - \widetilde{\sigma}(x)\widetilde{\pi}(x)\widetilde{\pi}(x)]a_k^\dagger(\beta)\,|0(\beta)\rangle\,.\end{aligned}$$

Using the expansion of the boson fields, $\sigma(x)$ and $\pi(x)$, in momentum space, Bogoliubov transformation and the commutation relations, various parts of the matrix elements are:

$$\begin{aligned}\langle 0(\beta)|\,\sigma(x)a_k^\dagger(\beta)\,|0(\beta)\rangle &= e^{-ikx}\cosh\theta_k,\\ -\langle 0(\beta)|\,\tilde{\sigma}(x)a_k^\dagger(\beta)\,|0(\beta)\rangle &= e^{-ikx}\sinh\theta_k,\\ \langle 0(\beta)|\,b_{k_2}(\beta)b_{k_1}(\beta)\pi(x)\pi(x)\,|0(\beta)\rangle &= e^{i(k_1+k_2)x}\cosh\theta_{k_1}\cosh\theta_{k_2},\\ \langle 0(\beta)|\,b_{k_2}(\beta)b_{k_1}(\beta)\tilde{\pi}(x)\tilde{\pi}(x)|0(\beta)\rangle &= e^{i(k_1+k_2)x}\sinh\theta_{k_1}\sinh\theta_{k_2}.\end{aligned}$$

Combining these factors, the amplitude for the process is

$$M_{fi}(\beta) = \lambda[\cosh\theta_k \cosh\theta_{k_1} \cosh\theta_{k_2} - \sinh\theta_k \sinh\theta_{k_1} \sinh\theta_{k_2}].$$

The decay rate for the σ-meson is given as

$$\begin{aligned}\Gamma(w) &= \frac{1}{2w}\int \frac{d^3k_1 d^3k_2 (2\pi)^4 \delta^4(k-k_1-k_2)}{(2w_1)(2w_2)(2\pi)^3(2\pi)^3} \left|M_{fi}(\beta)\right|^2 \\ &= \frac{\lambda^2}{32w\pi^2} I_\beta(T),\end{aligned}$$

where

$$I_\beta(T) = \int \frac{d^3k_1}{w_1}\frac{d^3k_2}{w_2}\delta^4(k-k_1-k_2) W_\beta(w;w_1,w_2), \tag{9.9}$$

$$W_\beta(w;w_1,w_2) = \left[\cosh\theta_k \cosh\theta_{k_1} \cosh\theta_{k_2} - \sinh\theta_k \sinh\theta_{k_1} \sinh\theta_{k_2}\right]^2,$$

with

$$w_i = \sqrt{\kappa_i^2 + m^2}, w = \sqrt{\mathbf{k}^2 + M^2}.$$

This expression simplifies as

$$\begin{aligned}&\delta(w-w_1-w_2) W_\beta(w;w_1,w_2) \\ &= n_1 n_2 n_w [e^{\beta(w+w_1+w_2)/2} - 1]^2 \delta(w-w_1-w_2) \\ &= n_1 n_2 n_w (e^{\beta w} - 1)\left(e^{\beta(w_1+w_2)} - 1\right)\delta(w-w_1-w_2) \\ &= n_1 n_2 n_w [\frac{1+n_w}{n_w} - 1]\{\frac{(1+n_1)(1+n_2)}{n_1 n_2} - 1\}\delta(w-w_1-w_2) \\ &= (1+n_1+n_2)\delta(w-w_1-w_2)\end{aligned}$$

where we have used $n_i = n_\beta(w_i)$, $i = 1, 2$, and $n_w = n_\beta(w)$, with $\sinh^2\theta_k = n_\beta(w)$ and $\cosh^2\theta_k = e^{\beta w} n_\beta(w)$, $n_\beta(w) = \left(e^{\beta w} - 1\right)^{-1}$.

The integral in Eq. (9.9) is calculated explicitly in the rest frame of the decaying particle: $w = M$, $\mathbf{k} = 0$, $w_i = \sqrt{\mathbf{k}_i^2 + m^2} = \sqrt{\mathbf{q}^2 + m^2} = w_q$,

$$\begin{aligned}I_B(\beta) &= \int \frac{d^3k_1}{w_1}\frac{d^3k_2}{w_2}\delta^4(k-k_1-k_2) W_\beta(w;w_1,w_2) \\ &= 4\pi \int \frac{dq q^2}{w_q^2}\delta(2w_q - M) W_\beta(M;w_q,w_q) \\ &= 8\pi\sqrt{\frac{1}{4} - (\frac{m}{M})^2} W_B(M;\frac{M}{2},\frac{M}{2}).\end{aligned}$$

Therefore, the ratio of the decay width at $T \neq 0$ and at $T = 0$ is

$$\frac{\Gamma(T\neq 0)}{\Gamma(T=0)} = W_\beta(M;\frac{M}{2},\frac{M}{2}) = (1 + 2n_B(\frac{M}{2})). \tag{9.10}$$

This result is checked by using the generalized Cutkosky rule.

At $T = 0$, the decay ratio relates to the discontinuity of the self-energy of the decaying particle. For finite temperature, these rules were generalized by Kobes and Semenoff [125]. To illustrate the utility of these rules, we consider the decay of σ-meson into two pions, ignoring the isospin factors. With the interaction Lagrangian given by Eq. (9.8), the generalized Cutkosky rules are applied to calculate the decay rates. The σ-meson is assumed to have a rest mass of M and four-momentum $k = (w, \mathbf{k})$ with $w = \sqrt{\mathbf{k}^2 + M^2}$. Then the decay rate is related to the self-energy by

$$\Gamma_{GCR}(w) = -\frac{1}{w}\mathrm{Im}\sum(k) = \frac{(e^{\beta w} - 1)}{w(e^{\beta w} + 1)}\mathrm{Im}\sum(k), \tag{9.11}$$

where

$$\sum(k) = \lambda^2 \int \frac{d^4p}{(2\pi)^4} iG^0_{11}(p)G^0_{11}(p-k).$$

From generalized Cutkosky rules, we get the imaginary part of the self-energy, $\sum(k)$, using the two contributions shown in Fig. 9.1 This leads to the expression

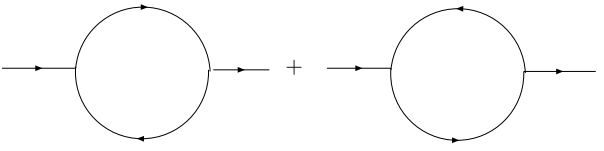


Fig. 9.1 Generalized Cutkosky rules for the imaginary part of the boson self-energy.

$$\begin{aligned}\sum(\kappa) = \frac{\lambda^2}{2}\int \frac{d^4p}{(2\pi)^4} \big[&iG^+_0(p)iG^-_0(p-k) \\ &+iG^-_0(p)iG^+_0(p-k)\big],\end{aligned} \tag{9.12}$$

where $iG^{\pm}_0(p) = 2\pi\left[\theta(\pm p_0) + n_B(p)]\delta(p^2 - m^2)\right]$. The two terms in the integrand are related by

$$iG^{\pm}_0(p) = ie^{\pm\beta p_0}G^{\mp}_0(p).$$

Therefore, we get

$$\begin{aligned}\Gamma_{GCR}(w) = \frac{(e^{\beta w} - 1)(e^{-\beta w} + 1)\lambda^2}{2w(e^{\beta w} + 1)} &\int \frac{d^4p}{(2\pi)^4}(2\pi)^2 \\ &\times\delta(p^2 - m^2)\delta((p-k)^2 - m^2)[\theta(p_0) + n_\beta(p_0)] \\ &\times[\theta(-p_0 + w) + n_\beta(p_0 - w)].\end{aligned} \tag{9.13}$$

Let us calculate this expression explicitly. It is to be noted that at $T \neq 0$ Lorentz invariance is lost and hence, the decay rate will not be invariant. It will be frame dependent. Let us choose the rest frame of the σ-meson so that $\mathbf{k} = 0$ and $k = (M, 0, 0, 0)$. The δ-functions reduce to

$$\delta(p^2 - m^2)\delta((p-k)^2 - m^2) = \frac{1}{4Mw_p}\delta(p_0 - w_p)\delta(w_p - \frac{M}{2}),$$

which is non-zero for $p_0 = w_p = M/2$. This follows since σ is at rest. The thermal factors, $F(\beta)$, in Eq. (9.13) reduce to

$$\begin{aligned} F(\beta) &= \frac{(e^{\beta w}-1)(e^{-\beta w}+1)\lambda^2}{(e^{\beta w}+1)}[\theta(p_0)+n_\beta(p_0)] \\ &\quad \times[\theta(-p_0+w)+n_\beta(p_0-w)] \\ &= (1-e^{\beta M})[1+n_\beta(M/2)]^2. \end{aligned}$$

The ratio for the decay rate at $T \neq 0$ and $T = 0$ is

$$\frac{\Gamma_{GCR}(T\neq 0)}{\Gamma(T=0)} = [1+n_\beta(M/2)]^2 - n_\beta^2(M/2) = \frac{[1+n_\beta(M/2)]^2}{1+n_\beta(M)}, \tag{9.14}$$

where we used

$$e^{-\beta M} = e^{-\beta M/2}e^{-\beta M/2}$$

and

$$e^{-\beta M} = \frac{n_\beta(w)}{1+n_\beta(w)}.$$

Therefore, the results for the decay of $\sigma \to \pi\pi$ agree with the direct calculation from the Feynman graphs.

9.4 Decay of Higgs meson

Here we consider the decay of a scalar Higgs meson, $h(x)$, into electron-positron pair. The interaction Lagrangian density is

$$\widehat{\mathcal{L}}_I = \mathcal{L}_I - \widetilde{\mathcal{L}}_{int} = -igh(x)\overline{\psi}(x)\psi(x) + ig\widetilde{h}(x)\widetilde{\overline{\psi}}(x)\widetilde{\psi}(x). \tag{9.15}$$

At the tree level the decay amplitude is

$$\langle f|\widehat{S}|i\rangle = i(-ig)\int d^4x \langle f|\left[h(x)\overline{\psi}(x)\psi(x) + \widetilde{h}(x)\widetilde{\overline{\psi}}(x)\widetilde{\psi}(x)\right]|i\rangle$$

and the transition amplitude reads

$$\begin{aligned} M_{fi}(\beta) &= (-ig)[\cos\theta_{k_1}\cos\theta_{-k_2}\cosh\theta_k \overline{u}(k_1)v(k_2) \\ &\quad -\sin\theta_{k_1}\sin\theta_{-k_2}\sinh\theta_k \widetilde{\overline{v}}(k_2)\widetilde{u}(k_1)], \end{aligned}$$

where $u(k_1)$ and $v(k_2)$ are the basic spinors (see Chapter 3). The decay rate is

$$\Gamma(w) = \frac{1}{2w}\int \frac{d^3k_1}{(2\pi)^3}\frac{d^3k_2}{(2\pi)^3}\frac{\delta^4(k-k_1-k_2)(2m)^2}{(2w_1)(2w_2)}\sum_{spins}|M_{fi}|^2,$$

where

$$\sum_{spins}|M_{fi}|^2 = g^2 W_F(w,w_1,w_2)\,\mathrm{Tr}\left[\frac{\gamma\cdot k_1+m}{2m}\frac{\gamma\cdot k_2+m}{2m}\right],$$

with

$$W_F(w, w_1, w_2) = \left[\cos\theta_{k_1}\cos\theta_{-k_2}\cosh\theta_k - \sin\theta_{k_1}\sin\theta_{-k_2}\sinh\theta_k\right]^2$$
$$= \cos^2\theta_{k_1}\cos^2\theta_{-k_2}\cosh^2\theta_k\left[1 - e^{-\beta(w+w_1+w_2)/2}\right]^2$$

where we use $\sin^2\theta_{\pm k} = \left[1 + e^{\beta(k_0 \mp \mu)}\right]^{-1}$, $\cos^2\theta_{\pm k} = e^{\beta(k_0 \pm \mu)/2}\sin^2\theta_{\pm k}$ with $\sin^2\theta_{+k} = n_F(k)$ and $\sin^2\theta_{-k} = \overline{n}_F(k)$. Here $n_F(\kappa)$ and $\overline{n}_F(\kappa)$ refer to the distribution function of fermions and anti-fermions respectively.

Hence the ratio of decay width is

$$\frac{\Gamma(T \neq 0)}{\Gamma(T = 0)} = W_F(w, w_1, w_2)$$
$$= \left[1 - n_F(M/2)\right]\left[1 - \overline{n}_F(M/2)\right]\left(1 - e^{\beta M}\right)$$

where M is the mass of the scalar particle.

9.5 The detailed balance

The decay rate of a boson into r bosons is

$$\Gamma(w) = \frac{1}{2w}\int \frac{d^3k_1 d^3k_2 ... d^3k_r}{(2w_1)(2w_2)...(2w_r)(2\pi)^3}\delta(k - k_1 - k_2 ... - k_r)\left|M_{fi}(\beta)\right|,$$

where

$$\left|M_{fi}(\beta)\right|^2 = \left[\cosh\theta_k\cosh\theta_{k_1}...\cosh\theta_{k_r} - \sinh\theta_k\sinh\theta_{k_1}...\sinh\theta_{k_r}\right]^2$$
$$= n_1...n_r n_w\left[1 - e^{-\beta w}\right]\left[1 - e^{-\beta(w_1+w_2+...+w_r)}\right]$$
$$= \left[(1+n_1)(1+n_2)...(1+n_r) - n_1 n_2 ... n_r\right],$$

with n_i is the boson distribution function. The total decay rate is

$$\Gamma(w) = \Gamma_d(w) - \Gamma_i(w),$$

where $\Gamma_d(w)$ and $\Gamma_i(w)$ are the forward and inverse process for the decay. These are related by the detailed balance principle

$$\frac{\Gamma_d(w)}{\Gamma_i(w)} = \frac{(1+n_1)(1+n_2)...(1+n_r)}{n_1 n_2 ... n_r}.$$

This is a relation discovered by Weldon [126].

It is important to remark that an experiment measures only the total decay rate, $\Gamma(w)$, and not any partial decay rates like $\Gamma_d(w)$ and $\Gamma_i(w)$. This follows from the fact that the total rate, $\Gamma(w)$, is connected to the pole of the one-particle Green function. The rates like $\Gamma_d(w)$ and $\Gamma_i(w)$ have no such direct relation to the physical quantities.

9.6 Scattering cross-section of $1 + 2 \to 1' + 2'$

The cross-section for the process $1+2 \to 1'+2'$, in terms of the transition amplitude, is

$$\frac{d\sigma}{d\Omega'} = \frac{|M_{fi}(\beta)|^2 \left[\prod_{j=1}^{2} 2mj\right] |\mathbf{k}'_1|^2}{64\pi^2 \nu_{rel} w_1 w_2 w'_1 w'_2} \{\frac{\delta\,(w'_1 + w'_2)}{\delta|\mathbf{k}'_1|}\}^{-1}$$

Therefore the ratio of cross-sections is

$$\frac{(d\sigma/d\Omega'|_{T\neq 0}}{(d\sigma/d\Omega'|_{T=0}} = \frac{|M_{fi}(T)|^2}{|M_{fi}(T=0)|^2} \equiv W(T)$$

Now we analyze some particular examples and evaluate the expression for $W\,(\beta)$.

9.6.1 *Boson-boson scattering*

Assume an interaction Lagrangian for two bosons a and b denoted by field ϕ_a and ϕ_b, respectively,

$$\mathcal{L}_I = \lambda \phi_a^2 \phi_b^2$$

and

$$\hat{\mathcal{L}}_I = \mathcal{L}_I - \widetilde{\mathcal{L}}_I.$$

Proceeding as in the case of the decays processes, the tree level amplitude can be obtained at finite temperature and the ratio is written as

$$W_{BB}(T) = \frac{|M_{fi}(T \neq 0)|^2}{|M_{fi}(T=0)|^2} = [C(T)S(T)]^2$$

where

$$C(T) = \cosh\theta_{k_1} \cosh\theta_{k_2} \cosh\theta_{k_3} \cosh\theta_{k_4},$$
$$S(T) = \sinh\theta_{k_1} \sinh\theta_{k_2} \sinh\theta_{k_3} \sinh\theta_{k_4}.$$

Using the notation $n_i = n_B(k_i)$ and $n'_i = n_B(k'_i)$, the expression $W_{BB}(T)$ is reduced to

$$W_{BB}(T) = [(1+n_1)(1+n_2) - n_1 n_2][(1+n'_1)(1+n'_2) - n'_1 n'_2]$$

Energy conservation, $w_1 + w_2 = w'_1 + w'_2$, is needed to get this relation.

9.6.2 *Fermion-fermion scattering*

Assume an interaction Lagrangian for two fermions a and b described by the fermi fields $\Psi_a(x)$ and $\Psi_b(x)$ respectively to be

$$\mathcal{L}_I = \lambda \bar{\Psi}_a(x) \Gamma_\alpha \Psi_a(x) \bar{\Psi}_b \Gamma^\alpha \Psi_b(x)$$

where Γ_α is an appropriate Dirac matrix. In this case the temperature dependent factor is

$$\begin{aligned} W_{FF}(\beta) &= \frac{|M_{fi}(T \neq 0)|^2}{|M_{fi}(T=0)|^2} \\ &= \left[\cos\theta_{k_1}\cos\theta_{k_2}\cos\theta_{k_1'}\cos\theta_{k_2'} - \sin\theta_{k_1}\sin\theta_{k_2}\sin\theta_{k_1'}\sin\theta_{k_2'}\right]^2 \\ &= n_F(k_1)\, n_F(k_2)\, n_F(k_1')\, n_F(k_2')\left[e^{\beta\left(w_1+w_2-\mu_1-\mu_2+w_1'+w_2'-\mu_1'-\mu_2'\right)}\right]. \end{aligned}$$

At equilibrium, $\mu_1 + \mu_2 = \mu_1' + \mu_2'$ and using the conservation of energy, $w_1 + w_2 = w_1' + w_2'$, this expression is simplified to

$$W_{FF}(\beta) = [(1-n_1)(1-n_2) - n_1 n_2][(1-n_1')(1-n_2') - n_1' n_2'],$$

where $n_i = n_F(k_i)$ and $n_1' = n_F(k_i')$ are fermion distribution functions.

9.7 Fermion-boson scattering

Assume an Lagrangian describing the interaction between a fermion ($\Psi(x)$) and a boson ($\phi(x)$) to have the form

$$\mathcal{L}_I = -g\bar{\Psi}(x)\Gamma\Psi(\lambda)\phi(x).$$

At the tree level, the temperature dependant factor has the form

$$\begin{aligned} W_{FB}(T) &= \frac{|M_{fi}(T \neq 0)|^2}{|M_{fi}(T=0)|^2} \\ &= \left[\cos\theta_{k_1}\cosh\theta_{k_2}\cos\theta_{k_1'}\cosh\theta_{k_2'} - \sin\theta_{k_1}\sinh\theta_{k_2}\sin\theta_{k_1'}\sinh\theta_{k_2'}\right]^2 \\ &= \left[(1-n_F(k_1)) + n_B(k_2)\right]\left[1-n_F(k_1') + n_B(k_2')\right]. \end{aligned}$$

Use of the energy conservation, $w_1 + w_2 = w_1' + w_2'$, is essential to prove this relation.

These examples show that calculations for decay rates, transition probability and reaction cross-sections at finite temperature are quite simple with TFD. It is important to note that these results are only useful in the study of matter at high temperatures. This is the case, for instance, for particles in the early days of the universe. Ultimately, these results have to be included in an equation like the Boltzmann equation in the collision term to describe the full process. A similar procedure, for instance, would be needed to describe the results from RHIC, heavy ion collider.

We have considered the decay and scattering amplitudes at the tree level. These can be extended to loop diagram contributions that require renormalization. However, it is possible to carry out the calculation to higher order perturbation theory. For particles in a many-body system at high temperature, it is not quite correct to use the Lagrangian density as obtained for decay of particles in free space. The particular problem arises since coupling constants and mass of particles change with temperature [127]. In such a case a self-consistent calculation has to be carried

out. A consistency can be achieved by using Ward-Takahashi relations at finite temperature. This assures that the results obey the symmetry of the interaction Lagrangian. Renormalization procedures and Ward-Takahashi relations at finite temperature are discussed in the next two chapters.

Chapter 10

Topics on Renormalization Theory

In this chapter we present some of the structural elements underlying renormalization theory. We concentrate ourselves on the massive $\lambda\phi^4$-theory, and skip almost all the proofs. For rigorous treatments of the presented topics, specific references are indicated throughout the chapter. Our plan is to be neither rigorous nor exhaustive, but to discuss the main aspects of the techniques of dealing with ultraviolet divergences in Feynman amplitudes. For the renormalization group and the Bogoliubov recurrence only an overview is presented. In particular, we analyze procedures of renormalization including the effect of temperature and spatial confinement.

10.1 Ultraviolet divergences

We start from the Lagrangian density,

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) + \frac{m^2}{2}\phi^2(x) + \frac{\lambda}{4!}\phi^4(x), \tag{10.1}$$

and let us examine some properties of Feynman integrals. The set of Feynman amplitudes with a given number of vertices, V and external lines N, is the coefficient of λ^V in the perturbative expansion of the N-point Green function. For the moment finiteness and dimension of the coupling constant are not considered, we just look at some formal properties of the integrals.

Products of fields at the same point are, in general, divergent, and the translation of this fact to Feynman diagrams in momentum space gives rise to divergences of the Feynman integrals over the momenta of independent loops at the upper limit. The structure of these divergences has been clarified and a way to treat them has been established with a recursive process, the Bogoliubov recurrence [128, 129]. This and similar procedures are known under the general denomination of renormalization. The underlying idea is to hide the infinities into unobservable bare parameters, that would describe phenomena at vanishingly small distances, or equivalently at extremely high energies. Unless some fundamental graininess of space-time is assumed, as could be the case of the Planck scale in string theory [130], these distances should truly vanish, corresponding to the product of fields at the same point, lead-

ing to infinities. The procedure then prescribes to add to the Lagrangian density equally infinite *counterterms*, such that lead to finite, physically observable, quantities. For a clear and pedagogical presentation on the subject see [130] and for a rigorous treatment for both commutative and non-commutative field theories, the reader is referred to [131].

But renormalization is not only a way to remove divergences by, at first sight, a rather artificial procedure. Renormalization was discovered to apply to condensed matter physics [132], besides particle physics. The important point is that precisely one of the disturbing aspects of the renormalization process in particle physics, the existence of an arbitrary scale parameter, plays a central role. The renormalization group (RG), was discovered to be the appropriate mathematical tool to move through the different scales of physics. RG techniques become a major tool for a better understanding of phase transitions, in particular of the universal character of critical exponents and the relations among them [133].

The simplest example of these divergences occurs in the diagram of Fig. 10.1(a), the first correction to the two-point function. More generally, any insertion of the type shown in Fig. 10.1(b) in a larger diagram does give rise to the same divergence. The diagram of Fig. 10.1(b) corresponds to an integral (in the 4-dimensional Euclidian space) given by

$$\int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2+m^2}. \tag{10.2}$$

This integral is quadratically divergent. As a second example, we consider the

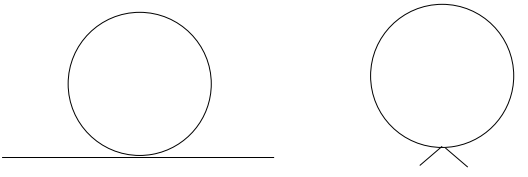


Fig. 10.1 Diagrams with the same type of divergence: (a) Mass correction diagram, (b) General diagram insertion.

diagram given in Fig. 10.2. The corresponding Feynman integral is given by

$$\int \frac{d^4k}{(2\pi)^4} \frac{1}{(k^2+m^2)[(p-k)^2+m^2]}, \tag{10.3}$$

which is logarithmically divergent at the upper limit.

As a third example, we consider the diagramatic insertion of Fig. 10.3, corresponding to the integral,

$$\int \frac{d^4k_1 d^4k_2}{(k_1^2+m^2)(k_1^2+m^2)[(p-k_1-k_2)^2+m^2]}, \tag{10.4}$$

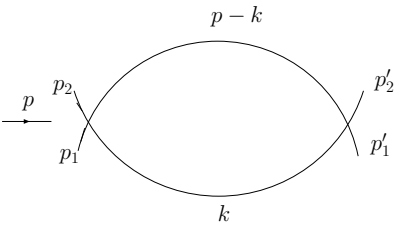


Fig. 10.2 Logarithmically divergent diagram.

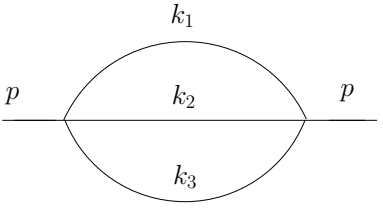


Fig. 10.3 Quadratically divergent diagram.

which is quadratically divergent at the upper limit.

In general in a D-dimensional Euclidian space, a diagramatic insertion G has an expression of the form (omitting external factors and coefficients)

$$A_G(\{p\}) = \int \prod_{i=1}^{I} \frac{d^D q_i}{(2\pi)^D} \prod_{i=1}^{I} \frac{1}{q_i^2 + m^2} \prod_{v=1}^{V} \delta(\sum_i \epsilon_{vi} q_i), \tag{10.5}$$

where $\{p\}$ stands for the set of external momenta, V is the number of vertices, I is the number of internal lines and q_i stands for the momentum of each internal line i. The quantity ϵ_{vi} is the *incidence matrix*, which equals 1 if the line i arrives at the vertex v, -1 if it starts at v and 0 otherwise. Performing the integrations over the internal momenta, leads to a choice of independent loop-momenta $\{k_l\}$ and we get,

$$A_G(\{p\}) = \int \prod_{l=1}^{L} \frac{d^D k_l}{(2\pi)^D} \prod_{i=1}^{I} \frac{1}{q_i^2(\{p\}, \{k_l\}) + m^2} \tag{10.6}$$

where L is the number of independent loops. The momentum q_i is a *linear* function of the independent internal momenta k_l and of the external momenta $\{p\}$. The integral is convergent if $DL - 2I < 0$; otherwise, if $DL - 2I \geq 0$, the integral is ultraviolet divergent in the upper integration limit. So, given a diagram G, we define the quantity

$$d(G) = DL(G) - 2I(G) \tag{10.7}$$

as the superficial divergence degree of the diagram. If $d(G) \geq 0$ the diagram will be ultraviolet divergent.

For any sub-diagram $S \subset G$ there are corresponding sub-integrations,

$$A_S(\{p\}) = \int \prod_{\alpha=1}^{L(S)} \frac{d^D k_l}{(2\pi)^D} \prod_{i=1}^{I(S)} \frac{1}{q_i^2(\{p\},\{k_l\}) + m^2} \tag{10.8}$$

where $L(S)$ and $I(S)$ are, respectively, the number of loops and the number of internal lines of the sub-diagram S. Then if the quantity

$$d(S) = DL(S) - 2I(S) \geq 0, \tag{10.9}$$

an ultraviolet divergence will appear associated with the sub-diagram S. Thus even if the diagram G is said to be superficially convergent, $d(G) < 0$, the Feynman integral A_G is divergent. For this, it is enough that there is a sub-diagram S such that $d(S) \geq 0$. This has been stated in [128] as:
If for all subdiagrams $S \subseteq G$ we have $d(S) < 0$ the Feynman integral A_G is ultraviolet convergent. If there is at least one $S \subseteq G$, such that $d(S) \geq 0$, A_G is ultraviolet divergent.
The divergent subdiagrams of a given diagram are called *renormalization parts*. For the full renormalization process, we need consider only non-overlaping renormalization parts [128, 129].

10.2 Regularization

Regularization is a procedure to replace divergent Feynman amplitudes with more general integrals by means of a set of supplementary parameters, such that the theory does not have ultraviolet divergences when these parameters belong to some domain. For a certain limit of these parameters we find the original theory with their divergences. This is a provisional procedure allowing to perform formal calculations to explore more precisely the divergences to be suppressed. Some types of regularization are described in the following.

- Cutoff in the momenta
  In this case we introduce an upper bound in the momentum modulus, that is $|k|^2 \leq \Lambda$, and the original theory is recovered when $\Lambda \to \infty$.
- Pauli-Villars regularization
  We introduce a mass parameter M by the correspondence
  $$\frac{1}{k^2+m^2} \to \frac{M^2-m^2}{(k^2+m^2)(k^2+M^2)}; \quad M \to \infty \tag{10.10}$$
- Analytic regularization
  By changing the propagators
  $$\frac{1}{k^2+m^2} \to \frac{1}{(k^2+m^2)^s}, \tag{10.11}$$
  the integrals converge for high enough values of $\{s\}$ and define regular functions of the variables s, for which one looks for the analytical continuation notably in the neighborhood of $\{s = 1\}$.

- Lattice regularization
  In this case we proceed with a discretization of the continuous space-time by introducing lattice characterized by a spacing parameter a between neighboring sites. The original theory is recovered by taking $a \to 0$. This method is an important tool particularly in the non-perturbative domain of non-abelian field theories.
- Dimensional regularization
  The central idea is to define the Feynman integrals in a generic space-time of dimension D for which the integrals are convergent. The divergences are recovered as poles of some functions. We will be particularly concerned with the integral,

$$\int \frac{d^D p}{(2\pi)^D} \frac{1}{(p^2+M)^s} = \frac{\Gamma\left(s-\frac{D}{2}\right)}{(4\pi)^{\frac{D}{2}}\Gamma(s)} \frac{1}{M^{s-\frac{D}{2}}}\,, \tag{10.12}$$

  This method was developed, independently, by Bollini and Giambiagi [134] and 't Hooft and Veltman [135]. In this book we largely employ this method.

Let us emphasize that regularization does not suppress the divergences. This will be performed by the renormalization procedure, a concept to be summarized in the next section.

10.3 Renormalization

Let us consider a primitively divergent diagram, that is, a diagram that is divergent but does not contain divergent sub-diagrams. Moreover we start with the simple case of a logarithmically divergent diagram. Let N be the number of external lines of a diagram G. The basis of the pertubative renormalization method is that the starting theory is not consistent as a physical model, and this fact manifests itself as divergences. Then one attempts to modify the theory, by introducing supplementary terms, *counter-terms*, in the original Lagrangian, in such a way to cancel the original divergences. It is outside the scope of this chapter to present all the steps of the proof of renormalizability. However we present some examples and will describe in a simplified manner the basic steps of the technique [128, 136].

In the simple case of a logarithmically primitive-divergent diagram, depicted in Fig. 10.4, we change the Lagrangian according to

$$\mathcal{L} \to \mathcal{L} + c_G \phi^N\,. \tag{10.13}$$

With this new Lagrangian, we have not only the amplitude A_G for the diagram in Fig. 10.4(a), but also the amplitude c_G for the new diagram in Fig. 10.4(b). Next we introduce anyone of the regularization methods described in the previous section, represented by a parameter η. We represent symbolically by $\eta \to 0$ the suppression of the regularization. Then it is verified that the regularized amplitude is written

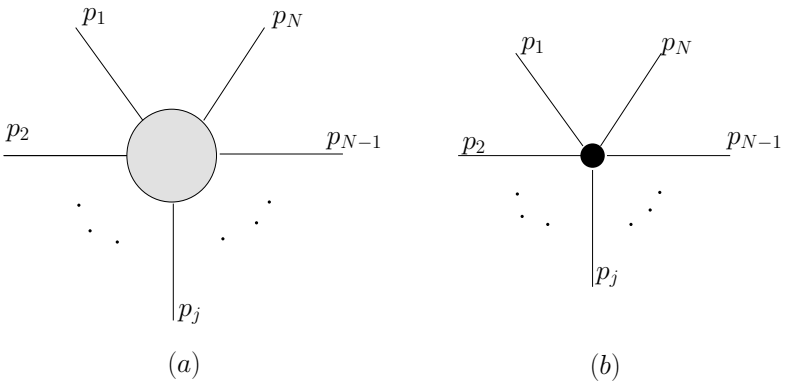


Fig. 10.4 Logarithmically primitive-divergent diagram.

in the form

$$A_G^{\mathrm{Reg}}(\{p\};\eta) = A_G^{\mathrm{Div}}(\eta) + A_G^{\mathrm{Ren}}(\{p\};\eta), \tag{10.14}$$

where

$$\lim_{\eta\to 0} A_G^{\mathrm{Div}}(\eta) = \infty\,; \quad \lim_{\eta\to 0} A_G^{\mathrm{Ren}}(\{p\};\eta) = A_G^{\mathrm{Ren}}(\{p\}) < \infty \tag{10.15}$$

If we choose in the Lagrangian $\mathcal{L}$ the coefficient c_G with the value $c_G = -A_G^{\mathrm{Div}}(\eta)$, we find that the sum of the amplitudes corresponding to Fig. 10.4(a,b) tends to the finite limit $A_G^{\mathrm{Ren}}(\{p\})$ when the regularization is suppressed. The amplitude $A_G^{\mathrm{Ren}}(\{p\})$ is said to be the renormalized amplitude. Before going to the general situation we give some examples of ultraviolet divergent diagrams, and how these divergences can be suppressed. Let us start by presenting some comments about dimensional analysis. We are presenting results in dimension 4. The action (energy $\times$ time) is measured in units of the Planck constant, $\hbar$, and velocity in units of the speed of light, c. We take $\hbar = c = 1$, the natural units. The Lagrangian density has the same dimension as the Hamiltonian density, i.e., $[\mathcal{L}] = [\mathcal{H}] = Energy/L^3$, where L stands for the linear dimension of space. Then energy has dimension of mass, M, i.e. $[energy] = M = L^{-1} = T^{-1}$, with T standing for time. As the action is dimensionless, then $[\mathcal{L}] = M^4$. For the scalar field, $\phi(x)$, we find $[\phi] = M$. Let us remark that, for the perturbative series to be meaningful, the coupling constant has to be dimensionless. This is true for the $\lambda\phi^4$ model in the 4-dimension space-time. If we use dimensional regularization, we need to take $D \neq 4$, and in this case we can choose a dimensionless coupling constant defined by $\lambda^{'} = \lambda\mu^{-4+D}$, where μ is an arbitrary constant with dimension of mass. This kind of arbitrariness is present also when we use other regularizations.

As a first example, we consider the tadpole diagram given by,

$$A_{Tadpole} \sim \lambda \int \frac{d^D k}{(2\pi)^D} \frac{1}{k^2 + m^2}$$
$$= \frac{\lambda' \mu^{-D+4}}{(2\pi)^D} \pi^{D/2} \, (m^2)^{\frac{D-2}{2}} \, \Gamma(\frac{2-D}{2}), \tag{10.16}$$

where we have used Eq. (10.12). If we take $D = 4$, $\Gamma(\frac{2-D}{2}) = \Gamma(-1)$, which is singular. Taking $D = 4 - 2\epsilon$ we have,

$$\Gamma(\frac{2-D}{2}) = \Gamma(-1 + \epsilon), \tag{10.17}$$

which can be expanded around $\epsilon = 0$ using the formula

$$\Gamma(-n + \epsilon) = \frac{(-1)^n}{n!} \left[\frac{1}{\epsilon} + \psi(n+1) + \mathcal{O}(\epsilon) \right], \tag{10.18}$$

where $\psi(z) = d \ln(z)/dz$.

Taking $n = 1$ in Eq. (10.18) and replacing it in Eq. (10.16), we get

$$A_{Tadpole} \sim -\frac{\lambda' \pi^{D/2}}{(2\pi)^D} \, (m^2)^{\frac{D-2}{2}} \frac{1}{\epsilon}$$
$$-\frac{\lambda' \pi^{D/2}}{(2\pi)^D} \left[\psi(2) - 2 \ln \left(\frac{m}{\mu} \right) + O(\epsilon) \right].$$

When $\epsilon \to 0$ the divergence is isolated in the term

$$A^{div}_{Tadpole} = -\frac{\lambda' \pi^{D/2}}{(2\pi)^D} \, (m^2)^{\frac{D-2}{2}} \frac{1}{\epsilon} \Big|_{D=4}$$
$$= -\frac{\lambda}{16\pi^2} \, m^2 \frac{1}{\epsilon}.$$

Let us now take a look at the contribution of the tadpole to the 2-point Green function, depicted in Fig. 10.5(a). We have,

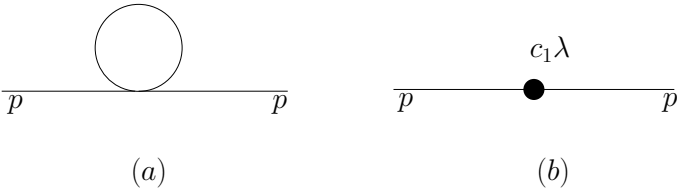


Fig. 10.5 Tadpole contribution to the 2-point Green function.

$$G^{(2)} = \left(\frac{1}{p^2 + m^2} \right)^2 \left\{ -\frac{\lambda' \pi^{D/2}}{(2\pi)^D} \, (m^2)^{\frac{D-2}{2}} \frac{1}{\epsilon} \right.$$
$$\left. -\frac{\lambda' \pi^{D/2}}{(2\pi)^D} \left[\psi(2) - 2 \ln \left(\frac{m}{\mu} \right) + O(\epsilon) \right] \right\}.$$

If we add to the Lagrangian a partial counterterm $c_1\lambda'\phi^2$ with the choice

$$c_1 = \frac{\lambda'\pi^{D/2}}{(2\pi)^D}\ (m^2)^{\frac{D-2}{2}}\frac{1}{\epsilon},$$

then it results that the renormalized two point Green function, given by the sum of the two diagrams in Figs. 10.5(a) and 10.5(b), in the limit of $\epsilon \to 0$, is

$$A^{\rm Ren}_{G^{(2)}} = \frac{\lambda\pi^2}{(2\pi)^4}\left\{\left[-\psi(2) + 2\ln\left(\frac{m}{\mu}\right)\right]\right\}. \tag{10.19}$$

This gives us a finite amplitude.

As a second example, let us analyze a two-loop contribution to the two-point function, depicted in Fig. 10.6(a). More involved calculations are required in this case. We find,

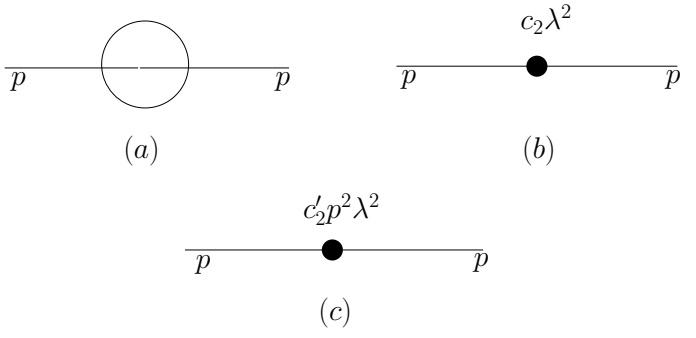


Fig. 10.6 2-loop contribution to the mass.

$$A_{G^{(2)}}(p;\epsilon) = \frac{\lambda^2}{6(16\pi^2)^2}\left[\frac{3m^2}{2\epsilon^2} + \frac{3m^2}{\epsilon}\left(\frac{3}{2} + \psi(1) + \ln\left(\frac{4\pi\mu^2}{m^2}\right)\right)\right] + \frac{\lambda^2}{6(24\pi^2)^2}\frac{p^2}{\epsilon} + A^{\rm Ren}_G(p;\epsilon),$$

where $A^{\rm Ren}_{G^{(2)}}(p;\epsilon)$ tends to a finite limit, $A^{\rm Ren}_G(p)$, when $\epsilon \to 0$. In this case, we have to add to the Lagrangian two partial counterterms of the form,

$$c_2\lambda^2\phi^2 + c_2'\lambda^2\partial_\mu\phi\partial^\mu\phi,$$

giving rise to the diagrams depicted in Figs. 10.6(b) and 10.6(c). With the choice

$$c_2 = -\frac{1}{6(16\pi^2)^2}\left[\frac{3m^2}{2\epsilon^2} + \frac{3m^2}{\epsilon}\left(\frac{3}{2} + \psi(1) + \ln\left(\frac{4\pi\mu^2}{m^2}\right)\right)\right] \tag{10.20}$$

and

$$c_2' = -\frac{1}{24(16\pi^2)^2}\frac{1}{\epsilon} \tag{10.21}$$

the sum of the three diagrams in Fig. 10.6(a–c) gives the finite result $A^{\rm Ren}_{G^{(2)}}(p)$.

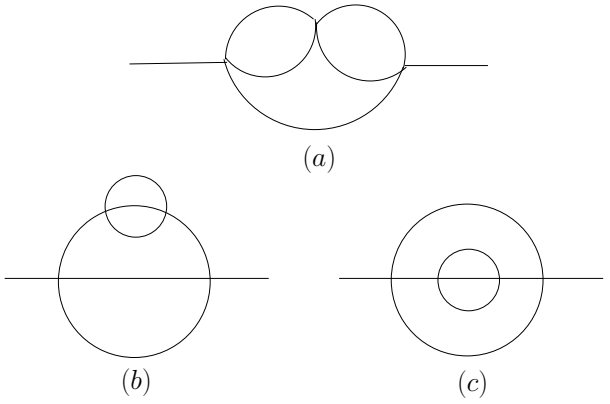


Fig. 10.7 Diagrams corresponding to counterterms given in Eqs. (10.22) and (10.23).

The diagrams in Figs. 10.7(a)–10.7(c) correspond to partial counterterms of the type

$$c_3\lambda^3\phi^2 + c_3'\lambda^3\partial_\mu\phi\partial^\mu\phi, \tag{10.22}$$

and

$$c_4\lambda^4\phi^2 + c_4'\lambda^4\partial_\mu\phi\partial^\mu\phi. \tag{10.23}$$

The definition of a 1PI (one-particle-irreducible) diagram, as a diagram such that it cannot be transformed into a disconnected diagram by cutting just one line, means that the diagrams considered above of order λ^2, λ^3 and λ^4 are 1PI diagrams.

If we represent by a full circle, as depicted in Fig. 10.8(a), the sum of all 1PI diagrams with two external lines cut, any insertion as represented in Fig. 10.8(b) can be written in the form

$$\Sigma(p)\frac{1}{p^2+m^2}\Sigma(p),$$

where $\Sigma(p)$ is the *sum* of all 1PI diagrams in Fig. 10.8(a). For complete evaluation of the 2-point Green function, we limit ourselves to just 1PI-diagrams.

The logical structure of the process tells us that in order to suppress the ultraviolet divergences of the two-point function, it is necessary to introduce two counterterms (not partial counterterms) of the form

$$c^{(2)}\lambda^2\phi^2 + c^{(2)\prime}\lambda^2\partial_\mu\phi\partial^\mu\phi$$

where each counterterm $c^{(2)}$ and $c^{(2)\prime}$, is an infinite series in λ corresponding to ultraviolet divergent diagrams to all orders, i.e.

$$c^{(2)}(\eta) = \lambda c_1^{(2)}(\eta) + \lambda^2 c_2^{(2)}(\eta) + \cdots + \lambda^n c_n^{(2)}(\eta) + \cdots,$$
$$c^{(2)\prime}(\eta) = \lambda c_1^{(2)\prime}(\eta) + \lambda^2 c_2^{(2)\prime}(\eta) + \cdots + \lambda^n c_n^{(2)\prime}(\eta) + \cdots,$$

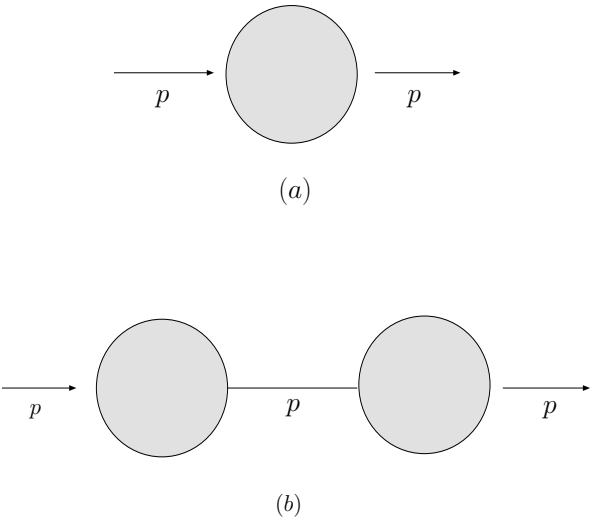


Fig. 10.8 Tadpole contribution to the 2-point Green function.

where $c_n^{(2)}(\eta)$ and $c_n^{(2)\prime}(\eta)$ are such that

$$\lim_{\eta\to 0} c_n^{(2)}(\eta) \to \infty$$
$$\lim_{\eta\to 0} c_n^{(2)\prime}(\eta) \to \infty,$$

in order to cancell the ultraviolet divergences of all the diagrams contributing to the two-point function. Each coefficient, $c_n^{(2)}(\eta)$ and $c_n^{(2)\prime}(\eta)$ is exactly what we have called partial counterterms.

Let us now consider the 4-point insertion to lowest order (Fig. 10.2), given by

$$A_{G^{(4)}} = \frac{(\mu^2)^{2-\frac{D}{2}}(\lambda')^2}{(2\pi)^D}\int \frac{d^D k}{[(p-k)^2+m^2](k^2+m^2)}. \tag{10.24}$$

This amplitude can be evaluated using the identity,

$$\frac{1}{A_1\cdots A_I} = \int_0^1 dx_{_1}\cdots dx_{_I}\,\delta\left(\sum_{i=1}^{I} x_i - 1\right) \times \frac{(I-1)!}{[x_1A_1+\cdots+x_IA_I]^I}, \tag{10.25}$$

and Eq. (10.12). By taking $D = 4-2\epsilon$, and using Eq. (10.18), we get

$$A_{G^{(4)}} = (\mu^2)^{2-\frac{D}{2}}\frac{(\lambda')^2}{16\pi^4\epsilon} + (\mu^2)^{2-\frac{D}{2}}\frac{(2\lambda')^2}{(32\pi)^2} \times\left[\psi(1) - \int_0^1 dx\,\ln\frac{m^2+p^2x(1-x)}{4\pi\mu^2}\right] + O(\epsilon). \tag{10.26}$$

The choice of the partial counterterm

$$c_2^{(4)} = -\frac{(\lambda')^2}{16\pi^4\epsilon} \tag{10.27}$$

suppresses the ultraviolet divergence of the diagram in the limit $\epsilon \to 0$.

Similarly, for higher order diagrams, we have respectively partial countertems of the form $\lambda^3 c_3^{(4)}$ and $\lambda^4 c_4^{(4)}$. This can be extended to all orders, which correspond to the addition of a counterterm of the type

$$c^{(4)}(\eta) = \lambda^2 c_2^{(4)}(\eta) + \cdots + \lambda^n c_n^{(4)}(\eta) + \cdots . \tag{10.28}$$

10.3.1 *Renormalization parts in the $\lambda\phi^4$ theory*

An essential aspect of renormalization is to determine how many counterterms must be introduced in the theory to make it convergent. In order to examine this point let us first note that for a given diagram G of the $\lambda\phi^4$ model, the number of independent loops $L(G)$, internal lines $I(G)$ and vertices $V(G)$ satisfies the topological formula,

$$L(G) = I(G) - V(G) + 1.$$

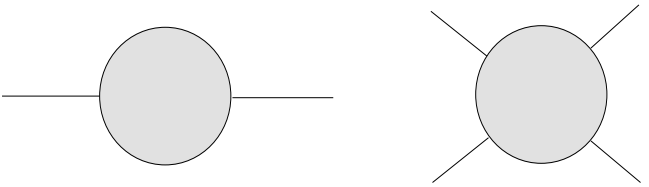
Moreover, if the diagram has $N(G)$ external lines, the relation

$$2I(G) + N(G) = 4V(G),$$

holds. Then the superficial degree of divergence $d(G) = DL(G) - 2I(G)$ becomes

$$d(G) = D - V(G)(D-4) + N(G)\left(1 - \frac{D}{2}\right). \tag{10.29}$$

For $D = 4$, we find that $d(G) \geq 0$ if, and only if, $N(G) \leq 4$. This implies that, to any order, the only ultraviolet divergent diagrams are those for which $N(G) = 2, 4$; see Fig. 10.9. Note that, as one infers from topological considerations, there are no diagrams with $N(G) = 3$ in the $\lambda\phi^4$ model.



(*a*) $d = 2$ (*b*) $d = 0$

Fig. 10.9 Tadpole contribution to the 2-point Green function.

The insertions $A_{G^{(2)}}$ and $A_{G^{(4)}}$ with 2 and 4 external lines respectively, and only those, are ultraviolet divergent. Thus for $D = 4$, we need to introduce only two counterterms, $c^{(2)}\phi^2 + c^{(2)\prime}\partial_\mu\phi\partial^\mu\phi$ and $c^{(4)}\phi^4$, to get a divergence free theory, at least as far as primitively divergent diagrams are concerned. We will see later

that this holds also in the general case. Recall that $c^{(2)}$ and $c^{(4)}$ are infinite series in the coupling constant, corresponding to the infinity of diagrams with 2 and 4 external lines. Theories of this type, in which we need to introduce a finite number of counterterms to render the theory finite, are called *renormalizable*, or strictly renormalizable.

10.3.2 *The Callan-Zimanzik equation*

Whenever regularization is not suppressed, amplitudes are finite to a given perturbative order. Trouble starts when we suppress the regulator. So, let us focus for the moment on our regularized objects (Feynman amplitudes, counterterms, etc) emerging from the "bare" Lagrangian density,

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi\,\partial^\mu\phi + \frac{m^2}{2}\phi^2 + \frac{\lambda}{4!}\phi^4. \tag{10.30}$$

Two sets of counterterms, corresponding to two distinct renormalization schemes (see Eqs. (10.40) and (10.41) in Sec. 10.4), or two values of the parameter μ in Eq. (10.26), differ by a finite counterterm. To completely define the theory this ambiguity has to be eliminated. This can be done by defining the theory by means of physical conditions, fixing the normalization of some Green functions. In the case of the $\lambda\phi^4$ theory it is enough to fix the two- and four-point functions.

The full two-point function, including corrections to all orders is

$$G^{(2)}(p) = \frac{1}{p^2 + m^2 + \Sigma(p)}.$$

Since $G^{(2)}(p)$ must have a pole at the physical mass, $p^2 = -\overline{m}^2$ we have $\left[p^2 + \Sigma(p) + m^2\right]\big|_{p^2=-\overline{m}^2} = 0$, and the residue of the pole is equal to 1. Analogously, we fix the physical coupling constant by means of a normalization condition, for instance, such that the amputated four-point function, including the correction from the counterterm $c^{(4)}$),

$$G^{(4)\text{amputaded}}(p_1, p_2, p_3, p_4) + c^{(4)}, \tag{10.31}$$

equals the physical coupling constant at the symmetric point $p_j^2 = \mu^2\,;\;\; (p_i + p_j)^2 = \frac{4\mu^2}{3}$. Then the theory is dependent on an arbitrary constant μ.

The renormalized Lagrangian density, is obtained from the bare Lagrangian by including the counterterms (10.24) and (10.28) as,

$$\mathcal{L}^{\text{Ren}} = \frac{\mathrm{Z}}{2}\partial_\mu\phi\,\partial^\mu\phi + \frac{\mathrm{Z}}{2}(m^2 + c^{(2)})\phi^2 + \frac{\mathrm{Z}^2(\lambda + \mathrm{c}^{(4)})}{4!}\phi^4, \tag{10.32}$$

where $\mathrm{Z} = \sqrt{1 + \mathrm{c}^{(2)\prime}}$. Z and the counterterms $c^{(2)}$ and $c^{(4)}$ are dependent on the regulator η and on the arbitrary parameter μ. With the rescaling of the field, $\overline{\phi} = \sqrt{\mathrm{Z}}\phi$ and defining the physical mass and renormalized constant by $\overline{m}^2 = m^2 + c^{(2)}$ and $\overline{\lambda} = \lambda + c^{(4)}$ respectively, we have,

$$\mathcal{L}^{\text{Ren}} = \frac{1}{2}\partial_\mu\overline{\phi}\,\partial^\mu\overline{\phi} + \frac{1}{2}\overline{m}^2\overline{\phi}^2 + \frac{\overline{\lambda}}{4!}\overline{\phi}^4. \tag{10.33}$$

When the regularization is suppressed, everything explodes: the counterterms and, for consistency, the bare mass and coupling constant diverge, in such a way as to provide *finite* physical mass and coupling constant. The Lagrangian given in Eq. (10.33) generates a perturbative series in the physical coupling constant $\overline{\lambda}$. All Feynman diagrams will have the factor $\overline{\lambda}$ at each vertex. Among them, those strictly containing subdiagrams with two and four external legs will have UV divergences to be subtracted along the lines described above. The main difference is that the series is in the physical coupling constant $\overline{\lambda}$.

Since there is a factor $\sqrt{\mathrm{Z}}$ for each field, the N-point renormalized amputated 1PI Green function is obtained from the non-renormalized one by,

$$\Gamma^{(N)}(\overline{\lambda}(\mu), \overline{m}(\mu), \mu, \eta) = \mathrm{Z}^{\frac{\mathrm{N}}{2}}(\eta, \mu)\Gamma_0^{(\mathrm{N})}(\lambda, \mathrm{m}, \eta). \tag{10.34}$$

In Eq. (10.34) $\Gamma_0^{(N)}$ is independent of μ but depends on the regulator η. When the regularization is suppressed, $\Gamma^{(N)}$ is independent of η, but depends explicitly on μ. Or, μ is an arbitrary parameter and we expect on physical grounds that results do not depend on it. We rewrite Eq. (10.34),

$$\Gamma_0^{(N)}(\lambda, m, \eta) = \mathrm{Z}^{-\frac{\mathrm{N}}{2}}(\eta, \mu)\Gamma^{(\mathrm{N})}(\overline{\lambda}(\mu), \overline{\mathrm{m}}(\mu), \mu). \tag{10.35}$$

The independence of $\Gamma_0^{(N)}$ on μ implies that the right hand side of Eq. (10.35) does not depend on this parameter,

$$\mu\frac{\partial}{\partial\mu}\left[\mathrm{Z}^{-\frac{\mathrm{N}}{2}}(\eta, \mu)\Gamma^{(\mathrm{N})}(\overline{\lambda}(\mu), \overline{\mathrm{m}}, \mu)\right] = 0, \tag{10.36}$$

which can be rewritten in the form,

$$\left[\mu\frac{\partial}{\partial\mu} + \beta(\overline{\lambda})\frac{\partial}{\partial\overline{\lambda}} + \beta_{\overline{m}}(\overline{\lambda})\frac{\partial}{\partial\overline{m}} - N\gamma(\overline{\lambda})\right]\Gamma^{(N)}(\overline{\lambda}, \mu) = 0, \tag{10.37}$$

where the functions β, γ and $\beta_{\overline{m}}$ are given by,

$$\beta(\overline{\lambda}) = \mu\frac{\partial\overline{\lambda}}{\partial\mu}; \quad \beta_{\overline{m}}(\overline{\lambda}) = \mu\frac{\partial\overline{m}}{\partial\mu}; \quad \gamma(\overline{\lambda}) = \mu\frac{\partial}{\partial\mu}\ln\sqrt{\mathrm{Z}}. \tag{10.38}$$

The independence of the renormalized Green functions on the arbitrary parameter μ is given in Eq. (10.37). It is known as the Callan-Symanzik or the renormalization group equation .

10.4 Bogoliubov recurrence

For a renormalizable theory, we look for the organization of the set of subtraction to be performed in order to define the complete set of counterterms. When a counterterm c_{S_1} for a subdiagram S_1, with N_1 external lines is present, the modified Lagrangian contains a new vertex with N_1 lines. For any $S_2 \supset S_1$, to subtract the divergent integration corresponding to S_1 is equivalent to considering the sum

$$A_{S_2}^{\mathrm{Ren}} = A_{S_2} + c_{S_1}A_{S_2/S_1},$$

where A_{S_2/S_1} is the reduced diagram obtained by shrinking the subdiagram S_1 to a point. If S_2 is superficially divergent (independently of the S_1-divergence), we must define another counterterm c_{S_2}, such that

$$A_{S_2}^{\mathrm{Ren}} = A_{S_2} + c_{S_1} A_{S_2/S_1} + c_{S_2}.$$

The process is continued in a recurrent manner, starting from the smaller diagram to the larger ones. It may be shown that, in order to obtain finite amplitudes, it is enough to take simultaneously all the non-overlapping subdiagrams S. This is the origin of the BPH (Bogoliubov, Parasiuk, Hepp) recursive process [128, 129, 136].

Suppose that we have defined all counterterms up to a given order n. Then for a diagram G of order $n+1$, we define the renormalized amplitude, A_G^{Ren}, by the formula

$$A_G^{\mathrm{Ren}} = \sum_{\{S\}} \left[A_{G/\{S\}} \prod_{S\in\{S\}} c_S \right] + c_G, \tag{10.39}$$

where c_G is present if G itself is superficially divergent. The sum in Eq. (10.39) is over all the families $\{S\}$ of superficially divergent non-overlapping subdiagrams of G, including the empty family, which corresponds to the term A_G. The amplitude $A_{G/\{S\}}$ corresponds to the diagram obtained by reducing to a point each subdiagram of the family $\{S\}$. In the recursive process, it is understood that the intermediary step of the regularization has been done, which is suppressed after the recurrence is performed up to a given order.

An equivalent way to introduce counterterms and implement renormalization using the Bogoliubov recurrence formula (10.39), consists in taking the regularized amplitude Taylor-subtracted at a fixed point in the external momenta, $\{p\} = \{\omega\}$; that is, for a logarithmically divergent diagram, for example, we subtract the zeroth order term in the Taylor expansion on the external momenta, around the point $\{\omega\}$. We can verify that the divergence is contained in the first term of the expansion. This procedure is in principle not unique, due to the arbitrariness of the choice of the point $\{\omega\}$. Consider now a primitively divergent subdiagram $S \subset G$ with $\{p_i\}$, $i = 1 \cdots N$, external momenta, for which $d(S) > 0$. In this case it is not enough to subtract only the zeroth order term in the Taylor expansion, but to subtract up to the order $d(S)$,

$$A_S^{\mathrm{Ren}}(\{p\}) = \lim_{\eta\to 0} \left[1 - \tau_S^{d(S)}(\omega)\right] A_S^{\mathrm{Reg}}(\{p\};\eta) \tag{10.40}$$

where $\tau_S^{d(S)}(\omega)$ is the Taylor operator up to order $d(S)$, around the point $\{\omega\}$; it is defined, in a simplified version, by

$$\begin{aligned}\tau_S^{d(S)}(\omega) A_S^{\mathrm{Reg}}(\{p\};\eta) = A_S^{\mathrm{Reg}}(\omega;\eta) + \sum_i (p_i - \omega_i)^{\mu_i} \left[\frac{\partial A_S^{\mathrm{Reg}}(\{p\}\eta)}{\partial p_i^{\mu_i}}\right]_{p_i=\omega_i} + \cdots \\ + \sum_{\{i\}} \frac{(p_1-\omega_1)^{\mu_{i_1}} \cdots (p_N - \omega_N)^{\mu_{i_N}}}{d(S)!} \left[\frac{\partial^{d(S)} A_S^{\mathrm{Reg}}(\{p\};\eta)}{\partial p^{\mu_1} \cdots \partial p^{\mu_N}}\right]_{\{p_i=\omega_i\}}.\end{aligned} \tag{10.41}$$

It is not a trivial task to show that this procedure can be generalized to take into account all renormalization parts of every diagram G. We define a *forest* $\mathcal{F}$ of G as a set $\{S_i \subseteq G\}$ of proper (connected and 1PI) subdiagrams such that for $S_i, S_j \in \mathcal{F}$, either $S_i \subset S_j$, $S_i \supset S_j$, or $S_i \cap S_j$. Then the renormalized amplitude of the diagram G can be written as

$$A_G^{\mathrm{Ren}}(\{p\}) = \lim_{\eta \to 0} \mathcal{R}\, A_G^{\mathrm{Reg}}(\{p\}; \eta), \tag{10.42}$$

where the renormalization operator, $\mathcal{R}$, is given by

$$\mathcal{R} = \sum_{\mathcal{F}} \prod_{S_i \in \mathcal{F}} \left(-\tau^{d(S_i)}\right) \tag{10.43}$$

and the sum extends to all forests $\mathcal{F}$ of G, including the empty forest $\emptyset$, which corresponds to the term 1.

In Eq. (10.42) the product of Taylor operators is to be performed following the ordering in each forest, that is from smaller to bigger diagrams. Each Taylor operator $\tau^{d(S_i)}$ takes the beginning of the Taylor expansion up to the order $d(S_i)$ in the *external* momenta of S_i which can be *internal* momenta of G or of a bigger diagram. The definition of $\mathcal{R}$ may therefore depend on the choice of momentum routing, that is, on the choice of the independent loop momenta solving the delta function in Eq. (10.5). This difficulty has lead to the definition for each diagram, of sets of *admissible* momenta and for these, to the statement of the theorem [128]:

Theorem: *The amplitude* $A_G^{\mathrm{Ren}}(\{p\})$ *in Eq. (10.42) is convergent for any diagram* G *in Euclidian space and its analytical continuation to the Minkowski space define tempered distributions.*

In Fig. 10.10(a) we have a 4th order diagram and the set of its renormalization parts is shown in Fig. 10.10(b). The list of forests of this diagram is,

$$\begin{aligned} &\emptyset\,, \{S_1\}\,, \{S_2\}\,, \{S_3\}\,, \{G\}\,, \{S_1, S_3\}\,, \{S_2, S_3\}\,, \\ &\{S_1, G\}\,, \{S_2, G\}\,, \{S_3, G\}\,, \{S_1, S_3, G\}\,, \{S_2, S_3, G\}. \end{aligned} \tag{10.44}$$

We invite the courageous reader to apply formula given in Eq. (10.42) to this case and verify that a finite amplitude is obtained [128, 137].

10.4.1 *Dimensional renormalization*

The simplest case of dimensional regularization consists in generalizing the dimension D in the formula given by Eq. (10.12) to complex values D', by considering the analytical extension of its right hand side. This may be done for more involved Feynman integrals, with the result that they become meromorphic functions of D', $A_G(D')$, and the ultraviolet divergences appear as poles of gamma functions at $D' = D$. The expansion around these poles allows us to define the *dimensional*

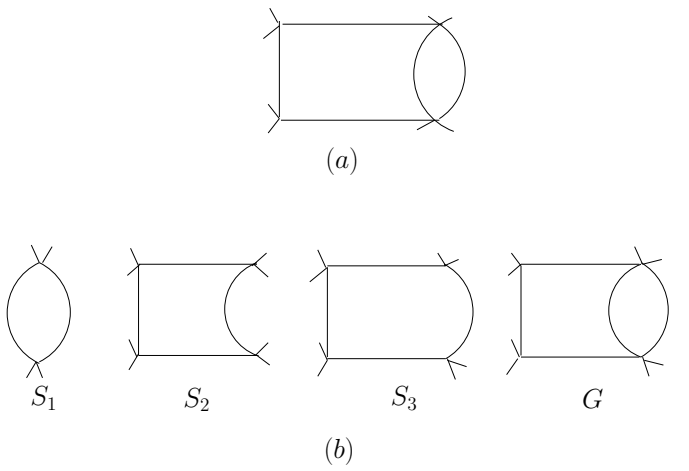


Fig. 10.10 (a) The 4th order diagram of the $\lambda\phi^4$ theory. (b) Renormalization parts of the diagram in (a).

renormalization: at each step in the BPH recurrence, we perform an expansion in powers of $D' - D = \epsilon$ of the dimensionally regularized amplitudes,

$$A_G^{\mathrm{DimReg}}(D') = \sum_{\{S\}} \left[A_{G/\{S\}}(D') \prod_{S\in\{S\}} c_S(D') \right] + A_G^{\mathrm{Ren}}(D')$$
$$= \sum_{m=1}^{m_{max}} \frac{a_m}{(D-D')^m} + A_G^{\mathrm{Ren}}(D'), \tag{10.45}$$

where

$$\lim_{D'\to D} A_G^{\mathrm{Ren}}(D') = A_G^{\mathrm{Ren}}(D) < \infty. \tag{10.46}$$

Dimensional renormalization consists, essentially, in subtracting the pole terms in the limit $D' \to D$, i.e. by subtracting the counterterms

$$-\sum_{m=1}^{m_{max}} \frac{a_m}{\epsilon^m}. \tag{10.47}$$

This is not obvious, but the counterterms are polynomials in the external momenta, in the dimension D, supposed to be an integer. It is worth mentioning that there is no convenient definition of the momentum in complex dimensions; actually it is hard to imagine a complex number of components of a vector. It is necessary to work with the invariants directly.

The main advantage of the dimensional renormalization is that, in general, it respects the symmetry properties of the theory, which are often dimensionally independent. On the contrary, in other renormalization schemes, one need usually to reestablish the symmetry by adding new finite counterterms. However, a defect of

the dimensional renormalization in practical applications is that it must be done following the Bogoliubov recurrence, step-by-step. A solution to this situation has been found with the BPHZ systematics [136], where an explicit global solution is obtained for the dimensional renormalization [138].

10.4.2 *Other renormalization procedures*

(i) *renormalization in the α-parametric representation*

The Bogoliubov-Schwinger parametric α-representation is introduced by expressing each propagator in Eq. (10.6) in the form,

$$\frac{1}{k_l^2+m^2} = \int_0^\infty d\alpha\, e^{-\alpha(k_l^2+m^2)} \tag{10.48}$$

Upon integration over each k_l the Feynman amplitude is expressed as [139]

$$A_G(\{p\}) = \int_0^\infty \frac{\prod_{l=1}^I d\alpha_l}{U^{d/2}(\alpha)} e^{-\sum_l \alpha_l m^2} e^{-N(s_K;\alpha)/U(\alpha)}, \tag{10.49}$$

where U and N are homogeneous polynomials in the α_l parameters, of order L and $L+1$, respectively, constructed with topological relations defined by the 1- and 2-trees of the diagram G:

$$U(\alpha) = \sum_T \prod_{l\notin T} \alpha_l, \qquad N(\alpha) = \sum_K s_K \left(\prod_{l\notin K} \alpha_l\right). \tag{10.50}$$

The symbols $\sum_T$ and $\sum_K$ denote, respectively, summation over the 1-trees T (a tree is a set of lines of the diagram connecting all the vertices without loops) and 2-trees K of G (a two-tree is a tree with two connect components); s_K is the cut-invariant of one of the two connected pieces of the 2-tree K, that is, the square of the total external momentum entering one piece of K (any one of them equivalently, by momentum conservation). U and N are known in the literature as the Symanzik polynomials.

The Bogoliubov-Schwinger parametric α-representation has been employed to provide a simpler proof of the Bogoliubov recurrence [137, 140].

(ii) *renormalization in the complete Mellin representation*

Starting from the parametric α-representation, we rewrite the Symanzik polynomials as [141, 142, 150],

$$u_{ij} = \begin{cases} 0 \text{ if the line } i \text{ belongs to the 1-tree } j \\ 1 \text{ otherwise} \end{cases} \tag{10.51}$$

and

$$n_{iK} = \begin{cases} 0 \text{ if the line } i \text{ belongs to the 2-tree } K \\ 1 \text{ otherwise} \end{cases} \tag{10.52}$$

with

$$\sum_i u_{ij} = L\,, \quad \forall\, j\,,$$
$$\sum_i n_{iK} = L+1\,, \quad \forall\, K\,.$$

The Feynman amplitude in Eq. (10.49) has a complete Mellin (CM) representation [142]. For convergent amplitudes it reads,

$$A_G(s_K) = \int_\Delta \frac{\prod_j \Gamma(-x_j)}{\Gamma(-\sum_j x_j)} \prod_K s_K^{y_K} \Gamma(-y_K) \prod_l \left(m^2\right)^{-\phi_l} \Gamma\left(\phi_l\right), \tag{10.53}$$

where Δ is the nonempty convex domain (σ and τ standing respectively for Re x_j and Re y_K),

$$\Delta = \left\{ \sigma, \tau \,\middle|\, \begin{array}{l} \sigma_j < 0;\ \tau_K < 0;\ \sum_j x_j + \sum_K y_K = -\frac{D}{2}; \\ \forall i,\ \text{Re}\ \phi_i \equiv \sum_j u_{ij}\sigma_j + \sum_K n_{iK}\tau_K + 1 > 0 \end{array} \right\} \tag{10.54}$$

and the symbol $\int_\Delta$ is defined by,

$$\int_\Delta \equiv \int_{-\infty}^{+\infty} \frac{\text{Im}\ x_j}{2\pi i} \frac{\text{Im}\ y_K}{2\pi i}. \tag{10.55}$$

If the Feynman integral, Eq. (10.6), is ultraviolet divergent, the domain Δ in the complete Mellin representation, Eq. (10.53), is empty. The renormalization procedure *does not alter the algebraic structure* of integrands of the CM representation [142, 143]. It only changes the set of relevant integration domains in the Mellin variable space. Actually, by the action of the renormalization operator $\mathcal{R}$, the integration domain Δ is split into a set of cells C corresponding to integration domains Δ_C in the Mellin variables, in such a way that the *renormalized* amplitude has the form,

$$\begin{aligned} A_G^{\text{Ren}}(s_K, m^2) &= \int_0^\infty \frac{\prod_{l=1}^I d\alpha_l}{U^{d/2}(\alpha)}\, \mathcal{R}\left(e^{-\sum_l \alpha_l m^2} e^{-N(s_K;\alpha)/U(\alpha)}\right) \\ &= \sum_C \mu_C \int_{\Delta_C} \frac{\prod_j \Gamma(-x_j)}{\Gamma(-\sum_j x_j)} \prod_K s_K^{y_K} \Gamma(-y_K) \prod_l \left(m^2\right)^{-\phi_l} \Gamma\left(\phi_l\right), \end{aligned} \tag{10.56}$$

where μ_C are numerical coefficients and

$$\Delta_C = \left\{ \sigma \in C, \tau \in C \,\middle|\, \begin{array}{l} \sigma_j < 0;\ \tau_K < 0;\ \sum_j x_j + \sum_K y_K = -\frac{D}{2}; \\ \forall i,\ \text{Re}\ \phi_i \equiv \sum_j u_{ij}\sigma_j + \sum_K n_{iK}\tau_K + 1 > 0 \end{array} \right\}. \tag{10.57}$$

10.4.3 *Borel summability*

Perturbation theory makes sense if the coupling constant is small and dimensionless. The renormalizaton procedure gives a way to get finite coefficients of the perturbative expansion (Feynman diagrams) at any order in the physical coupling constant, but nothing is said about the convergence of the expansion itself. On the contrary, there are indications that some physically relevant perturbative series asymptotically diverge [144], but even so, very precise predictions can be made using the perturbation theory. QED is an example of this. However, in spite of its remarkable achievements, there are situations where the use of the perturbative method is not possible, or is of little use. These situations have led to attempts to improve analytical methods to circumvent the limitations of the perturbation theory. In particular, non-perturbative renormalization methods in constructive field theory have been improved [144].

In perturbation theory there are a number of successful attempts to solve the problem. There are methods that perform resummations of perturbative series, even if they are divergent, which amounts in some cases to extending the weak-coupling regime to a strong-coupling domain [145–149]. For instance, starting from a series in powers of a coupling constant g, *not necessarily convergent*,

$$f(g) = \sum_{n=0}^{\infty} a^n g^n, \tag{10.58}$$

it is possible under the assumption of the validity of the Watson-Nevanlinna-Sokal theorem [144] to define its associated Borel transform series in the Borel variable, say b,

$$B(b) = \sum_{n=0}^{\infty} \frac{a^n}{n!} b^n. \tag{10.59}$$

It can be easily verified that the inverse Borel transform,

$$\overline{B}(g) = \frac{1}{g} \int_0^{\infty} db\, e^{-(b/g)}\, B(b), \tag{10.60}$$

reproduces, formally, the original series in g. From a physical point of view, the important point is that the Borel series in b can be convergent and can be summed even if the original series in g diverges. In this case, the inverse Borel transform defines a *function* of g, which can be taken as the sum of the divergent series in g. This function is defined for values of g not necessarily small and, in this sense, an extension from a weak to a strong-coupling regime can be performed.

10.5 Temperature effects

We now address the question about the renormalizability of a theory at finite temperature. Specifically, we indicate how to use dimensional regularization and analytic zeta function techniques to calculate Feynman amplitudes at $T \neq 0$. Let us

start with Eq. (10.6), written in the form

$$A_G(\{p\}) \sim \int \prod_{\alpha=1}^{L} \frac{d^D k_\alpha}{(2\pi)^D} \prod_{i=1}^{I} \frac{1}{A_i}, \tag{10.61}$$

where $A_i = q_i^2(\{p\},\{k\}) + m^2$. Using the identity Eq. (10.25) and the fact that each q_i is a linear function of the internal momenta, Eq. (10.61) becomes

$$A_G(\{p\}) = \int_0^1 dx_{_1} \cdots dx_{_{I-1}} \int \prod_{\alpha=1}^{L} \frac{d^D k_\alpha}{(2\pi)^D} \frac{(I-1)!}{[k_1^2 + \cdots + k_L^2 + \Delta^2]^I},$$

where

$$\Delta^2 = \Delta^2(\{p\},\{x_j\}; m)$$

is a function of the external momenta, $\{p\}$, of the Feynman parameters, $\{x_i\}$, and of the mass m [31].

As pointed out in Chapter 8, the thermal (TFD) free-boson propagator, Eq. (8.11), fulfills the KMS conditions and is periodic in the imaginary time, with period $\beta = T^{-1}$. Thus, in its Fourier expansion, k^0 takes values on the discrete set of Matsubara frequencies, $\{\omega_n = 2\pi n/\beta\}$. For an amplitude with L independent loops, A_G, the Matsubara prescription should be applied to all k_α^0 to get the finite temperature expression,

$$A_G(\{p\};\beta) = \frac{1}{\beta^L} \sum_{\{l_\alpha = -\infty\}}^{\infty} \int_0^1 dx_{_1} \cdots dx_{_{I-1}} \int \prod_{\alpha=1}^{L} \frac{d^{D-1}\mathbf{k}_\alpha}{(2\pi)^{D-1}} \times \frac{(I-1)!}{[\mathbf{k}_1^2 + \cdots + \mathbf{k}_L^2 + \sum_{\alpha=1}^{L} \frac{4\pi^2 l_\alpha^2}{\beta^2} + \Delta^2]^I}.$$

We rewrite this equation as

$$A_G(\{p\};\beta) = \frac{1}{\beta^L} \sum_{\{l_\alpha = -\infty\}}^{\infty} \int_0^1 dx_{_1} \cdots dx_{_{I-1}} B_G(\{p\},\{x_j\};\{l_\alpha\},\beta),$$

where

$$B_G(\{p\},\{x_j\};\{l_\alpha\},\beta) = \int \prod_{\alpha=1}^{L} \frac{d^{D-1}\mathbf{k}_\alpha}{(2\pi)^{D-1}} \frac{(I-1)!}{[\mathbf{k}_1^2 + \cdots + \mathbf{k}_L^2 + \sum_{\alpha=1}^{L} b^2 l_\alpha^2 + \Delta^2]^I}, \tag{10.62}$$

with

$$b = \frac{2\pi}{\beta}\,.$$

To perform the integration in Eq. (10.62), we proceed by recurrence. We start by rewriting Eq. (10.62) as

$$B_G(\{p\},\{x_j\};\{l_\alpha\},\beta) = \int \prod_{\alpha=1}^{L} \frac{d^{D-1}\mathbf{k}_\alpha}{(2\pi)^{D-1}} \frac{(I-1)!}{[\mathbf{k}_1^2 + \Delta_1^2]^I},$$

with Δ_1^2 given by

$$\begin{aligned}\Delta_1^2 &= \Delta_1^2(\{p\},\{x_j\};\{l_\alpha\},\beta;\{\mathbf{k}_{\alpha>1}\})\\ &= \mathbf{k}_2^2+\cdots+\mathbf{k}_L^2+\sum_{\alpha=1}^{L} b^2 l_\alpha^2+\Delta^2(\{p\},\{x_j\};m).\end{aligned}$$

Then, we perform the integration over $\mathbf{k}_1$ by using the formula given in Eq. (10.12) and obtain

$$B_G(\{p\},\{x_j\};\{l_\alpha\},\beta)=\frac{\Gamma\left(I-\frac{D-1}{2}\right)}{(4\pi)^{\frac{D-1}{2}}}\int\prod_{\alpha=2}^{L}\frac{d^{D-1}\mathbf{k}_\alpha}{(2\pi)^{D-1}}\,\frac{1}{[\mathbf{k}_2^2+\Delta_2^2]^{I-\frac{D-1}{2}}},$$

where

$$\begin{aligned}\Delta_2^2 &= \Delta_2^2(\{p\},\{x_j\};\{l_\alpha\},\beta;\{\mathbf{k}_{\alpha>2}\})\\ &= \mathbf{k}_3^2+\cdots+\mathbf{k}_L^2+\sum_{\alpha=1}^{L} b^2 l_\alpha^2+\Delta^2.\end{aligned}$$

The second step is to integrate over the momentum $\mathbf{k}_2$, again using Eq. (10.12). The result is

$$B_G(\{p\},\{x_j\};\{l_\alpha\},\beta)=\frac{\Gamma\left(I-2\left[\frac{D-1}{2}\right]\right)}{(4\pi)^{2\left[\frac{D-1}{2}\right]}}\int\prod_{\alpha=3}^{L}\frac{d^{D-1}\mathbf{k}_\alpha}{(2\pi)^{D-1}}\,\frac{1}{[\mathbf{k}_3^2+\Delta_3^2]^{I-2\left[\frac{D-1}{2}\right]}},$$

where

$$\begin{aligned}\Delta_3^2 &= \Delta_3^2(\{p\},\{x_j\};\{l_\alpha\},\beta;\{\mathbf{k}_{\alpha>3}\})\\ &= \mathbf{k}_4^2+\cdots+\mathbf{k}_L^2+\sum_{\alpha=1}^{L} b^2 l_\alpha^2+\Delta^2(\{p\},\{x_j\};m).\end{aligned}$$

This procedure is continued until we have integrated over all momenta. The final result is

$$\begin{aligned}A_G(\{p\};\beta) &= \frac{1}{\beta^L}\,\frac{\Gamma\left(I-L\left[\frac{D-1}{2}\right]\right)}{(4\pi)^{L\left[\frac{D-1}{2}\right]}}\\ &\quad\times\int_0^1 dx_{_1}\cdots dx_{_{I-1}}\sum_{\{l_\alpha=-\infty\}}^{\infty}\frac{1}{[\Delta_L^2]^{I-L\left[\frac{D-1}{2}\right]}},\end{aligned}\tag{10.63}$$

where

$$\begin{aligned}\Delta_L^2 &= \Delta_L^2(\{p\},\{x_j\};m,\beta)\\ &= \sum_{\alpha=1}^{L} b^2 l_\alpha^2+\Delta^2(\{p\},\{x_j\};m).\end{aligned}$$

We recognize the sum over the set $\{l_\alpha\}$ in Eq. (10.63) as one of the multivariable Epstein-Hurwitz zeta function defined by

$$A_d^{c^2}(\nu;a_1,\ldots,a_d)=\sum_{\{n_j=-\infty\}}^{+\infty}\frac{1}{\left(\sum_{r=1}^{d}a_r^2n_r^2+c^2\right)^{\nu}}\,.\tag{10.64}$$

This function can be analytically continued to the whole complex ν-plane. We postpone to Chapter 18 the full construction of such an analytic extension [284] and present now only the result:

$$A_d^{c^2}(\nu;\{a_j\}) = \frac{\pi^{\frac{d}{2}}}{a_1\cdots a_d\,\Gamma(\nu)}\left[\Gamma\left(\nu-\frac{d}{2}\right)c^{d-2\nu}+F\left(\nu-\frac{d}{2};\{a_j\},c\right)\right], \quad (10.65)$$

where the function $F\left(\nu-d/2;\{a_j\},c\right)$ is the finite part, which is expressed by sums with j indices (and $1\leq j\leq d$) involving modified Bessel functions, $K_{\nu-d/2}$ (see Chapter 20), while the first term, proportional to $\Gamma\left(\nu-d/2\right)$, has simple poles at the values $\nu=-n+d/2$, $n\in\mathbb{N}$.

Now, if we take

$$d=L\,,\quad a_1=\cdots=a_L=b\,,\quad c^2=\Delta^2(\{p\},\{x_j\};m)\,,\quad \nu=I-L\left(\frac{D-1}{2}\right)$$

in the above expression, the L-loop amplitude, Eq. (10.63), becomes

$$A_G(\{p\};\beta)=\frac{1}{2^{LD}\pi^{L(D-1)}}\left[\Gamma\left(I-\frac{LD}{2}\right)\int_0^1 dx_{_1}\cdots dx_{_{I-1}}\left[\Delta(\{p\},\{x_j\};m)\right]^{LD-2I}\right.$$
$$\left.+\int_0^1 dx_{_1}\cdots dx_{_{I-1}}\,F\left(\nu-\frac{d}{2};\beta,\Delta(\{p\},\{x_j\};m)\right)\right]. \quad (10.66)$$

The first term in this expression does not depend on the temperature, β^{-1}, and carries a singularity for space-time dimensions D satisfying $I-LD/2=0,-1,-2,\ldots$. The second term is finite. To get the renormalized amplitude, this term should be added to the finite part that remains when the pole of the first term is suppressed. Applications of this method will be presented in Chapters 18 to 21.

The general aspects of the topic presented here can be extended to models where the matter field (bosons or fermions) is coupled with a gauge field. In these theories, an important role is played by the gauge symmetry in the discussion of perturbative renormalization. The Ward-Takahashi relations, that manifestly contain the full implications of the symmetry, are discussed in the next chapter.

Chapter 11

Ward-Takahashi Relations and Gauge Symmetry

Ward [151] established a relationship between the vertex and the propagator for quantum electrodynamics. It played a fundamental role in the renormalization theory and the theory of spontaneous symmetry breaking. This relationship was generalized by Takahashi [152] to many particle Green's functions. These non-perturbative results, called Ward-Takahashi (W-T) relations, have played an important role in keeping perturbative schemes in quantum field theory and many-particle systems consistent with the underlying symmetry properties. Quantum electrodynamics (QED) with a $U(1)$ gauge symmetry leads to the continuity conditions on the current, i.e. $\partial_\mu j^\mu(x) = 0$. Similar relation exists for the axial current J_μ^A which is only partially conserved, i.e. $\partial^\mu J_\mu^A(x) = C\phi(x)$ where ϕ is a pseudo-scalar field that is taken to be the pion field.

Relationships of the type mentioned above provide a limitation on the longitudinal part of the vertex function. The transverse part is not determined by the W-T relations. In order to study gauge theories through Dyson-Schwinger equation [153], a complete knowledge of the vertex function is required. A great deal of effort has been devoted to gain a better understanding, and thus construct the transverse part of the vertex function. Perturbative schemes [154–161] have been devised to get a handle on the transverse part. However these attempts are not unique since these are not based on a basic symmetry property of the system. It is possible to establish a proper constraint on the transverse part of the vertex by a WT-type relation as is possible for the longitudinal part of the vertex, by a method suggested by Takahashi [162].

This chapter provides a detailed operator relationship that gives W-T relations at $T = 0$ and at finite temperature. First we present an analysis of the W-T relationship that gives the longitudinal part of the vertex function. These are exact results, only ones available for quantum field theory. Then we establish a WT-type relationship for the transverse part of the vertex [163] and these are obtained to one-loop level. Again these results are used for both $T = 0$ and finite temperature.

11.1 Ward relation

The Ward relation in momentum space is obtained from the definition of the Feynman propagator for a fermion

$$S_F(p) = \frac{1}{\gamma \cdot p - m},$$

then

$$\frac{\partial}{\partial p_\mu} S_F(p) = -S_F(p)\,\gamma_\mu S_F(p). \tag{11.1}$$

This relation has proved very useful in understanding the connection between renormalization constants defined by Dyson and then indicated that all divergences in quantum electrodynamics may be removed by a renormalization of charge and mass. Dyson conjectured that $Z_1 = Z_2$ and the above identity led to a formal proof of this equivalence by Ward. However this started a search for a generalized Ward relation valid for arbitrary momentum transfer q that was discovered by Takahashi.

11.2 Ward-Takahashi relations

The Ward relation has played a fundamental role in canonical quantum field theory. Now we will discuss the generalization as given by Takahashi. In canonical field theory, the Lagrangian depends on the field operators, $\phi_\alpha(x)$, their conjugate, $\phi^\dagger_\alpha(x)$, and their derivatives, $\partial_\mu\phi_\alpha(x)$ and $\partial_\mu\phi^\dagger_\alpha(x)$. Consider an infinitesimal transformation of the field operator

$$\phi_\alpha(x) \to \phi'_\alpha(x) = \phi_\alpha(x) + \delta\phi_\alpha(x). \tag{11.2}$$

The Lie derivative of the transformation is defined as

$$\begin{aligned}\delta^L\phi_\alpha(x) &\equiv \phi'_\alpha(x) - \phi_\alpha(x) \\ &= \delta\phi_\alpha(x) - \delta x^\mu \partial_\mu\phi_\alpha(x).\end{aligned} \tag{11.3}$$

It follows that

$$\partial_\mu\delta^L\phi_\alpha(x) = \delta^L\partial_\mu\phi_\alpha(x)$$

and

$$\begin{aligned}\delta^L T(\phi_\alpha(x_1)\,\phi_\beta(x_2)\cdots) = {} & T\left(\delta^L\phi_\alpha(x_1)\,\phi_\beta(x_2)\cdots\right) \\ & + T\left(\phi_\alpha(x_1)\,\delta^L\phi_\beta(x_2)\cdots\right) + \cdots\end{aligned} \tag{11.4}$$

where T is the time-ordering operator. Then the current is defined by the relation

$$\begin{aligned}\partial_\mu J^\mu - g(x) = {} & \delta^L\phi^\dagger_\alpha(x)\left\{\frac{\partial\mathcal{L}}{\partial\phi^\dagger_\alpha(x)} - \partial_\mu\frac{\partial\mathcal{L}}{\partial\partial_\mu\phi^\dagger_\alpha(x)}\right\} \\ & + \left\{\frac{\partial\mathcal{L}}{\partial\phi^\dagger_\alpha(x)} - \partial_\mu\frac{\partial\mathcal{L}}{\partial\partial_\mu\phi^\dagger_\alpha(x)}\right\}\delta\phi_\alpha(x)\end{aligned} \tag{11.5}$$

where $g(x)$ should not have any time derivatives of the canonical variables. The Euler-Lagrange equation i.e the dynamical equation, has not been used in defining this equation for a given Lie derivative.

The relation for the current is not unique; divergence of an anti-symmetric tensor would still satisfy this relation. The generator of the transformation given by Eq. (11.2) leads to the quantization conditions of the field, $\phi_\alpha(x)$,

$$-i\delta^L\phi_\alpha(x) = [\phi_\alpha(x), G(\sigma)] \tag{11.6}$$

where x lies on the space-like surface σ and $G(\sigma)$ is the generator of the transformation given as

$$G(\sigma) = \int d\sigma_\mu(x) J^\mu(x). \tag{11.7}$$

Thus the field quantization is given by the two equations: Eq. (11.5) determines the form of the generating current for a given transformation and a given Lagrangian and Eq. (11.6) provides a restriction on the algebra satisfied by the field operator.

We are ready to define the generalized Ward-Takahashi relations. The Lie derivatives of the field operator is written as

$$\begin{aligned}
-i\delta^L\phi_\alpha(x) &= \phi_\alpha(x) G(\sigma) - G(\sigma)\phi_\alpha(x) \\
&= \phi_\alpha(x)[G(\sigma) - G(-\infty)] - [G(\sigma) - G(+\infty)]\phi_\alpha(x) \\
&\quad + \phi_\alpha(x) G(-\infty) - G(+\infty)\phi_\alpha(x) \\
&= \int d^4x' \left\{T\left(\phi_\alpha(x)\partial'_\mu J^\mu(x')\right) - \partial'_\mu T\left(\phi_\alpha(x) J^\mu(x')\right)\right\}.
\end{aligned} \tag{11.8}$$

This relation may be generalized to arbitrary number of field operators with a time-ordering operator, T, leading to

$$\begin{aligned}
-i\delta^L T(\phi_\alpha(x_1)\phi_\beta(x_2)\cdots) = \int d^4x' \partial'_\mu T(\phi_\alpha(x_1)\phi_\beta(x_2)\cdots J^\mu(x')) \\
-T\left(\phi_\alpha(x_1)\phi_\beta(x_2)\cdots\partial'_\mu J^\mu(x')\right).
\end{aligned} \tag{11.9}$$

It is important to make a few remarks about these relations.

The Euler-Lagrange equations, the dynamical equations for the field operators, have not been used. The use of the field equations implies that the right-hand side of Eq. (11.5) is zero, and we get

$$\partial_\mu J^\mu(x) = g(x). \tag{11.10}$$

Using this relation in Eq. (11.9) we obtain

$$\begin{aligned}
-i\delta^L T(\phi_\alpha(x_1)\phi_\beta(x_2)\cdots) = \int d^4x' \left\{\partial'_\mu T(\phi_\alpha(x_1)\phi_\beta(x_2)\cdots J^\mu(x'))\right. \\
\left.-T(\phi_\alpha(x_1)\phi_\beta(x_2)\cdots g(x'))\right\}.
\end{aligned} \tag{11.11}$$

This defines the most general Ward-Takahashi relation. It is clear that for a gauge theory, the current $J^\mu(x)$ is conserved,

$$\partial_\mu J^\mu(x) = 0$$

and $g(x) = 0$. However it is well-known that for weak interactions, the axial current is partially conserved while the vector current is conserved. For the axial current we have

$$\partial^\mu J_\mu^A(x) = C\phi_\pi(x)$$

where C is a constant and $\phi_\pi(x)$ is the pion field. In such a case the generalized W-T relations given by Eq. (11.11) provide a relation between the fields interacting with the axial current and the pion field. Such relations for many particle systems have been analyzed. These have proved very useful in providing important information about perturbation schemes and cancelation among several different contributions.

The generalized W-T relations, being the only exact relations in quantum field theory, have proved very useful not only for gauge theories but also for fields that have a partial conservation of the current. The generalized W-T relation given in Eq. (11.9) is an operator relation. The Ward relation given by Eq. (11.1) is for the expectation values of the product of operators i.e. for Green functions. The operator form provides a much wider applications not only for quantum field theory at zero temperature but also for finite temperature quantum field theory. In defining the Green functions, the operator form of the generalized W-T relation requires the vacuum state to find the expectation value. Applications to finite temperature are considered later.

11.3 Applications of generalized Ward-Takahashi relations

The generalized W-T relations are completely equivalent to the canonical quantization conditions. These relations have played a fundamental role in quantum field theory. Some of the important applications of the W-T relations for the longitudinal component of the generating current are to the Dyson equation and the dynamical rearrangement of symmetry that is connected to the Goldstone theorem and to the presence of Goldstone bosons in cases of spontaneous breaking of a symmetry of the ground state. These aspects have been studied in detail [164].

11.3.1 *W-T relations for the case of n-body current amplitudes*

An explicit form for the case of the Noether current and its divergence is given by a Lagrangian. Assume that

$$J_\mu^A = \xi_{A\alpha} J_{\mu\,\alpha}^A \tag{11.12}$$

and

$$J_\mu^V = \xi_{V\alpha} J_{\mu\,\alpha}^V, \tag{11.13}$$

where $\xi_{A\alpha}$ and $\xi_{V\alpha}$ are infinitesimal parameters for the axial-vector and vector transformations in the chiral-spin space. The subscript α indicates the isospin

components. Assumptions for low-energy hadron physics lead to conservation of vector current (CVC) and partially conservation of axial current (PCAC), i.e.

$$\partial^{\mu} J^{V}_{\mu\,\alpha} = 0, \tag{11.14}$$

$$\partial^{\mu} J^{A}_{\mu\,\alpha} = \mu^2 f_{\pi} \phi_{\pi}, \tag{11.15}$$

where μ is the pion mass and f_{π} is the pion decay constant. A simple Lagrangian to allow the relation for axial current is the linear σ-model [165]. The equation of motion of the nucleon field becomes

$$\delta_A \psi(x) = i\xi_{A\alpha}\tau_{\alpha}\gamma_5 \psi(x), \tag{11.16}$$

$$\delta_A \overline{\psi}(x) = i\overline{\psi}(x)\gamma_5 \xi_{A\alpha}\tau_{\alpha}, \tag{11.17}$$

and

$$\delta_V \psi(x) = i\xi_{V\alpha}\tau_{\alpha}\psi(x), \tag{11.18}$$

$$\delta_V \overline{\psi}(x) = i\overline{\psi}(x)\tau_{\alpha}\xi_{V\alpha}. \tag{11.19}$$

The generalized n-particle W-T relations for the axial current [166] are

$$\sum_i \left\{\delta^4(x_i - z)\gamma_5^i \tau_{\alpha}^i M + M\tau_{\alpha}^i \gamma_5^i \delta^4(x_i - z)\right\} = \mu^2 f_{\pi} M_{(\pi)\alpha} - \partial_z^{\mu} M_{\mu\alpha}, \tag{11.20}$$

where

$$\begin{aligned} M &= T\left[\psi_1(x_1)\cdots\psi_i(x_i)\cdots\psi_n(x_n)\,\overline{\psi}_1(x_1')\cdots\overline{\psi}_n(x_n')\right], \\ M_{(\pi)\alpha} &= T\left[\psi_1(x_1)\cdots\psi_i(x_i)\cdots\psi_n(x_n)\,\overline{\psi}_1(x_1')\cdots\overline{\psi}_n(x_n')\,\pi_{\alpha}(z)\right], \\ M_{\mu\alpha} &= T\left[\psi_1(x_1)\cdots\psi_i(x_i)\cdots\psi_n(x_n)\,\overline{\psi}_1(x_1')\cdots\overline{\psi}_n(x_n')\,J^{A}_{\mu\,\alpha}(z)\right]. \end{aligned}$$

Taking an expectation value with zero temperature vacuum state we get the general relation

$$\begin{aligned} \partial_z^{\mu}\Gamma^{(n)}_{A\mu\alpha}(x_i,\ldots,x_n;x_1',\ldots,x_n';z) &= \mu^2 f_{\pi} \\ &\times \int dz' \Gamma^{(n)}_{\pi\beta}(x_i,\ldots,x_n;x_1',\ldots,x_n';z')\,\Delta_{\beta\alpha}(z'-z) \\ &- \sum_i \left[\mathcal{S}^{-1}\delta^4(x_i'-z)\gamma_5^i\tau_{\alpha}^i + \tau_{\alpha}^i\gamma_5^i\delta^4(x_i'-z)\,\mathcal{S}^{-1}\right], \end{aligned}$$

where

$$\mathcal{S} \equiv S^{(n)}(x_i,\ldots,x_n;x_1',\ldots,x_n') = \langle 0|\,M\,|0\rangle.$$

The proper current functions are defined as

$$\langle 0|\,M_{\mu\alpha}\,|0\rangle = \int \prod_{i=1}^{n} d^4y_i d^4y_i' \mathcal{S}\Gamma^{(n)}_{A\mu\alpha}(y_1,\ldots,y_n;y_1',\ldots,y_n';z)\,\mathcal{S},$$

$$\langle 0|\,M_{(\pi)\alpha}\,|0\rangle = \int \prod_{i=1}^{n} d^4y_i d^4y_i' dz' \mathcal{S}\Delta_{\alpha\beta}(z-z')\,\Gamma^{(n)}_{\pi\beta}(y_1,\ldots,y_n;y_1',\ldots,y_n';z')\,\mathcal{S}$$

and

$$\Delta_{\alpha\beta}(z-z') = \langle 0|\, T\left[\pi_\alpha(z)\,\pi_\beta(z')\right]|0\rangle\,.$$

It is easy to find the familiar results to one-body system, i.e. for the weak decay of a nucleon in momentum space,

$$\begin{aligned} q^\mu \Gamma^{(1)}_{A\mu\alpha}(k;k+q;q) = {} & i\mu^2 f_\pi \Gamma^{(1)}_{\pi\beta}(k;k+q;q)\,\Delta_{\alpha\beta}(q) \\ & -i\left[S^{-1}(k)\,\gamma_5\tau_\alpha + \tau_\alpha\gamma_5 S^{-1}(k+q)\right]. \end{aligned} \tag{11.21}$$

This is to be compared to the one-body W-T relations for the case of vector current, i.e. QED, that is conserved

$$q^\mu \Gamma^{(1)}_{\mu}(k;k+q;q) = -i\left[S^{-1}(k)\,\tau_\alpha - \tau_\alpha S^{-1}(q+k)\right]. \tag{11.22}$$

It is important to note the difference in sign for CVC while for PCAC the last two terms in Eq. (11.21) have the same sign. This implies that for Eq. (11.22)

$$\lim_{q\to 0} q^\mu \Gamma^{(1)}_{\mu}(k;k+q;q) \to 0, \tag{11.23}$$

while for the axial-vector current, the right-hand side of Eq. (11.21) does not vanish in the limit $q \to 0$. This leads to a relation for the pion radiative amplitude

$$\mu^2 f_\pi \Gamma_{\pi\beta}(k;k;0)\,\Delta_{\beta\alpha}(0) = \left\{S^{(1)-1}, \gamma_5\pi_\alpha\right\} \tag{11.24}$$

where $\{A,B\} = AB + BA$. This relation was obtained as a consistency condition by Adler and Dothan [167].

11.3.2 *Ward-Takahashi relations at finite temperature*

So far we have presented W-T relations at zero temperature where the operator relations are sandwiched between $T = 0$ vacuum states. However we have learned that at finite temperature the Lagrangian density, $\mathcal{L}$, is replaced by $\widehat{\mathcal{L}}$ given as

$$\widehat{\mathcal{L}} = \mathcal{L} - \widetilde{\mathcal{L}}. \tag{11.25}$$

In order to write the W-T relations in a compact form, we consider Eq. (11.5) and write the Noether current, $J_\mu(x)$, in terms of change in the Lagrangian

$$\int d^4x'\mathcal{L}\left[\phi'(x'), \partial'_\mu\phi'(x')\right] - \int d^4x\,\mathcal{L}\left[\phi(x), \partial_\mu\phi(x)\right] = \epsilon\int d^4x\,\delta\mathcal{L}(x)\,, \tag{11.26}$$

where ϵ is an infinitesimal constant. Now using the relation

$$\partial(x'_1x'_2x'_3x'_4)/\partial(x_1x_2x_3x_4) = 1 + \epsilon\partial^\lambda\delta x_\lambda$$

leads to

$$\epsilon\delta\mathcal{L} = \mathcal{L}\left[\phi'(x'), \partial'_\mu\phi'(x')\right] - \mathcal{L}\left[\phi(x), \partial_\mu\phi(x)\right] + \epsilon\partial^\lambda\delta x_\lambda\mathcal{L}(x)\,. \tag{11.27}$$

With the definition

$$\partial'_\mu\phi'(x') = \partial_\mu\phi(x) + \epsilon\partial_\mu\delta\phi(x) - \epsilon\partial^\nu\phi(x)\,\partial_\mu x_\nu, \tag{11.28}$$

we find

$$\delta\mathcal{L}(x) = \frac{\partial\mathcal{L}}{\partial\phi}\delta\phi(x) + \frac{\partial\mathcal{L}}{\partial\partial_\mu\phi}\delta\partial_\mu\phi(x) - \frac{\partial\mathcal{L}}{\partial\partial_\mu\phi}\partial^\nu\phi\partial_\mu\delta x_\nu + \partial^\nu\delta x_\nu\mathcal{L}.$$
$$= \partial_\mu\left[\frac{\partial\mathcal{L}}{\partial\partial_\mu\phi}\delta\phi(x)\right] - \frac{\partial\mathcal{L}}{\partial\partial_\mu\phi}\partial^\nu\phi\partial_\mu\delta x_\nu + \partial^\nu\delta x_\nu\mathcal{L}. \tag{11.29}$$

Using the Heisenberg equation we get

$$\delta\mathcal{L}(x) = \partial_\mu\left\{\frac{\partial\mathcal{L}}{\partial\partial_\mu\phi}\left(\delta\phi(x) - \partial^\nu\phi\delta x_\nu\right) + \delta x^\mu\mathcal{L}\right\}. \tag{11.30}$$

This defines the Noether current $\mathcal{N}_\mu$ as

$$\mathcal{N}_\mu = \frac{\partial\mathcal{L}}{\partial\partial_\mu\phi}\delta^L\phi(x) + \delta x^\mu\mathcal{L} \tag{11.31}$$

and it satisfies the relation

$$\partial_\mu\mathcal{N}^\mu(x) = \delta\mathcal{L}(x). \tag{11.32}$$

Then the generator of transformations is given as

$$\mathcal{N}(t) = \int d^3x\,\mathcal{N}_0(x). \tag{11.33}$$

Here $\mathcal{N}_\mu(x)$ is the same as $J_\mu(x)$ defined in Eq. (11.10).

The W-T relation may be written in the following form

$$\frac{\partial}{\partial t}\langle 0|T\left[\mathcal{N}(t)\phi(x_1)\cdots\phi(x_n)\right]|0\rangle = \sum_{i=1}^{n}\delta(t-t_i)$$
$$\times\langle 0|T\left[\phi(x_1)\cdots\left[\mathcal{N}(t),\phi(x_i)\right]\cdots\phi(x_n)\right]|0\rangle \tag{11.34}$$
$$+\langle 0|T\left[\dot{\mathcal{N}}(t)\phi(x_1)\cdots\phi(x_n)\right]|0\rangle. \tag{11.35}$$

Since

$$\dot{\mathcal{N}} = \int d^3x\,\delta\mathcal{L},$$

we get

$$\frac{\partial}{\partial t}\langle 0|T\left[\mathcal{N}(t)\phi(x_1)\cdots\phi(x_n)\right]|0\rangle = -i\hbar\sum_{i=1}^{n}\delta(t-t_i)$$
$$\times\langle 0|T\left[\phi(x_1)\cdots\delta^0\phi(x_i)\cdots\phi(x_n)\right]|0\rangle$$
$$+\int d^3x\,\langle 0|T\left[\delta\mathcal{L}(x)\phi(x_1)\cdots\phi(x_n)\right]|0\rangle.$$

The left-hand side vanishes leading to

$$i\hbar\sum_{i=1}^{n}\delta(t-t_i)\langle 0|T\left[\phi(x_1)\cdots\delta^0\phi(x_i)\cdots\phi(x_n)\right]|0\rangle$$
$$= \int d^3x\,\langle 0|T\left[\delta\mathcal{L}(x)\phi(x_1)\cdots\phi(x_n)\right]|0\rangle. \tag{11.36}$$

To find a compact expression for W-T relations, define

$$\overline{\mathcal{L}} = \int d^4x f_i(x)\,\psi_i(x) \tag{11.37}$$

where $f(x)$ is a c-number. Then using the transformation given by Eq. (11.28) we get

$$\begin{aligned}\overline{\mathcal{L}}' &= \int d^4x' f_i'(x')\,\psi_i'(x') \\ &= \int d^4x f_i(x)\,\psi_i(x) + \epsilon \int d^4x f_i(x)\,\delta^0\psi_i(x) \\ &= \overline{\mathcal{L}} + \epsilon \int d^4x f_i(x)\,\delta^0\psi_i(x)\,. \end{aligned} \tag{11.38}$$

This leads to

$$\begin{aligned}\delta\overline{\mathcal{L}} &= \left(\overline{\mathcal{L}}' - \overline{\mathcal{L}}\right)\frac{1}{\epsilon} \\ &= \int d^4x f_i(x)\,\delta^0\psi_i(x)\,. \end{aligned} \tag{11.39}$$

Now multiplying Eq. (11.36) by $f_1(x_1)\cdots f_n(x_n)$ and then integrating over $x_1,\ldots,x_n$ we get

$$\sum_n i\hbar n \langle 0|\,T\left[\delta\overline{\mathcal{L}}\left(\overline{\mathcal{L}}\right)^{n-1}\right]|0\rangle = \int d^4x \langle 0|\,T\left[\delta\mathcal{L}(x)\left(\overline{\mathcal{L}}\right)^n\right]|0\rangle\,. \tag{11.40}$$

With sum over n on the left side we get

$$\langle 0|\,T\left[i\delta\overline{\mathcal{L}}\exp\left(\frac{i}{\hbar}\overline{\mathcal{L}}\right)\right]|0\rangle = -\int d^4x \langle 0|\,T\left[i\delta\mathcal{L}(x)\,e^{\left(\frac{i}{\hbar}\overline{\mathcal{L}}\right)}\right]|0\rangle\,. \tag{11.41}$$

In order to get W-T relation for different number of field operators, n, take functional derivative with $-i\frac{\delta}{\delta f(x_1)}$ n-times then take $f(x)\to 0$. For example for $n=1$, we find

$$\langle 0|\,\delta^0\phi(x_1)\,|0\rangle = -\int d^4x \langle 0|\,T\left[i\delta\mathcal{L}(x)\,\phi(x_1)\right]|0\rangle \tag{11.42}$$

and for $n=2$,

$$\begin{aligned}&\langle 0|\,\delta^0\phi(x_1)\,\phi(x_2)\,|0\rangle + \langle 0|\,\phi(x_1)\,\delta^0\phi(x_2)\,|0\rangle \\ &\quad = -\int d^4x \langle 0|\,T\left[i\delta\mathcal{L}(x)\,\phi(x_1)\,\phi(x_2)\right]|0\rangle\,. \end{aligned} \tag{11.43}$$

In this way we can get W-T relations with an arbitrary number of fields.

Now we can make two changes to write down the W-T relations at finite temperature: (i) change the vacuum state, $|0\rangle$, to finite temperature vacuum state, $|0(\beta)\rangle$ and (ii) change the Lagrangian $\mathcal{L}$ to $\widehat{\mathcal{L}} = \mathcal{L} - \widetilde{\mathcal{L}}$. Then the W-T relation is written as

$$\langle 0(\beta)|\,T\left[\frac{i}{\hbar}\delta\widehat{\overline{\mathcal{L}}}\exp\left(\frac{i}{\hbar}\widehat{\overline{\mathcal{L}}}\right)\right]|0(\beta)\rangle = -\int d^4x \langle 0(\beta)|\,T\left[\frac{i}{\hbar}\delta\widehat{\mathcal{L}}\exp\left(\frac{i}{\hbar}\widehat{\overline{\mathcal{L}}}\right)\right]|0(\beta)\rangle \tag{11.44}$$

where

$$\widehat{\widetilde{\mathcal{L}}} = \int d^4x \left[f_i^{\alpha\dagger}(x)\, \phi_i^{\alpha}(x) + \phi_i^{\alpha\dagger}(x)\, f_i^{\alpha}(x) \right],$$

$$\delta\widehat{\widetilde{\mathcal{L}}} = \int d^4x \left[f_i^{\alpha\dagger}(x)\, \delta^0\phi_i(x) + \delta^0\phi_i^{\dagger}(x)\, f_i^{\alpha}(x) \right]$$

and

$$\delta\widehat{\widetilde{\mathcal{L}}} = \delta\mathcal{L} - \delta\widetilde{\mathcal{L}}.$$

Here doublet notation for the field, $\phi_i(x)$, is used i.e.

$$\psi_i' = \psi_i, \qquad \psi_i^L = \widetilde{\psi}_i^{\dagger}$$

and $\delta\mathcal{L}$ and $\delta\widetilde{\mathcal{L}}$ define the change due to the transformation in $\mathcal{L}$ and $\widetilde{\mathcal{L}}$ respectively.

It is important to note that the operators need to be in the finite temperature form using Bogoliubov transformations and then use of the vacuum at $T \neq 0$ leads to an explicit form for the W-T relations. These relations are essential to check whether the perturbation expansion obeys the symmetry properties of the model to any order.

11.4 Transverse Ward-Takahashi relations

We have discussed the Ward-Takahashi relations for the Noether current that follows from the gauge symmetry and is, thus, conserved

$$\partial^{\mu} J_{\mu} = 0.$$

This implies that the relationship established here refers to the longitudinal component of the current and thus leads to W-T relations, at $T = 0$ or $T \neq 0$, put restriction on the longitudinal components and no restriction on the transverse component. This implies that if we wish any limitation on these components we are forced to use the Euler-Lagrange equations of motion.

In order to obtain the transverse W-T relations we define the Lie transformation for a fermion field

$$\delta_{\mu\nu}^{L}\psi(x) = \sigma_{\mu\nu}\psi(x) \tag{11.45}$$

and

$$\delta_{\mu\nu}^{L}\overline{\psi}(x) = \overline{\psi}(x)\,\sigma_{\mu\nu}, \tag{11.46}$$

where $\sigma_{\mu\nu} = \frac{i}{2}[\gamma_{\mu}, \gamma_{\nu}]$. This would imply that

$$\delta^{L}\psi(x) = \frac{1}{2}\epsilon^{\mu\nu}\sigma_{\mu\nu}\psi(x) \equiv \frac{1}{2}\epsilon^{\mu\nu}\delta_{\mu\nu}^{L}\psi(x),$$

$$\delta^{L}\overline{\psi}(x) = \frac{1}{2}\epsilon^{\mu\nu}\overline{\psi}(x)\,\sigma_{\mu\nu} \equiv \frac{1}{2}\epsilon^{\mu\nu}\delta_{\mu\nu}^{L}\overline{\psi}(x),$$

$$J_\lambda(x)=\frac{1}{2}\epsilon^{\mu\nu}\left\{\left(\overline{\psi}(x)\gamma_\mu\psi(x)\right)\delta_{\lambda\nu}-\left(\overline{\psi}(x)\gamma_\nu\psi(x)\right)\delta_{\lambda\mu}\right\}$$

and

$$q(x)=\frac{1}{2}\epsilon^{\mu\nu}\left\{2m\overline{\psi}(x)\sigma_{\mu\nu}\psi(x)-\epsilon_{\mu\nu\lambda\rho}\overline{\psi}(x)i\gamma_5\gamma^\rho\left(\partial^\lambda-\overleftarrow{\partial}^\lambda\right)\psi(x)\right\}. \quad (11.47)$$

This leads to the transverse W-T relation

$$\begin{aligned}
&i\delta^L_{\mu\nu}T\left(\psi(x_1)\cdots\psi(x_n)\overline{\psi}(y_1)\cdots\overline{\psi}(y_n)\right)\\
&=\int d^4x'\left[\partial'_\mu T\left[\psi(x_1)\cdots\psi(x_n)\overline{\psi}(y_1)\cdots\overline{\psi}(y_n)J_\nu(x')\right]\right.\\
&\quad-\partial'_\nu T\left[\psi(x_1)\cdots\psi(x_n)\overline{\psi}(y_1)\cdots\overline{\psi}(y_n)J_\mu(x')\right]\\
&\quad-T\left[\psi(x_1)\cdots\psi(x_n)\overline{\psi}(y_1)\cdots\overline{\psi}(y_n)\partial'_\mu J_\nu(x')\right]\\
&\quad\left.-T\left[\psi(x_1)\cdots\psi(x_n)\overline{\psi}(y_1)\cdots\overline{\psi}(y_n)\partial'_\nu J_\mu(x')\right]\right] \quad (11.48)
\end{aligned}$$

The first two terms on the right hand side are similar to the curl operation on the current operator.

It is important to emphasize that both the longitudinal and transverse W-T relations are obtained by using the Lie derivatives in canonical field theory. Next we will give the example of $U(1)$ gauge theory i.e. quantum electrodynamics.

Example: $U(1)$ gauge theory

We construct the time-ordered product of the three-point function for the $U(1)$ gauge theory with the fermion-gauge boson vertex

$$T\left(j^\mu(x)\psi(x_1)\overline{\psi}(x_2)\right) \quad (11.49)$$

with $j^\mu(x)=\overline{\psi}(x)\gamma^\mu\psi(x)$. The longitudinal W-T relations relate the divergence of the current operator and the transverse W-T relations arise from the curl of the current operator. Therefore we need to calculate

$$\partial^\mu_x T\left[j^\nu(x)\psi(x_1)\overline{\psi}(x_2)\right]-\partial^\nu_x T\left[j^\mu(x)\psi(x_1)\overline{\psi}(x_2)\right]. \quad (11.50)$$

In order to obtain an explicit expression we need the identity

$$\begin{aligned}
\delta^L T\left[\phi_\alpha(x_1)\phi_\alpha(x_2)\cdots\right]&=T\left[\delta^L\phi_\alpha(x_1)\phi_\alpha(x_2)\cdots\right]\\
&\quad+T\left[\phi_\alpha(x_1)\delta^L\phi_\alpha(x_2)\cdots\right]+\cdots \quad (11.51)
\end{aligned}$$

and a bilinear covariant current operator

$$\begin{aligned}
V^{\lambda\mu\nu}(x)&=\frac{1}{2}\overline{\psi}(x)\left[\gamma^\lambda,\sigma^{\mu\nu}\right]\psi(x),\\
&=i\left(g^{\lambda\mu}j^\nu(x)-g^{\lambda\nu}j^\mu(x)\right), \quad (11.52)
\end{aligned}$$

where we have used the anti-commutator $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$. In order to calculate the curl of the three point function we note the general identity

$$\begin{aligned}
&\partial_\mu^x T\left[J_\mu(x)\,\psi(x_1)\cdots\psi(x_n)\,\overline{\psi}(y_1)\cdots\overline{\psi}(y_n)\right] \\
&= \delta_{\mu 0}\sum_{i=1}^{n} T\left[\left\{\left[J_\mu(x),\psi(x_i)\right]\overline{\psi}(y_i)\,\delta\left(x^0-x_i^0\right)\right.\right. \\
&\qquad\left.\left.+\psi(x_i)\left[J_\mu(x),\overline{\psi}(y_i)\right]\delta\left(x^0-y_i^0\right)\right\}\right. \\
&\qquad\left.\psi(x_1)\cdots\psi(x_n)\,\overline{\psi}(y_1)\cdots\overline{\psi}(y_n)\,\widehat{\psi(x_i)\,\overline{\psi}(y_i)}\right] \\
&\quad+T\left[\partial_\mu^x J_\mu(x)\,\psi(x_1)\cdots\psi(x_n)\,\overline{\psi}(y_1)\cdots\overline{\psi}(y_n)\right] \qquad (11.53)
\end{aligned}$$

where the symbol $\widehat{\ }$ implies that $\psi(x_i)\,\overline{\psi}(y_i)$ are omitted in the preceding set of field operators. The curl-like terms for the three-point functions may be written as

$$\begin{aligned}
&i\partial_x^\mu T\left[j^\nu(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] - i\partial_x^\nu T\left[j^\mu(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \\
&= \delta^4(x-x_1)\,\frac{1}{2}\left(\gamma^0\sigma^{\mu\nu}\gamma^0-\sigma^{\mu\nu}\right)T\left(\psi(x_1)\,\overline{\psi}(x_2)\right) \\
&\quad+\delta^4(x-x_2)\,T\left(\psi(x_1)\,\overline{\psi}(x_2)\right)\frac{1}{2}\left(\gamma^0\sigma^{\mu\nu}\gamma^0-\sigma^{\mu\nu}\right) \\
&\quad+T\left[\overline{\psi}(x)\left(\overleftarrow{\partial}_x\sigma^{\mu\nu}-\sigma^{\mu\nu}\overrightarrow{\partial}_x\right)\psi(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \\
&\quad+T\left[\overline{\psi}(x)\,S^{\lambda\mu\nu}\left(\overrightarrow{\partial}_\lambda^{\,x}-\overleftarrow{\partial}_\lambda^{\,x}\right)\psi(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \qquad (11.54)
\end{aligned}$$

where

$$S^{\lambda\mu\nu} = \frac{1}{2}\left\{\gamma^\lambda,\sigma^{\mu\nu}\right\} = -\epsilon^{\lambda\mu\nu\rho}\gamma_\rho\gamma_5.$$

In order to express the right-hand side of Eq. (11.54) in terms of Green functions, we have to take the derivative operation outside the time-ordered product by making the right and left derivatives for x and x'. Furthermore to recover the gauge invariant expression we include the line integral so that the last term becomes

$$\left(\partial_\lambda^x-\partial_\lambda^{x'}\right)T\left[\overline{\psi}(x')\,S^{\lambda\mu\nu}\exp\left(-ig\int_x^{x'}A_\rho(y)\,dy^\rho\right)\psi(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \qquad (11.55)$$

where $A_\rho(y)$ is the gauge field and g is the coupling constant between fermions and the gauge boson. For the $U(1)$ gauge field, QED, $g = e$ and $A_\rho(y)$ is the photon field. For the $SU(3)$ gauge field, QCD, $A_\rho = A_\rho^a t^a$, A_ρ^a is the gluon field and t^a are the generators of the $SU(3)$ color group. Explicitly Eq. (11.55) becomes

$$\begin{aligned}
&\left(\partial_\lambda^x-\partial_\lambda^{x'}\right)T\left[\overline{\psi}(x')\,S^{\lambda\mu\nu}U_P(x',x)\,\psi(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \\
&= T\left(\left[\left(\partial_\lambda^x-\partial_\lambda^{x'}\right)\overline{\psi}(x')\,S^{\lambda\mu\nu}\psi(x)\right]U_P(x',x)\,\psi(x_1)\,\overline{\psi}(x_2)\right) \\
&+\delta^4(x-x_2)\,T\left(\overline{\psi}(x')\,U_P(x',x)\,\psi(x_1)\right)\gamma^0 S^{\lambda\mu\nu} \\
&+\delta^4(x'-x_1)\,S^{0\mu\nu}\gamma^0 T\left(\psi(x)\,\overline{\psi}(x_2)\,U_P(x',x)\right) \\
&-2\delta^4(x-x')\,\mathrm{Tr}(\gamma^0 S^{0\mu\nu})T\left(\psi(x_1)\,\overline{\psi}(x_2)\right) \\
&+T\left[\overline{\psi}(x')\,S^{\lambda\mu\nu}\left(\left(\partial_\lambda^x-\partial_\lambda^{x'}\right)U_P(x',x)\right)\psi(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \qquad (11.56)
\end{aligned}$$

where

$$U_P(x',x) \equiv T\left[\exp\left(-ig\int_x^{x'} A_\rho(y)\,dy^\rho\right)\right]$$

with T being the time ordering operator so that functions from right to left are ordered with increasing time.

Combining all the terms we get

$$\begin{aligned}
&\partial_x^\mu T\left[j^\nu(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] - \partial_x^\nu T\left[j^\mu(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \\
&= iT\left(\psi(x_1)\,\overline{\psi}(x_2)\right)\sigma^{\mu\nu}\delta^4(x-x_2) + i\sigma^{\mu\nu}T\left(\psi(x_1)\,\overline{\psi}(x_2)\right)\delta^4(x-x_1) \\
&+ \lim_{x\to x'} i\left(\overrightarrow{\partial}_\lambda^{\,x} - \overleftarrow{\partial}_\lambda^{\,x}\right) T\left[\overline{\psi}(x')\,\epsilon^{\lambda\mu\nu\rho}\gamma_\rho\gamma_5 U_P(x',x)\,\psi(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \\
&+ T\left[\overline{\psi}(x)\left(\sigma^{\mu\nu}i\overrightarrow{\not{D}}_x - i\overleftarrow{\not{D}}_x\sigma^{\mu\nu}\right)\psi(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \qquad (11.57)
\end{aligned}$$

where $\overrightarrow{D}_\mu = \overrightarrow{\partial}_\mu + igA_\mu$ and $\overleftarrow{D}_\mu = \overleftarrow{\partial}_\mu - igA_\mu$ are covariant derivatives and $\not{D} = D_\mu\gamma^\mu$.

Now using the fact that the dynamics for the fermion field i.e. the Euler-Lagrange equation implies that

$$\left(i\overrightarrow{D} - m\right)\psi = 0 \qquad \text{and} \qquad \overline{\psi}\left(i\overleftarrow{D} + m\right) = 0.$$

These equations are valid for both QED and QCD. Finally we arrive at the W-T relation for the transverse fermion-gauge boson vertex to be

$$\begin{aligned}
&\partial_x^\mu T\left[j^\nu(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] - \partial_x^\nu T\left[j^\mu(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \\
&= iT\left(\psi(x_1)\,\overline{\psi}(x_2)\right)\sigma^{\mu\nu}\delta^4(x-x_2) \\
&+ i\sigma^{\mu\nu}T\left(\psi(x_1)\,\overline{\psi}(x_2)\right)\delta^4(x-x_1) \\
&+ \lim_{x\to x'} i\left(\overrightarrow{\partial}_\lambda^{\,x} - \overleftarrow{\partial}_\lambda^{\,x}\right)\epsilon^{\lambda\mu\nu\rho}T\left[\overline{\psi}(x')\,\gamma_\rho\gamma_5 U_P(x',x)\,\psi(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \\
&+ 2mT\left[\overline{\psi}(x)\,\sigma^{\mu\nu}\psi(x)\,\psi(x_1)\,\overline{\psi}(x_2)\right] \qquad (11.58)
\end{aligned}$$

The transverse vertex depends on tensor and axial-vector vertex. In addition the line integral in the axial-vector makes the calculations complicated and has to be considered loop-wise [168]. This operator equation may be converted into a Ward-Takahashi relation between Green functions by taking its vacuum expectation value.

11.5 Transverse W-T relation in momentum space

The transverse W-T relation has a simpler form in the momentum space. As usual the three-point function in momentum space is defined as

$$\begin{aligned}
&\int d^4x d^4x_1 d^4x_2 e^{i(p_1\cdot x_1 + p_2\cdot x_2 + p_3\cdot x_3)}\left\langle 0\right|j_\Lambda(x)\,\psi(x_1)\,\overline{\psi}(x_2)\left|0\right\rangle \\
&\qquad = (2\pi)^4\,\delta(p_1 - p_2 - q)\,iS_F(p_1)\,\Gamma_\Lambda(p_1,p_2)\,iS_F(p_2) \qquad (11.59)
\end{aligned}$$

where the subscript $\Lambda = V, A, T$, denote vector, axial-vector and tensor vertices respectively for Γ_Λ. The corresponding currents are:

$$j_\mu^V = \overline{\psi}\gamma_\mu\psi\,, \quad j_\mu^A = \overline{\psi}\gamma_\mu\gamma_5\psi\,, \quad j_{\mu\nu}^T = \overline{\psi}\sigma_{\mu\nu}\psi\,.$$

This now leads to the transverse W-T identity in momentum space

$$\begin{aligned} iq^\mu\Gamma_V^\nu(p_1,p_2) - iq^\nu\Gamma_V^\mu(p_1,p_2) = {} & S_F^{-1}(p_1)\,\sigma^{\mu\nu} + \sigma^{\mu\nu}S_F^{-1}(p_2) \\ & + 2m_F\Gamma_T^{\mu\nu}(p_1,p_2) \\ & + (p_{1\lambda}+p_{2\lambda})\,\epsilon^{\lambda\mu\nu\rho}\,\Gamma_{A\rho}(p_1,p_2) \end{aligned} \tag{11.60}$$

where $q = p_1 - p_2$ and m_F is the mass of the fermion. Again the axial-vector vertex has the line integral, which forces a perturbative analysis. This equation is valid at tree level. For loop corrections, Wilson loops have to be included.

11.5.1 *Full vertex for the fermion-gauge boson vertex*

The longitudinal W-T relation in Eq. (11.22) after multiplying with q^μ is

$$q^\mu q^\nu\Gamma_\nu(p_1,p_2) = q^\mu\left(S_F^{-1}(p_1) - S_F^{-1}(p_2)\right) \tag{11.61}$$

while the transverse W-T relation is

$$q_\nu q^\nu\Gamma^\mu(p_1,p_2) - q_\nu q^\mu\Gamma^\nu(p_1,p_2) = iq_\nu h^{\mu\nu} \tag{11.62}$$

where $h_{\mu\nu}$ is the expression on the right-hand side of Eq. (11.60). Combining the last two expressions we get

$$q^2\Gamma^\mu(p_1,p_2) = q^\mu\left(S_F^{-1}(p_1) - S_F^{-1}(p_2)\right) + iq_\nu h^{\mu\nu}. \tag{11.63}$$

The full vertex for the gauge theory has two components: longitudinal (first term) and transverse (second term). Explicitly the full vertex is given as

$$\begin{aligned} \Gamma_V^\mu(p_1,p_2) = {} & q^{-2}q^\mu\left(S_F^{-1}(p_1) - S_F^{-1}(p_2)\right) \\ & + iS_F^{-1}(p_1)\,q^{-2}q_\nu\sigma^{\mu\nu} + q^{-2}q_\nu\sigma^{\mu\nu}iS_F^{-1}(p_2) \\ & + 2im_F q^{-2}q_\nu\Gamma_T^{\mu\nu}(p_1,p_2) \\ & + q^{-2}q_\nu\,(p_{1\lambda}+p_{2\lambda})\,\epsilon^{\lambda\mu\nu\rho}\Gamma_{A\rho}(p_1,p_2)\,. \end{aligned} \tag{11.64}$$

This shows that the vector vertex depends on the axial-vector and the tensor vertices in addition to the fermion propagator. However for QCD in the chiral limit, $m_F = 0$, the dependance on the tensor vertex disappears.

It is interesting to note that in the case of bare vertices and free propagators, the transverse W-T relation reduces to

$$\begin{aligned} i\,(q^\mu\gamma^\nu - \gamma^\nu q^\mu) = {} & (\not{p}_1 - m)\,\sigma^{\mu\nu} + \sigma^{\mu\nu}\,(\not{p}_2 - m) \\ & + 2m\sigma^{\mu\nu} + (p_{1\lambda}+p_{2\lambda})\,\epsilon^{\lambda\mu\nu\rho}\gamma_\mu\gamma_5 \end{aligned} \tag{11.65}$$

which is a trivial identity of the γ-matrices. The longitudinal W-T relation at tree level is similarly a trivial identity

$$q_\mu\gamma^\mu = (\not{p}_1 - m) - (\not{p}_2 - m)\,. \tag{11.66}$$

Thus the transverse, longitudinal and total vertices for gauge fields satisfy generalized W-T relations. It is to be stressed again that the longitudinal and transverse W-T relations have to be considered differently, in the sense, that the former is a consequence of the gauge symmetry while the latter depends on Euler-Lagrange equations and does not emerge from any symmetry considerations. There are previous attempts to obtain the transverse component of the vertex. They met with limited success [169–172].

11.5.2 *Tranverse W-T relation for axial current*

By a procedure used to calculate the W-T relation for vector current, a similar relation is obtained for the axial current, $\overline{\psi}(x)\gamma_\mu\gamma_5\psi(x)$, as

$$\begin{aligned}\partial_x^\mu T\left[j_5^\nu(x)\psi(x_1)\overline{\psi}(x_2)\right] &= \partial_x^\nu T\left[j_5^\mu(x)\psi(x_1)\overline{\psi}(x_2)\right] \\ &+ i\sigma^{\mu\nu}\gamma_5 T\left[\psi(x_1)\overline{\psi}(x_2)\right]\delta^4(x_1-x) \\ &- iT\left[\psi(x_1)\overline{\psi}(x_2)\right]\sigma^{\mu\nu}\gamma_5\delta^4(x_1-x) \\ &+ i\lim_{x'\to x}\left(\partial_\lambda^x-\partial_\lambda^{x'}\right)\epsilon^{\lambda\mu\nu\rho} \\ &\times T\left[\overline{\psi}(x')\gamma_\rho U_P(x',x)\psi(x)\psi(x_1)\overline{\psi}(x_2)\right].\end{aligned}$$

After taking the expectation value of this expression between vacuum states the transverse W-T relation in momentum space is

$$\begin{aligned}&iq^\mu\Gamma_A^\nu(p_1,p_2)-iq^\nu\Gamma_A^\mu(p_1,p_2) \\ &= S_F^{-1}(p_1)\sigma^{\mu\nu}\gamma_5-\sigma^{\mu\nu}\gamma_5 S_F^{-1}(p_2) \\ &+(p_{1\lambda}+p_{2\lambda})\epsilon^{\lambda\mu\nu\rho}\Gamma_{V\rho}(p_1,p_2).\end{aligned}$$

This is valid at tree level. For corrections at loop level, Wilson loops have to be considered. Thus we find that the transverse vector and axial vertex functions are connected. These relations have been shown to be accurate to one-loop order [168].

11.5.3 *Transverse W-T relation at finite temperature*

In order to get the transverse W-T relation at finite temperature, the expectation value of the expression in Eq. (11.58) is taken between finite temperature vacuum, $|0(\beta)\rangle$, state. This suggests the versatility of the W-T relations that are operator relations. Taking expectations value between finite temperature vacuum transverse relations are obtained. Bogoliubov transformation has to be applied to the operators in transverse W-T relations.

11.6 W-T relations and spontaneous symmetry breaking

It is possible to relate W-T relations and spontaneous symmetry breaking and thus deduce that Goldstone boson has zero mass. It was shown by Takahashi [164] and

the results are similar to those obtained elsewhere [173].

From Noether current we obtain for the Lie derivative of a field to be

$$-i\delta^L\phi(x) = \int d^4x' T\left[\phi(x)\,\partial'_\mu J^\mu(x')\right] - \int d^4x' \partial'_\mu T\left[\phi(x)\,J^\mu(x')\right].$$

An invariant transformation implies that

$$\partial_\mu J^\mu(x) = 0.$$

Therefore we have

$$i\delta^L\phi(x) = \int d^4x' \partial'_\mu T\left[\phi(x)\,J^\mu(x')\right].$$

If the vacuum expectation value of $\delta^L\psi(x)$ is non-zero, i.e.

$$\langle 0|\,\delta^L\phi(x)\,|0\rangle = a \neq 0$$

where a is a c-number then

$$\int d^4x' \partial'_\mu T\left[\phi(x)\,J^\mu(x')\right] = ia \tag{11.67}$$

However we can write the left-hand side in terms of its spectral representation by using

$$\int d^4x' T\left[\phi(x)\,J^\mu(x')\right] = -i\int_0^\infty dk^2\rho_J\left(k^2\right)\partial_\mu\Delta^+\left(x-x';k^2\right)$$

which gives for current conservation condition

$$k^2\rho_J\left(k^2\right) = 0. \tag{11.68}$$

However we wish to write

$$\begin{aligned}\partial'_\mu\langle 0|\,T\left[\phi(x)\,J^\mu(x')\right]|0\rangle &= i\int_0^\infty dk^2\rho_J\left(k^2\right)\Box\Delta_c\left(x-x';k^2\right)\\ &= i\int_0^\infty dk^2\rho_J\left(k^2\right)k^2\Delta_c\left(x-x';k^2\right)\\ &\quad + i\int_0^\infty dk^2\rho_J\left(k^2\right)\delta\left(x-x'\right).\end{aligned}$$

Therefore we get the following expression for a

$$a = \int d^4x'\int_0^\infty dk^2\rho_J\left(k^2\right)k^2\Delta_c\left(x-x';k^2\right) + \int_0^\infty dk^2\rho_J\left(k^2\right).$$

However $k^2\rho_J\left(k^2\right) = 0$, leading to

$$a = \int_0^\infty dk^2\rho_J\left(k^2\right).$$

Therefore this relation along with the one in Eq. (11.68), we have that there exists a massless boson. This is the Goldstone theorem.

It is important to remark that the presentation in this chapter has focussed on quantum field theories with $U(1)$ gauge symmetry. This provides longitudinal W-T relations for the vertex function. The transverse W-T relations are studied by looking at an expression that appears curl-like. The combination gives the complete vertex function. These have proved very useful in assuring that the perturbative calculations are gauge-invariant at every order. However these ideas are much more general and are equally applicable to a perturbative study of many-body systems. The W-T relations provide a consistency condition so that all conservation laws are obeyed. Such procedures have been used for spin systems among others. As mentioned earlier, the W-T relations provide us relations for renormalization constants in quantum electrodynamics. These relations are important for studies at low energies and other gauge theory. For many-body systems, the sum rules can be easily derived by using W-T relations.

Ending this chapter we close the second part of this book, where we consider the quantum field theory at finite temperature from symmetry bases. Now we explore some consequences of the thermal states that we have introduced. In particular we analyze the meaning of the different thermal states, by studying their non-classical properties.

PART III

Applications to Quantum Optics

Chapter 12

Thermalized States of a Field Mode

Thermofield dynamics formalism provides a general prescription to define thermalized states of a boson oscillator. We shall show that TFD states, obtained by repeated action of $a^\dagger(\beta)$ on the thermal vacuum $|0(\beta)\rangle$ and their linear combinations, correspond to physical states of a field mode which incorporate thermal effects. We also show how these states are represented within the density matrix formalism of quantum mechanics and investigate procedures to determine expectation values of physical observables in order to discuss their nonclassical properties. Other classes of elements of the thermal Hilbert space $\mathcal{H}_T$ are also considered.

12.1 Thermalized states

Consider the thermal Hilbert space, $\mathcal{H}_T$, of a boson oscillator at a given temperature $T = \beta^{-1}$. As we have discussed earlier, this space is spanned by vectors of the type

$$|n, \widetilde{m}; \beta\rangle = U(\beta)\,|n, \widetilde{m}\rangle = \frac{1}{\sqrt{n!}\sqrt{m!}}\left[a^\dagger(\beta)\right]^n \left[\tilde{a}^\dagger(\beta)\right]^m |0(\beta)\rangle\,, \tag{12.1}$$

with $n, m = 0, 1, 2, \ldots$; that is, $\mathcal{H}_T$ corresponds to the application of the Bogoliubov transformation $U(\beta)$ to the doubled space $\mathcal{H}\otimes\widetilde{\mathcal{H}}$. It is easy to verify that, fixing the value of $\widetilde{m} = m_0$ say, the subspace of $\mathcal{H}_T$ spanned by $\{|n, m_0; \beta\rangle\ , n = 0, 1, 2, \ldots\}$ is isomorphic to the physical Hilbert space ($\mathcal{H}$) of the boson oscillator. Among all these subspaces, we initially detach the one for which $m_0 = 0$, corresponding to the subspace $\mathcal{H}_\beta$ that is spanned by the set of vectors $\left\{\left[a^\dagger(\beta)\right]^n |0(\beta)\rangle\ , n = 0, 1, 2, \ldots\right\}$. The isomorphism between $\mathcal{H}_\beta$ and the usual zero-temperature Hilbert space of a single mode of the electromagnetic field, $\mathcal{H}$, can be directly demonstrated from the correspondence

$$a^{\dagger n}\,|0\rangle \longleftrightarrow \left[a^\dagger(\beta)\right]^n |0(\beta)\rangle\ ,\ \ \left[a, a^\dagger\right] = 1 \longleftrightarrow \left[a(\beta), a^\dagger(\beta)\right] = 1\,.$$

Therefore, we can construct thermal states of a field mode by mimicking states usually considered in quantum optics [174–177] with the zero-temperature formalism. As we are going to show later, such states are physical states of a field mode that carry temperature effects. Before treating this physical interpretation, however, we work out some basic examples.

12.1.1 *Thermal number states*

Let us first write the hat Hamiltonian for a boson oscillator as $\widehat{H} = \widehat{H}(\beta) = H(\beta) - \widetilde{H}(\beta)$, where

$$H(\beta) = \omega a^\dagger(\beta) a(\beta) \tag{12.2}$$

and, similarly, $\widetilde{H}(\beta) = \omega \tilde{a}^\dagger(\beta)\tilde{a}(\beta)$. It is then easy to check that $[H(\beta), a(\beta)] = -\omega a(\beta)$ and $\left[H(\beta), a^\dagger(\beta)\right] = \omega a^\dagger(\beta)$, so that $a(\beta)$ and $a^\dagger(\beta)$ are annihilation and creation operators of quanta of $H(\beta)$, respectively. Now, since $a(\beta)\,|0(\beta)\rangle = 0$, the normalized eigenstates of $H(\beta)$ are given by

$$|n(\beta)\rangle = \frac{1}{\sqrt{n!}} \left[a^\dagger(\beta)\right]^n |0(\beta)\rangle \;\;,\;\; n = 0, 1, 2, \dots \,, \tag{12.3}$$

with the corresponding eigenvalues being $n\omega$. Naturally, these states are also eigenstates of the thermal number operator $N(\beta) = a^\dagger(\beta)a(\beta)$, i.e.

$$N(\beta)\,|n(\beta)\rangle = n\,|n(\beta)\rangle\,.$$

Also, the action of $a(\beta)$ and $a^\dagger(\beta)$ on the thermal number states $|n(\beta)\rangle$ is given by

$$\begin{aligned} a(\beta)\,|n(\beta)\rangle &= \sqrt{n}\;|(n-1)(\beta)\rangle\,, \\ a^\dagger(\beta)\,|n(\beta)\rangle &= \sqrt{n+1}\;|(n+1)(\beta)\rangle\,. \end{aligned}$$

Note that, being non-degenerate eigenstates of a hermitian operator, these thermal number states are orthonormal, that is

$$\begin{aligned} \langle m(\beta)|n(\beta)\rangle &= \delta_{m,n}\,, \\ \sum_{n=0}^{\infty} |n(\beta)\rangle\,\langle n(\beta)| &= \mathbf{1}. \end{aligned}$$

Therefore, an arbitrary normalized state $|\Psi(\beta)\rangle$ of $\mathcal{H}_\beta$ can be written as

$$|\Psi(\beta)\rangle = \sum_{n=0}^{\infty} c_n\,|n(\beta)\rangle\,, \tag{12.4}$$

where $c_n = \langle n(\beta)|\Psi(\beta)\rangle$ and $\sum_{n=0}^{\infty} |c_n|^2 = 1$.

12.1.2 *Thermal coherent states*

Similarly to the zero-temperature case, we define displacement operators acting on states of $\mathcal{H}_\beta$ and then introduce the notion of coherent states. The unitary thermal displacement operator, $D(\alpha;\beta)$, is defined by

$$D(\alpha;\beta) = \exp\left[\alpha a^\dagger(\beta) - \alpha^* a(\beta)\right], \tag{12.5}$$

where α is an arbitrary complex number. Notice that $D^\dagger(\alpha;\beta) = D^{-1}(\alpha;\beta) = D(-\alpha;\beta)$. The name "displacement operator" comes from the property

$$D^\dagger(\alpha;\beta)\,a(\beta)\,D(\alpha;\beta) = a(\beta) + \alpha, \tag{12.6}$$

which is readily verified by using the normal ordered form of $D(\alpha;\beta)$,

$$D(\alpha;\beta) = e^{-|\alpha|^2/2} \exp\left[\alpha a^\dagger(\beta)\right] \exp\left[-\alpha^* a(\beta)\right]. \tag{12.7}$$

This expression is a particular case of the Baker-Campbell-Hausdorff operator identity

$$e^{A+B} = e^A e^B e^{-[A,B]/2},$$

which holds only if $[A,[A,B] = [B,[A,B]] = 0$. It also follows from this identity that the repeated action of thermal displacement operators corresponds, apart from a phase factor, to a displacement by the sum of the complex parameters, that is

$$D(\gamma;\beta)D(\alpha;\beta) = e^{i\mathrm{Im}[\gamma\alpha^*]}\, D(\gamma+\alpha;\beta). \tag{12.8}$$

Multiplying Eq. (12.6) from the left by $D(\alpha;\beta)$ and applying the resulting operator identity to the thermal vacuum $|0(\beta)\rangle$, one obtains

$$a(\beta)D(\alpha;\beta)\,|0(\beta)\rangle = D(\alpha;\beta)\,(a(\beta)+\alpha)\,|0(\beta)\rangle = \alpha D(\alpha;\beta)\,|0(\beta)\rangle\,.$$

This means that the state

$$|\alpha(\beta)\rangle = D(\alpha;\beta)\,|0(\beta)\rangle \tag{12.9}$$

is an eigenstate of the thermal annihilation operator $a(\beta)$ with eigenvalue given by α. Notice that the eigenvalues of $a(\beta)$ are complex numbers in accordance with its nonhermiticity. We shall refer to states of the kind presented in Eq. (12.9) as thermal coherent states. By construction, due to the unitarity of the thermal displacement operator $D(\alpha;\beta)$, the thermal coherent states are normalized,

$$|\langle\alpha(\beta)|\alpha(\beta)\rangle|^2 = 1.$$

The expansion of thermal coherent states in the thermal number basis of $\mathcal{H}_\beta$ is found by directly applying the thermal displacement operator, in the normal form (12.7), to the thermal vacuum $|0(\beta)\rangle$; one gets,

$$|\alpha(\beta)\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}\,|n(\beta)\rangle\,. \tag{12.10}$$

Also, it follows that the scalar product between two thermal coherent states is a nonvanishing complex number given by

$$\langle\gamma(\beta)|\alpha(\beta)\rangle = \exp\left[-\frac{1}{2}\left(|\alpha|^2+|\gamma|^2\right)+\alpha\gamma^*\right], \tag{12.11}$$

implying that distinct coherent states are not orthogonal. The square of the absolute value of this scalar product is

$$|\langle\gamma(\beta)|\alpha(\beta)\rangle|^2 = e^{-|\alpha-\gamma|^2},$$

which shows that the coherent states $|\alpha(\beta)\rangle$ and $|\gamma(\beta)\rangle$ can be taken as approximately orthogonal only if α and γ are very distant apart complex numbers, i.e. when $|\alpha-\gamma| \gg 1$.

For a given β, the set of thermal coherent states, which is labeled by a two-dimensional continuous parameter, constitutes an overcomplete basis of $\mathcal{H}_\beta$. In fact,

$$\frac{1}{\pi}\int d^2\alpha\,|\alpha(\beta)\rangle\langle\alpha(\beta)| = \frac{1}{\pi}\sum_{n,m=0}^{\infty}\frac{|n(\beta)\rangle\langle m(\beta)|}{\sqrt{n!m!}}\int d^2\alpha\,e^{-|\alpha|^2}\alpha^n\alpha^{*m} = \mathbf{1}, \quad (12.12)$$

since

$$\int d^2\alpha\,e^{-|\alpha|^2}\alpha^n\alpha^{*m} = \pi n!\,\delta_{nm},$$

where $d^2\alpha = d\mathrm{Re}(\alpha)d\mathrm{Im}(\alpha)$. Thus, an arbitrary normalized thermal state is written in the thermal coherent basis as

$$|\Psi(\beta)\rangle = \frac{1}{\pi}\int d^2\alpha\,\langle\alpha(\beta)|\Psi(\beta)\rangle|\alpha(\beta)\rangle. \quad (12.13)$$

Particularly, we find that any thermal coherent state $|\gamma(\beta)\rangle$ is written as

$$|\gamma(\beta)\rangle = \frac{e^{-|\gamma|^2/2}}{\pi}\int d^2\alpha\,e^{-(|\alpha|^2-2\gamma\alpha^*)/2}|\alpha(\beta)\rangle.$$

12.1.3 *Thermal displaced number states*

In a similar fashion as thermal coherent states are defined as displacements of the thermal vacuum, we can introduce thermal displaced number states by applying the thermal displacement operator to thermal number states, i.e.

$$|n(\beta);\alpha\rangle = D(\alpha;\beta)\,|n(\beta)\rangle\,. \quad (12.14)$$

These states are eigenstates of the thermal displaced number operator,

$$N_\alpha(\beta)|n(\beta);\alpha\rangle \equiv a^\dagger_\alpha(\beta)a_\alpha(\beta)|n(\beta);\alpha\rangle = n|n(\beta);\alpha\rangle,$$

where

$$a_\alpha(\beta) = D(\alpha;\beta)a(\beta)D^\dagger(\alpha;\beta) = a(\beta) - \alpha,$$
$$a^\dagger_\alpha(\beta) = D(\alpha;\beta)a^\dagger(\beta)D^\dagger(\alpha;\beta) = a^\dagger(\beta) - \alpha^*,$$

are the thermal displaced annihilation and creation operators, respectively. From these relations, we find that the thermal displaced number state can also be expressed as

$$|n(\beta);\alpha\rangle = \frac{1}{\sqrt{n!}}\left[a^\dagger(\beta) - \alpha^*\right]^n|\alpha(\beta)\rangle\,. \quad (12.15)$$

The unitarity of the thermal displacement operator, together with the orthonormality of the thermal number states, implies that the set of thermal displaced number states, for an arbitrary but fixed value of α, constitutes a discrete orthonormal basis of $\mathcal{H}_\beta$, i.e.

$$\langle m(\beta);\alpha|n(\beta);\alpha\rangle = \delta_{m,n}\ , \quad \sum_{n=0}^{\infty}|n(\beta);\alpha\rangle\,\langle n(\beta);\alpha| = \mathbf{1}.$$

The projection of the thermal displaced number state $|n(\beta);\alpha\rangle$ onto the thermal number state $|m(\beta)\rangle$, which corresponds to the matrix element of the thermal displacement operator in the thermal number basis, is given by

$$\langle m(\beta)|n(\beta);\alpha\rangle = (-\alpha^*)^{n-m}\sqrt{\frac{m!}{n!}}L_m^{(n-m)}(|\alpha|^2)e^{-|\alpha|^2/2}\,, \quad \text{if } n \geq m\,,$$
$$\langle m(\beta)|n(\beta);\alpha\rangle = \left[\langle n(\beta)|m(\beta);-\alpha\rangle\right]^*\,, \quad \text{for } n < m\,,$$

where $L_r^{(s)}(z)$ denote Laguerre polynomials.

On the other hand, the overlap of $|n(\beta);\alpha\rangle$ with the thermal coherent state $|\gamma(\beta)\rangle$ is found from Eq. (12.8) to be

$$\begin{aligned}\langle\gamma(\beta)|n(\beta);\alpha\rangle &= \big\langle 0(\beta)|D^\dagger(\gamma;\beta)D(\alpha;\beta)|n(\beta)\big\rangle \\ &= \frac{(\gamma^*-\alpha^*)^n}{\sqrt{n!}}\,\exp\left[-\frac{1}{2}\left(|\gamma|^2+|\alpha|^2\right)+\gamma^*\alpha\right]. \end{aligned} \tag{12.16}$$

We notice that two displaced thermal states, with the same value of n but distinct values of the displacement parameter, are not orthogonal to each other; in fact, it follows from Eq. (12.8) that

$$\begin{aligned}\langle n(\beta);\gamma|n(\beta);\alpha\rangle &= e^{-i\mathrm{Im}(\gamma\alpha^*)}\,\langle n(\beta)|D(\alpha-\gamma;\beta)|n(\beta)\rangle \\ &= e^{-i\mathrm{Im}(\gamma\alpha^*)}\,{}_1F_1(-n,1;|\alpha-\gamma|^2),\end{aligned}$$

where ${}_1F_1(p,q;z)$ is the Kummer confluent hypergeometric function. Also, expanding $|n(\beta);\alpha\rangle$ in the thermal coherent basis by using (12.16), one can show that

$$\frac{1}{\pi}\int d^2\alpha\,|n(\beta);\alpha\rangle\langle n(\beta);\alpha| = \mathbf{1};$$

therefore, for fixed n, the set of all thermal displaced number states (with $\alpha\in\mathbb{C}$) forms an overcomplete basis of $\mathcal{H}_\beta$.

12.1.4 *Thermal squeezed states*

The thermal version of the unitary squeezing operator, acting on $\mathcal{H}_\beta$, has the form

$$S(\xi;\beta) = \exp\left(\frac{1}{2}\xi^* a^2(\beta) - \frac{1}{2}\xi a^{\dagger 2}(\beta)\right), \tag{12.17}$$

where

$$\xi = re^{i\varphi}$$

is a complex parameter. It is such that $S^\dagger(\xi;\beta) = S(-\xi;\beta)$. Using the operator identity

$$e^{\eta(A+B)} = e^{(\tanh\eta)B}\,e^{\ln(\cosh\eta)[A,B]}\,e^{(\tanh\eta)A},$$

with $\eta = r$, $A = \frac{1}{2}e^{-i\varphi}a^2(\beta)$ and $B = -\frac{1}{2}e^{i\varphi}a^{\dagger 2}(\beta)$, the thermal squeezing operator is written in normal-ordered form as follows

$$S(\xi;\beta) = \frac{1}{\sqrt{\mu}}\,\exp\left[-\frac{\nu}{2\mu}\,a^{\dagger 2}(\beta)\right]\,e^{-(\ln\mu)\,a^\dagger(\beta)a(\beta)}\,\exp\left[\frac{\nu^*}{2\mu}\,a^2(\beta)\right], \tag{12.18}$$

where

$$\mu = \cosh r \ , \quad \nu = e^{i\varphi} \sinh r$$

and, therefore, $\mu^2 - |\nu|^2 = 1$. Under the action of $S(\xi;\beta)$, the thermal annihilation and creation operators transform accordingly

$$a_\xi(\beta) = S(\xi;\beta) a(\beta) S^\dagger(\xi;\beta) = \mu\, a(\beta) + \nu\, a^\dagger(\beta), \tag{12.19}$$

$$a^\dagger_\xi(\beta) = S(\xi;\beta) a^\dagger(\beta) S^\dagger(\xi;\beta) = \mu\, a^\dagger(\beta) + \nu^*\, a(\beta). \tag{12.20}$$

We have $[a_\xi(\beta), a^\dagger_\xi(\beta)] = 1$, since $S(\xi;\beta)$ is unitary.

Many states of $\mathcal{H}_\beta$ can be formed with the use of the operator $S(\xi;\beta)$. For example, the thermal squeezed vacuum state is defined by

$$|\xi, 0; \beta\rangle = S(\xi;\beta)\, |0(\beta)\rangle\, . \tag{12.21}$$

More generally, thermal squeezed coherent states are generated by first displacing the thermal vacuum and then applying the thermal squeezing operator; that is,

$$|\xi, \alpha; \beta\rangle = S(\xi;\beta) D(\alpha;\beta)\, |0(\beta)\rangle = S(\xi;\beta)\, |\alpha(\beta)\rangle\, . \tag{12.22}$$

One naturally wonders whether inverting the order of these operations, i.e. first squeezing the vacuum and then displacing, would lead to a distinct type of state. To answer this question, first observe that the thermal squeezed coherent state, Eq. (12.22), corresponds to the displacement of the thermal squeezed vacuum implemented with the transformed thermal displacement operator, that is

$$|\xi, \alpha; \beta\rangle = D_\xi(\alpha;\beta)\, |\xi, 0; \beta\rangle\, ,$$

where, using Eqs. (12.19) and (12.20), we have

$$\begin{aligned} D_\xi(\alpha;\beta) &= S(\xi;\beta) D(\alpha;\beta) S^\dagger(\xi;\beta) \\ &= \exp\left[\alpha a^\dagger_\xi(\beta) - \alpha^* a_\xi(\beta)\right] \\ &= \exp\left[\alpha_\xi a^\dagger(\beta) - \alpha^*_\xi a(\beta)\right] = D(\alpha_\xi;\beta), \end{aligned} \tag{12.23}$$

with

$$\alpha_\xi = \mu\alpha - \nu\alpha^*. \tag{12.24}$$

Therefore, the state defined by Eq. (12.22) can also be written as

$$|\xi, \alpha; \beta\rangle = D(\alpha_\xi;\beta) S(\xi;\beta)\, |0(\beta)\rangle\, . \tag{12.25}$$

Conversely, the state

$$|\gamma, \xi; \beta\rangle = D(\gamma;\beta) S(\xi;\beta)\, |0(\beta)\rangle$$

is the same as the state

$$|\xi, \gamma_{-\xi}; \beta\rangle = S(\xi;\beta) D(\gamma_{-\xi};\beta)\, |0(\beta)\rangle\, ,$$

where

$$\gamma_{-\xi} = \mu\gamma + \nu\gamma^*.$$

In other words, changing the order of squeezing and displacing operations acting on the thermal vacuum leads to the same kind of state but with a modified displacement parameter.

It is important to note that, since $S(\xi;\beta)$ and $D(\alpha;\beta)$ are unitary operators, all these thermal squeezed states are normalized. Moreover, it follows that the set of all thermal squeezed coherent states, for a fixed value of the squeezing parameter ξ, constitutes an overcomplete basis of $\mathcal{H}_\beta$. In fact, from Eqs. (12.12) and (12.22) we have

$$\frac{1}{\pi}\int d^2\alpha\,|\xi,\alpha;\beta\rangle\langle\xi,\alpha;\beta| = S(\xi;\beta)\left[\frac{1}{\pi}\int d^2\alpha\,|\alpha(\beta)\rangle\langle\alpha(\beta)|\right]S^\dagger(\xi;\beta) = \mathbf{1},$$

and, also,

$$\begin{aligned}\langle\xi,\gamma;\beta|\xi,\alpha;\beta\rangle &= \big\langle\gamma(\beta)|S^\dagger(\xi;\beta)S(\xi;\beta)|\alpha(\beta)\big\rangle \\ &= \exp\left[-\frac{1}{2}(|\alpha|^2+|\gamma|^2)+\gamma^*\alpha\right].\end{aligned}$$

Furthermore, the overlap between the thermal squeezed coherent state $|\xi,\alpha;\beta\rangle$ and the thermal coherent state $\gamma(\beta)$ is given by

$$\langle\gamma(\beta)|\xi,\alpha;\beta\rangle = \frac{1}{\sqrt{\mu}}\exp\left(-\frac{|\alpha|^2+|\gamma|^2}{2}+\frac{2\gamma^*\alpha-\nu\gamma^{*2}+\nu^2\alpha^2}{2\mu}\right),$$

while the projection of the state $|\xi,\alpha;\beta\rangle$ onto the thermal number state $|n(\beta)\rangle$ is

$$\langle n(\beta)|\xi,\alpha;\beta\rangle = \sqrt{\frac{\nu^n}{2^n\mu^{n+1}n!}}\exp\left[-\frac{1}{2}\left(|\alpha|^2-\frac{\nu^*}{\mu}\alpha^2\right)\right]H_n\left(\frac{\alpha}{\sqrt{2\mu\nu}}\right),$$

where $H_n(z)$ denotes the Hermite polynomial of order n.

12.2 Physical interpretation

In the preceding section we have presented examples of basic thermalized states that are constructed mimicking some zero-temperature states. Although these states were consistently introduced and form bases of $\mathcal{H}_\beta$, a natural question emerges relative to their meanings. We address this question with the goal of providing a physical interpretation for a general thermalized state $|\Psi(\beta)\rangle$; that is, to find what such a state represents in the standard quantum mechanical description, where the Hilbert space does not carry any thermal degree of freedom and thermal effects appear in the density matrix representation of states. In other words, we would pursue the search for the density matrix associated with the thermal state $|\Psi(\beta)\rangle$.

We start by recalling the density matrix description of the thermal vacuum $|0(\beta)\rangle$. By construction, given any observable A acting on $\mathcal{H}$, we have

$$\langle 0(\beta)|A|0(\beta)\rangle = \mathrm{Tr}\left(\frac{1}{Z(\beta)}\,e^{-\beta\omega a^\dagger a}A\right),$$

where

$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta\omega n} = \frac{1}{1 - e^{-\beta\omega}}$$

is the partition function for the boson oscillator system. This means that the density matrix associated with the thermal vacuum state is the density matrix of the thermal (chaotic or Bose-Einstein) mixed state of the boson oscillator, that is

$$\begin{aligned} \rho_{|0(\beta)\rangle} \equiv \rho_\beta &= \frac{1}{Z(\beta)} \exp\left(-\beta\omega a^\dagger a\right) \\ &= \frac{1}{1+\bar{n}(\beta)} \sum_{n=0}^{\infty} \left(\frac{\bar{n}(\beta)}{1+\bar{n}(\beta)}\right)^n |n\rangle\langle n|. \end{aligned} \tag{12.26}$$

Here we use the notation

$$\bar{n}(\beta) = \frac{1}{e^{\beta\omega} - 1}$$

for the mean number of thermal photons in the chaotic state at temperature β^{-1}.

Following this observation, we associate with a general thermalized state $|\Psi(\beta)\rangle$ the density matrix $\rho_{|\Psi(\beta)\rangle}$ defined such that, for an arbitrary operator A acting on the physical Hilbert space $\mathcal{H}$, we have

$$\langle\Psi(\beta)|A|\Psi(\beta)\rangle = \mathrm{Tr}\left(\rho_{|\Psi(\beta)\rangle}\, A\right). \tag{12.27}$$

On general grounds, this can be accomplished if we manage to write $|\Psi(\beta)\rangle$ in the form

$$|\Psi(\beta)\rangle = f(a, a^\dagger; \beta)\, |0(\beta)\rangle\,, \tag{12.28}$$

in which case we get

$$\begin{aligned} \langle\Psi(\beta)|A|\Psi(\beta)\rangle &= \left\langle 0(\beta)|f^\dagger(a,a^\dagger;\beta)Af(a,a^\dagger;\beta)|0(\beta)\right\rangle \\ &= \mathrm{Tr}\left[\rho_\beta f^\dagger(a,a^\dagger;\beta)Af(a,a^\dagger;\beta)\right] \\ &= \mathrm{Tr}\left[f(a,a^\dagger;\beta)\rho_\beta f^\dagger(a,a^\dagger;\beta)A\right], \end{aligned}$$

leading to the identification

$$\rho_{|\Psi(\beta)\rangle} = f(a,a^\dagger;\beta)\rho_\beta f^\dagger(a,a^\dagger;\beta). \tag{12.29}$$

Note that the density operator $\rho_{|\Psi(\beta)\rangle}$ will have unit trace as a consequence of the normalization of the state $|\Psi(\beta)\rangle$.

Before proceeding with the analysis for the case of a general state $|\Psi(\beta)\rangle$, we have to calculate the density matrix associated with basis states. Consider, initially, the thermal number state $|n(\beta)\rangle$. The expectation value of an arbitrary physical operator A, $\langle n(\beta)|A|n(\beta)\rangle$, is calculated as follows. First, recall that

$$a^\dagger(\beta) = u(\beta)a^\dagger - v(\beta)\tilde{a}$$

and that

$$\tilde{a}|0(\beta)\rangle = \frac{v(\beta)}{u(\beta)} a^\dagger |0(\beta)\rangle,$$

which is a consequence of $\tilde{a}(\beta)|0(\beta)\rangle = 0$. These relations imply that

$$a^\dagger(\beta)|0(\beta)\rangle = \frac{1}{u(\beta)} a^\dagger |0(\beta)\rangle. \tag{12.30}$$

Thus, since $[a^\dagger(\beta), a^\dagger] = 0$, the thermal number state $|n(\beta)\rangle$ can be obtained by repeated applications of $a^\dagger$ on the thermal vacuum as

$$|n(\beta)\rangle = \frac{1}{\sqrt{n!}\,[u(\beta)]^n}\, a^{\dagger n}\, |0(\beta)\rangle\,. \tag{12.31}$$

Now, it follows that

$$\begin{aligned}\langle n(\beta)|A|n(\beta)\rangle &= \left\langle 0(\beta)\left|\frac{1}{n![u(\beta)]^{2n}}\, a^n A a^{\dagger n}\right| 0(\beta)\right\rangle \\ &= \mathrm{Tr}\left(\rho_\beta \frac{1}{n![u(\beta)]^{2n}}\, a^n A a^{\dagger n}\right) \\ &= \mathrm{Tr}\left(\left[\frac{1}{n![u(\beta)]^{2n}}\, a^{\dagger n}\rho_\beta a^n\right] A\right).\end{aligned} \tag{12.32}$$

Therefore, the density matrix associated with the thermal number state $|n(\beta)\rangle$ is given by

$$\rho_{_{|n(\beta)\rangle}} = \frac{1}{n![u(\beta)]^{2n}}\, a^{\dagger n}\rho_\beta a^n. \tag{12.33}$$

Taking $A = \mathbf{1}$ in Eq. (12.32) leads immediately to $\mathrm{Tr}\,\rho_{_{|n(\beta)\rangle}} = 1$ as a consequence of the normalization of $|n(\beta)\rangle$. However, it is instructive to check directly whether the operator $\rho_{_{|n(\beta)\rangle}}$, given by Eq. (12.33), does indeed correspond to an acceptable density matrix. In fact, working in the number basis and taking into account that $a^n|m\rangle = 0$, if $n > m$, while

$$a^n|m\rangle = \sqrt{m(m-1)\cdots(m-n+1)}\,|m-n\rangle \quad \text{, if } n \le m\,,$$

$\rho_{_{|n(\beta)\rangle}}$ can be written as

$$\rho_{_{|n(\beta)\rangle}} = \left(\frac{1}{1+\bar{n}(\beta)}\right)^{n+1} \sum_{r=0}^{\infty} \left(\frac{\bar{n}(\beta)}{1+\bar{n}(\beta)}\right)^r \frac{(n+r)!}{n!\,r!} |n+r\rangle\langle n+r|, \tag{12.34}$$

where we have used $u^2(\beta) = 1 + \bar{n}(\beta)$. Now, with the aid of the identity

$$\sum_{r=0}^{\infty} \frac{(n+r)!}{r!}\,\vartheta^r = \frac{n!}{(1-\vartheta)^{n+1}},$$

which holds for $\vartheta < 1$, one easily demonstrates that

$$\sum_{l=0}^{\infty} \langle l|\rho_{_{|n(\beta)\rangle}}|l\rangle = 1.$$

The density matrix written in Eq. (12.34) has appeared before [178] referred to as the number-chaotic state, since it is seen as a state interpolating between the number state $|n\rangle$ (when $T = \beta^{-1} = 0$, i.e. $\bar{n}(\beta) = 0$) and the chaotic state (when

$n = 0$). From Eq. (12.33), we notice that this state also corresponds to the n-photon added thermal state [179] of a field mode.

We now determine the density matrix associated with the general state $|\Psi(\beta)\rangle$ by working with its representation in the thermal number basis, Eq. (12.4). In fact, using Eq. (12.31) we have

$$|\Psi(\beta)\rangle = \sum_{n=0}^{\infty} \frac{c_n}{\sqrt{n!}\,[u(\beta)]^n}\, a^{\dagger n}\,|0(\beta)\rangle\,, \tag{12.35}$$

so that

$$\begin{aligned}\langle\Psi(\beta)|A|\Psi(\beta)\rangle &= \sum_{n,m=0}^{\infty} \frac{c_m^* c_n}{\sqrt{m!}\sqrt{n!}}\,\frac{1}{[u(\beta)]^{m+n}}\,\langle 0(\beta)|a^m A a^{\dagger n}|0(\beta)\rangle \\ &= \sum_{n,m=0}^{\infty} \frac{c_m^* c_n}{\sqrt{m!}\sqrt{n!}}\,\frac{1}{[u(\beta)]^{m+n}}\,\mathrm{Tr}\left[\rho_\beta a^m A a^{\dagger n}\right] \\ &= \mathrm{Tr}\left[\left(\sum_{n,m=0}^{\infty} \frac{c_m^* c_n}{\sqrt{m!}\sqrt{n!}}\,\frac{1}{[u(\beta)]^{m+n}}\,a^{\dagger n}\rho_\beta a^m\right) A\right],\end{aligned}$$

which implies that

$$\rho_{|\Psi(\beta)\rangle} = \sum_{n,m=0}^{\infty} \frac{c_m^* c_n}{\sqrt{m!}\sqrt{n!}}\,\frac{1}{[u(\beta)]^{m+n}}\,a^{\dagger n}\rho_\beta a^m. \tag{12.36}$$

Again, $\mathrm{Tr}\rho_{|\Psi(\beta)\rangle} = 1$ follows directly from the normalization of $|\Psi(\beta)\rangle$. But, also, we readily verify that the operator (12.36) has unit trace by using the formula

$$\mathrm{Tr}\left[a^{\dagger n}\rho_\beta a^m\right] = n![u(\beta)]^{2n}\delta_{nm},$$

which is a consequence of ρ_β being diagonal in the number basis and $\mathrm{Tr}\rho_{|n(\beta)\rangle} = 1$. Therefore, any normalized linear combination of states belonging to $\mathcal{H}_\beta$ is associated with a unit trace density matrix and so corresponds to a physical mixed state of the boson oscillator that incorporates thermal effects.

Consider, as another specific example, the thermal coherent state $|\alpha(\beta)\rangle$. Using the normal-ordered thermal displacement operator, Eq. (12.7), we rewrite $|\alpha(\beta)\rangle$ in the form of Eq. (12.28) as

$$|\alpha(\beta)\rangle = e^{-|\alpha|^2/2}\exp\left[\alpha a^\dagger(\beta)\right]|0(\beta)\rangle = e^{-|\alpha|^2/2}\exp\left[\frac{\alpha}{u(\beta)}a^\dagger\right]|0(\beta)\rangle\,. \tag{12.37}$$

From this expression for the thermal coherent state, using the general procedure described above, we get its corresponding density matrix,

$$\rho_{|\alpha(\beta)\rangle} = e^{-|\alpha|^2}\,\exp\left[\frac{\alpha}{u(\beta)}a^\dagger\right]\rho_\beta\,\exp\left[\frac{\alpha^*}{u(\beta)}a\right]. \tag{12.38}$$

Naturally, this density matrix can be obtained directly from Eq. (12.36), by gathering the coefficients of the expansion of $|\alpha(\beta)\rangle$ in the thermal number basis,

Eq. (12.10), in the form that corresponds to the Taylor expansion of the exponentials in Eq. (12.38). Also, if we consider the expansion of a general state $|\Psi(\beta)\rangle$ in the thermal coherent basis, Eq. (12.13), we have

$$\rho_{|\Psi(\beta)\rangle} = \frac{1}{\pi^2}\int d^2\alpha\, d^2\gamma\, \langle\Psi(\beta)|\gamma(\beta)\rangle\langle\alpha(\beta)|\Psi(\beta)\rangle\, e^{-(|\alpha|^2+|\gamma|^2)/2}\, e^{\frac{\alpha}{u(\beta)}a^\dagger}\rho_\beta e^{\frac{\gamma^*}{u(\beta)}a}. \tag{12.39}$$

We now determine the density matrix associated with the thermal displaced number state. Notice initially that, using $a(\beta) = u(\beta)a - v(\beta)\tilde{a}^\dagger$ and the corresponding expression for $a^\dagger(\beta)$ in Eq. (12.5), the thermal displacement operator is written as

$$D(\alpha;\beta) = D(u(\beta)\alpha)\widetilde{D}(v(\beta)\alpha^*), \tag{12.40}$$

where $\widetilde{D}(\gamma) = \exp(\gamma\tilde{a}^\dagger - \gamma^*\tilde{a})$ is the displacement operator acting on $\widetilde{\mathcal{H}}$. Furthermore, writing $\widetilde{D}(v(\beta)\alpha^*)$ in the normal-ordered form and considering that

$$\tilde{a}|0(\beta)\rangle = \frac{v(\beta)}{u(\beta)}a^\dagger|0(\beta)\rangle$$

and

$$\tilde{a}^\dagger|0(\beta)\rangle = \frac{u(\beta)}{v(\beta)}a|0(\beta)\rangle,$$

it is shown that

$$\widetilde{D}(v(\beta)\alpha^*)|0(\beta)\rangle = e^{-|\alpha|^2/2}D^\dagger(u(\beta)\alpha)\exp\left[\frac{\alpha}{u(\beta)}a^\dagger\right]|0(\beta)\rangle. \tag{12.41}$$

Therefore, using Eqs. (12.31), (12.40) and (12.41), the thermal displaced number state is written as

$$|n(\beta);\alpha\rangle = \frac{e^{-|\alpha|^2/2}}{\sqrt{n!}[u(\beta)]^n}\, D(u(\beta)\alpha)a^{\dagger n}D^\dagger(u(\beta)\alpha)\exp\left[\frac{\alpha}{u(\beta)}a^\dagger\right]|0(\beta)\rangle,$$

which leads to the density matrix

$$\begin{aligned}\rho_{|n(\beta);\alpha\rangle} = {} & \frac{e^{-|\alpha|^2}}{n![u(\beta)]^{2n}}\, D(u(\beta)\alpha)a^{\dagger n}D^\dagger(u(\beta)\alpha) \\ & \times \exp\left[\frac{\alpha}{u(\beta)}a^\dagger\right]\rho_\beta\exp\left[\frac{\alpha^*}{u(\beta)}a\right]D(u(\beta)\alpha)a^nD^\dagger(u(\beta)\alpha).\end{aligned}$$

Using that

$$D(\gamma)a^nD^\dagger(\gamma) = [a-\gamma]^n,$$

we rewrite $\rho_{|n(\beta);\alpha\rangle}$ in the form

$$\begin{aligned}\rho_{|n(\beta);\alpha\rangle} = {} & \frac{e^{-|\alpha|^2}}{n![u(\beta)]^{2n}}\,[a^\dagger - u(\beta)\alpha^*]^n \\ & \times \exp\left[\frac{\alpha}{u(\beta)}a^\dagger\right]\rho_\beta\exp\left[\frac{\alpha^*}{u(\beta)}a\right][a-u(\beta)\alpha]^n.\end{aligned} \tag{12.42}$$

This simpler form can be obtained, alternatively, using directly Eqs. (12.15) and (12.37).

To obtain the density matrices corresponding to thermal squeezed states, we start by considering the thermal squeezed vacuum state, $|\xi, 0; \beta\rangle$. Taking the thermal squeezing operator $S(\xi; \beta)$ in the normal-order form, Eq. (12.18), the thermal squeezed vacuum state, Eq. (12.21), is written as

$$\begin{aligned} |\xi, 0; \beta\rangle &= \frac{1}{\sqrt{\mu}} \exp\left[-\frac{\nu}{2\mu} a^{\dagger 2}(\beta)\right] |0(\beta)\rangle \\ &= \frac{1}{\sqrt{\mu}} \exp\left[-\frac{\nu}{2\mu} \frac{1}{[u(\beta)]^2} a^{\dagger 2}\right] |0(\beta)\rangle \,, \end{aligned}$$

so that the associated density matrix is

$$\rho_{|\xi,0;\beta)\rangle} = \frac{1}{\mu} \exp\left[-\frac{\nu}{2\mu} \frac{1}{[u(\beta)]^2} a^{\dagger 2}\right] \rho_\beta \exp\left[-\frac{\nu^*}{2\mu} \frac{1}{[u(\beta)]^2} a^2\right]. \tag{12.43}$$

Now consider the thermal squeezed coherent state

$$|\xi, \alpha; \beta\rangle = |\alpha_\xi, \xi; \beta\rangle = D(\alpha_\xi; \beta)|\xi, 0; \beta\rangle,$$

where $\alpha_\xi = \mu\alpha - \nu\alpha^*$ as in Eq. (12.24). Using Eqs. (12.40) and (12.41) with α replaced by α_ξ, and taking $|\xi, 0; \beta\rangle$ in the form (12.43), we obtain

$$\begin{aligned} |\xi, \alpha; \beta\rangle = \frac{e^{-|\alpha_\xi|^2/2}}{\sqrt{\mu}} D(u(\beta)\alpha_\xi) \exp\left[-\frac{\nu}{2\mu} \frac{1}{[u(\beta)]^2} a^{\dagger 2}\right] \\ \times D^\dagger(u(\beta)\alpha_\xi) \exp\left[\frac{\alpha_\xi}{u(\beta)} a^\dagger\right] |0(\beta)\rangle \,. \end{aligned}$$

Thus, the density matrix associated with thermal squeezed coherent state is

$$\begin{aligned} \rho_{|\xi,\alpha;\beta)\rangle} = \frac{e^{-|\alpha_\xi|^2}}{\mu} D(u(\beta)\alpha_\xi) \exp\left[-\frac{\nu}{2\mu} \frac{1}{[u(\beta)]^2} a^{\dagger 2}\right] D^\dagger(u(\beta)\alpha_\xi) \\ \times \exp\left[\frac{\alpha_\xi}{u(\beta)} a^\dagger\right] \rho_\beta \exp\left[\frac{\alpha_\xi^*}{u(\beta)} a\right] \\ \times D(u(\beta)\alpha_\xi) \exp\left[-\frac{\nu^*}{2\mu} \frac{1}{[u(\beta)]^2} a^2\right] D^\dagger(u(\beta)\alpha_\xi). \end{aligned} \tag{12.44}$$

Before closing this section a word must be said about these states in the zero- and the infinite-temperature limits. Consider initially the density matrix associated with the thermal vacuum $|0(\beta)\rangle$, given by Eq. (12.26). As $T \to 0$ (i.e. $\beta \to \infty$), $u(\beta) \to 1$ and $\bar{n}(\beta) \to 0$. Then it follows from Eq. (12.26) that, in the limit $T \to 0$, the density matrix ρ_β reduces to that of the pure vacuum state of the Hilbert space $\mathcal{H}$, that is $\lim_{T\to 0} \rho_\beta = |0\rangle\langle 0|$. Using this fact, one finds that the density matrix corresponding to the thermal number state $|n(\beta)\rangle$, given by Eq. (12.34), tends to that of the single number state $|n\rangle$ of $\mathcal{H}$, that is $\rho_{|n(\beta)\rangle} \to |n\rangle\langle n|$. This argument can be readily generalized to show that the density matrix associated with the general state $|\Psi(\beta)\rangle$ of $\mathcal{H}_\beta$ reduces, as $T \to 0$, to the general state of $\mathcal{H}$ having

the same coefficients, that is, as follows from Eq. (12.36), $\rho_{_{|\Psi(\beta)\rangle}} \to |\Psi\rangle\langle\Psi|$ where $|\Psi\rangle = \sum_{n=0}^{\infty} c_n|n\rangle$. In other words, density matrices of all thermalized states we have discussed so far reduce to the corresponding pure states of $\mathcal{H}$ as $T \to 0$.

The other limit to be considered is the infinite-temperature limit. As $T \to \infty$ (i.e. $\beta \to 0$), $u(\beta) \to \infty$ and $\bar{n}(\beta) \to \infty$, which implies that the density matrix ρ_β tends to the mixed state where all Fock states are occupied with the same weight, that is

$$\lim_{T\to\infty} \rho_\beta = \lim_{N\to\infty} \frac{1}{\sqrt{N}} \sum_{n=0}^{N} |n\rangle\langle n|;$$

of course, such a "hell" state possesses infinite energy. Also, in this limit, none of the states we have discussed makes any sense at all, since they have been defined from actions taken over the thermal state.

12.3 Other possibilities of thermalized states

States belonging to the subspace $\mathcal{H}_\beta$ of the thermal Hilbert space $\mathcal{H}_T$, which is spanned by the set $\{a^{\dagger n}(\beta)|0(\beta)\rangle, n \in \mathbb{N}\}$ have been considered so far. A natural question emerges about the meaning of other states belonging to $\mathcal{H}_T$ but not to $\mathcal{H}_\beta$. In fact, taking the set of states pertaining to $\mathcal{H}_T$ of the form $U(\beta)|n, \widetilde{m}\rangle$ with either n or $\widetilde{m}$ fixed, we get a subspace that is isomorphic to $\mathcal{H}$ and, therefore, also isomorphic to $\mathcal{H}_\beta$. From all those subspaces, we choose to look specifically at the one with $n = 0$ fixed, that is, we consider the subspace $\widetilde{\mathcal{H}}_\beta$ spanned by $\{\tilde{a}^{\dagger m}|0(\beta)\rangle, m = 0, 1, 2, \dots\}$. Other interesting possibility is to take states of $\mathcal{H}_T$ of the form $U(\beta)|\phi, \widetilde{\phi}\rangle$, where $|\widetilde{\phi}\rangle$ is a "replica" of the state $|\phi\rangle$ in the tilde Hilbert space; such type of states will be considered later.

12.3.1 *Thermal tilde states*

To begin, let us construct the Fock basis of $\widetilde{\mathcal{H}}_\beta$. The normalized thermal tilde number state is defined by

$$|\widetilde{m}(\beta)\rangle = \frac{1}{\sqrt{m!}} \left[\tilde{a}^\dagger(\beta)\right]^m |0(\beta)\rangle, \tag{12.45}$$

where $m \in \mathbf{N}$, the thermal vacuum state corresponding to $m = 0$. These states are eigenstates of the thermal tilde number operator $\widetilde{N}(\beta) = \tilde{a}^\dagger(\beta)\tilde{a}(\beta)$, that is

$$\widetilde{N}(\beta)|\widetilde{m}(\beta)\rangle = m|\widetilde{m}(\beta)\rangle.$$

They are also eigenstates of the tilde Hamiltonian $\widetilde{H}(\beta) = \omega\tilde{a}^\dagger(\beta)\tilde{a}(\beta)$, with eigenvalues $m\omega$. Notice that the action of the thermal tilde annihilation and creation operators on $|\widetilde{m}(\beta)\rangle$ is given by

$$\begin{aligned}
\tilde{a}(\beta)\,|\widetilde{m}(\beta)\rangle &= \sqrt{m}\;|(\widetilde{m}-1)(\beta)\rangle\,, \\
\tilde{a}^\dagger(\beta)\,|\widetilde{m}(\beta)\rangle &= \sqrt{m+1}\;|(\widetilde{m}+1)(\beta)\rangle\,.
\end{aligned}$$

The set of states defined by Eq. (12.45) constitutes a complete orthonormal basis for $\widetilde{\mathcal{H}}_\beta$, so that an arbitrary normalized state $|\widetilde{\Psi}(\beta)\rangle$ can be written as

$$|\widetilde{\Psi}(\beta)\rangle = \sum_{m=0}^{\infty} c_m \, |\widetilde{m}(\beta)\rangle \, , \tag{12.46}$$

where $\sum_{m=0}^{\infty} |c_m|^2 = 1$.

Similarly to thermal coherent states described in the last section, we can introduce thermal tilde coherent states by applying the thermal tilde displacement operator,

$$\widetilde{D}(\alpha;\beta) = \exp\left[\alpha \tilde{a}^\dagger(\beta) - \alpha^* \tilde{a}(\beta)\right] , \tag{12.47}$$

on the thermal vacuum state, that is

$$|\widetilde{\alpha}(\beta)\rangle = \widetilde{D}(\alpha;\beta)|0(\beta)\rangle. \tag{12.48}$$

This state is an eigenstate of the thermal tilde annihilation operator with eigenvalue α, i.e.

$$\tilde{a}(\beta)|\widetilde{\alpha}(\beta)\rangle = \alpha|\widetilde{\alpha}(\beta)\rangle.$$

Its expansion in the thermal tilde number basis is given by

$$|\widetilde{\alpha}(\beta)\rangle = e^{-|\alpha|^2/2} \sum_{m=0}^{\infty} \frac{\alpha^m}{\sqrt{m!}} \, |\widetilde{m}(\beta)\rangle \, , \tag{12.49}$$

which allows us to conclude that distinct thermal tilde coherent states are not orthogonal to each other but satisfy

$$\langle\widetilde{\gamma}(\beta)|\widetilde{\alpha}(\beta)\rangle = \exp\left[-\frac{1}{2}\left(|\alpha|^2 + |\gamma|^2\right) + \alpha\gamma^*\right].$$

The scalar product above shows explicitly that the thermal tilde coherent states are normalized, $|\langle\widetilde{\alpha}(\beta)|\widetilde{\alpha}(\beta)\rangle|^2 = 1$. Also, the set of thermal tilde coherent states, for a fixed value of β, constitutes an overcomplete basis of $\widetilde{\mathcal{H}}_\beta$, with the completeness relation given by

$$\frac{1}{\pi}\int d^2\alpha |\widetilde{\alpha}(\beta)\rangle\langle\widetilde{\alpha}(\beta)| = \mathbf{1}.$$

It is worth mentioning that the thermal tilde displacement operator defined by Eq. (12.47) is such that $\widetilde{D}(\alpha;\beta) = [D(\alpha^*;\beta)]\tilde{}$, since α is a complex number and so $\widetilde{\alpha} = \alpha^*$.

With the same underlying structure as presented in the last section, we introduce thermal tilde displaced-number states defined by

$$|\widetilde{m}(\beta);\alpha\rangle = \widetilde{D}(\alpha;\beta)|\widetilde{m}(\beta)\rangle. \tag{12.50}$$

All the relations presented for the displaced thermal number states in subsection 12.1.3 can be written down by just replacing $a(\beta)$ $(a^\dagger(\beta))$ by $\tilde{a}(\beta)$ $(\tilde{a}^\dagger(\beta))$.

Similarly, thermal tilde squeezed states can be defined: the thermal tilde squeezed-vacuum state is given by

$$|\xi, \widetilde{0}; \beta\rangle = \widetilde{S}(\xi;\beta)|0(\beta)\rangle, \tag{12.51}$$

while the thermal tilde squeezed-coherent state is introduced as

$$|\xi, \widetilde{\alpha}; \beta\rangle = \widetilde{S}(\xi;\beta)\widetilde{D}(\alpha;\beta)|0(\beta)\rangle = \widetilde{S}(\xi;\beta)|\widetilde{\alpha}(\beta)\rangle, \tag{12.52}$$

where $\widetilde{S}(\xi;\beta)$ is the thermal tilde squeezed operator,

$$\widetilde{S}(\xi;\beta) = \exp\left(\frac{1}{2}\xi^*\tilde{a}^2(\beta) - \frac{1}{2}\xi\tilde{a}^{\dagger 2}(\beta)\right). \tag{12.53}$$

Again, all relations stated in subsection 12.1.4 apply to the present case if the thermal annihilation and creation operators, and the thermal squeezed states, are replaced by their thermal tilde counterparts.

12.3.2 *Physical meaning of the thermal tilde states*

The introduction of thermal tilde states was performed simply by relying on the isomorphism that exists between $\mathcal{H}_\beta$ and $\widetilde{\mathcal{H}}_\beta$, that is, *mutatis mutandis* by replacing the algebra of the thermal annihilation and creation operators by the isomorphic algebra of the thermal tilde annihilation and creation operators. However, a fundamental question left out from this isomorphism concerns the physical meaning of these thermal tilde states. Since we are assigning physical significance to the Hilbert space $\mathcal{H}$, and the operators acting on it, we expect that corresponding thermal and thermal tilde states are associated with density matrices possessing distinct characteristics.

To obtain the density matrix associated with an arbitrary thermal tilde state, we must be able to write it in a form similar to Eq. (12.28), that is

$$|\widetilde{\Psi}(\beta)\rangle = g(a, a^\dagger; \beta)|0(\beta)\rangle. \tag{12.54}$$

This can be implemented, in general, if we manage to write the action of $\tilde{a}^\dagger(\beta)$ on $|0(\beta)\rangle$ in terms of a and $a^\dagger$ acting on the thermal vacuum. In fact, from $a(\beta)|0(\beta)\rangle = 0$, we infer that

$$\tilde{a}^\dagger|0(\beta)\rangle = \frac{u(\beta)}{v(\beta)}a|0(\beta)\rangle.$$

Then, from

$$\tilde{a}^\dagger(\beta) = u(\beta)\tilde{a}^\dagger - v(\beta)a,$$

we find that

$$\tilde{a}^\dagger(\beta)|0(\beta)\rangle = \frac{1}{v(\beta)}a|0(\beta)\rangle \tag{12.55}$$

and

$$\left[\tilde{a}^\dagger(\beta), a\right] = 0. \tag{12.56}$$

These relations permit us to write $|\widetilde{\Psi}(\beta)\rangle$ in the form shown in Eq. (12.54).

Let us start searching for the density matrix associated with the thermal tilde number state. Using Eqs. (12.55) and (12.56), we write $|\widetilde{m}(\beta)\rangle$ in the form

$$|\widetilde{m}(\beta)\rangle = \frac{1}{\sqrt{m!}\,[v(\beta)]^m} a^m |0(\beta)\rangle. \tag{12.57}$$

Then it follows that, for an arbitrary physical observable $A = A(a, a^\dagger)$,

$$\begin{aligned}\langle\widetilde{m}(\beta)|A|\widetilde{m}(\beta)\rangle &= \left\langle 0(\beta)\left|\frac{1}{m!\,[v(\beta)]^{2m}}\, a^{\dagger m} A a^m\right|0(\beta)\right\rangle \\ &= \mathrm{Tr}\left(\rho_\beta \frac{1}{m!\,[v(\beta)]^{2m}}\, a^{\dagger m} A a^m\right) \\ &= \mathrm{Tr}\left(\left[\frac{1}{m!\,[v(\beta)]^{2m}}\, a^m \rho_\beta a^{\dagger m}\right] A\right).\end{aligned}$$

Thus, we find the density matrix associated with the thermal tilde number state as

$$\rho_{|\widetilde{m}(\beta)\rangle} = \frac{1}{m!\,[v(\beta)]^{2m}}\, a^m \rho_\beta a^{\dagger m}. \tag{12.58}$$

From this expression we verify that the thermal tilde state $|\widetilde{m}(\beta)\rangle$ corresponds to the m-photon subtracted thermal state.

This density matrix is clearly diagonal in the number basis of $\mathcal{H}$ since ρ_β is diagonal in this basis. Using

$$a^{\dagger m}|r\rangle = \sqrt{(r+1)(r+2)\cdots(r+m)}\,|r+m\rangle,$$

Eq. (12.26) leads to the following representation of the density matrix $\rho_{|\widetilde{m}(\beta)\rangle}$ in the number basis

$$\rho_{|\widetilde{m}(\beta)\rangle} = \left(\frac{1}{1+\bar{n}(\beta)}\right)^{m+1} \sum_{r=0}^{\infty} \left(\frac{\bar{n}(\beta)}{1+\bar{n}(\beta)}\right)^r \frac{(m+r)!}{m!\,r!}\,|r\rangle\langle r|. \tag{12.59}$$

Although this expression looks similar to Eq. (12.34), the nature of the mixed state described by $\rho_{|\widetilde{m}(\beta)\rangle}$ is very distinct from that of $\rho_{|n(\beta)\rangle}$. In fact, we find that $\rho_{|\widetilde{m}(\beta)\rangle} \to |0\rangle\langle 0|$ as $T \to 0$, independently of the value of m, while $\rho_{|n(\beta)\rangle}$ reduces to the number state $|n\rangle$ in this limit.

For a general thermal tilde state, using Eq. (12.57), we have

$$|\widetilde{\Psi}(\beta)\rangle = \sum_{m=0}^{\infty} \frac{c_m}{\sqrt{m!}\,[v(\beta)]^m}\, a^m |0(\beta)\rangle, \tag{12.60}$$

so that

$$\begin{aligned}\langle\widetilde{\Psi}(\beta)|A|\widetilde{\Psi}(\beta)\rangle &= \sum_{n,m=0}^{\infty} \frac{c_n^* c_m}{\sqrt{n!}\sqrt{m!}} \frac{1}{[v(\beta)]^{n+m}} \langle 0(\beta)|a^{\dagger n} A a^m|0(\beta)\rangle \\ &= \sum_{n,m=0}^{\infty} \frac{c_n^* c_m}{\sqrt{n!}\sqrt{m!}} \frac{1}{[v(\beta)]^{n+m}} \mathrm{Tr}\left[\rho_\beta\, a^{\dagger n} A a^m\right],\end{aligned}$$

which leads to the identification

$$\rho_{|\tilde{\Psi}(\beta)\rangle} = \sum_{n,m=0}^{\infty} \frac{c_n^* c_m}{\sqrt{n!}\sqrt{m!}} \frac{1}{[v(\beta)]^{n+m}} \, a^m \rho_\beta a^{\dagger n}. \tag{12.61}$$

That $\rho_{|\tilde{\Psi}(\beta)\rangle}$ is a physical density matrix, with unit trace, follows from the normalization of the state $|\widetilde{\Psi}(\beta)\rangle$. This can be proved directly from the above expression if one uses

$$\mathrm{Tr}\left[a^m \rho_\beta a^{\dagger n}\right] = m![v(\beta)]^{2m}\delta_{mn}.$$

Also, using the number basis representation of ρ_β, Eq. (12.26), it can be shown that

$$\lim_{T\to 0} \rho_{|\tilde{\Psi}(\beta)\rangle} = |0\rangle\langle 0|$$

for all thermal tilde states.

We can work out various cases as we did for thermal states. For example, using the normal-order form of $\widetilde{D}(\alpha;\beta)$ and Eq. (12.55), the thermal tilde coherent state is written as

$$|\widetilde{\alpha}(\beta)\rangle = e^{-|\alpha|^2/2} \exp\left[\alpha \tilde{a}^\dagger(\beta)\right] |0(\beta)\rangle = e^{-|\alpha|^2/2} \exp\left[\frac{\alpha}{v(\beta)} a\right] |0(\beta)\rangle \, .$$

Therefore, the density matrix associated with $|\widetilde{\alpha}(\beta)\rangle$ is

$$\rho_{|\tilde{\alpha}(\beta)\rangle} = e^{-|\alpha|^2} \, \exp\left[\frac{\alpha}{v(\beta)} a\right] \rho_\beta \, \exp\left[\frac{\alpha^*}{v(\beta)} a^\dagger\right]. \tag{12.62}$$

This expression is very similar to that for $\rho_{|\alpha(\beta)\rangle}$; we can get one from the other just by making the replacements $a^\dagger \leftrightarrow a$ and $v(\beta) \leftrightarrow u(\beta)$. This is not a particular feature for coherent states but rather a general consequence of the fact that $\widetilde{\mathcal{H}}_\beta$ and $\mathcal{H}_\beta$, being isomorphic to $\mathcal{H}$, are themselves isomorphic. This can be inferred by comparing $\rho_{|\Psi(\beta)\rangle}$ and $\rho_{|\tilde{\Psi}(\beta)\rangle}$, Eqs. (12.36) and (12.61), and it is a result of the comparison of the actions of $a^\dagger(\beta)$ and $\tilde{a}^\dagger(\beta)$ on $|0(\beta)\rangle$, Eqs. (12.30) and (12.55). Therefore, properly using these replacements, we can find the density matrix associated with a thermal tilde state if we know the density matrix of the corresponding, non-tilde, thermal state.

12.3.3 *General states of $\mathcal{H}_T$*

We now address the question about the construction of the density matrix corresponding to states of $\mathcal{H}_T$ which can, in general, be written as linear superpositions of the states $|n,\widetilde{m};\beta\rangle = U(\beta)\,|n,\widetilde{m}\rangle$. The thermalized Fock states $|n,\widetilde{m};\beta\rangle$ were used to treat the Jaynes-Cummings model [180] in the context of thermofields [75]. Among the general states of $\mathcal{H}_T$, the class of states of the type

$$|\alpha,\widetilde{\gamma};\beta\rangle = U(\beta)|\alpha,\widetilde{\gamma}\rangle, \tag{12.63}$$

where $|\alpha\rangle$ and $|\widetilde{\gamma}\rangle$ are coherent states in $\mathcal{H}$ and $\widetilde{\mathcal{H}}$, respectively, has been widely used, particularly to discuss the interplay between thermalization and coherence

[75, 181, 76, 182, 183] and generalizations of uncertainty relations to include both quantum and thermal fluctuations [77, 184, 185]. Also, states of the type

$$|\phi,\widetilde{\phi};\beta\rangle = U(\beta)|\phi,\widetilde{\phi}\rangle, \tag{12.64}$$

where $|\widetilde{\phi}\rangle$ ($\in \widetilde{\mathcal{H}}$) is a replica of the state $|\phi\rangle$ ($\in \mathcal{H}$), can be considered as an alternative thermalization of the state $|\phi\rangle$.

Let us analyze a simple case, considering the state

$$|1,\tilde{1};\beta\rangle = a^{\dagger}(\beta)\tilde{a}^{\dagger}(\beta)|0(\beta)\rangle. \tag{12.65}$$

Using Eqs. (12.30) and (12.55), and the commutation relation

$$\left[a^{\dagger}(\beta),a\right] = -u(\beta)\,,\ \ \left[\tilde{a}^{\dagger}(\beta),a^{\dagger}\right] = -v(\beta)\,, \tag{12.66}$$

we find

$$\begin{aligned}
|1,\tilde{1};\beta\rangle &= \frac{1}{v(\beta)}\,a^{\dagger}(\beta)\,a\,|0(\beta)\rangle \\
&= \frac{1}{v(\beta)}\left[aa^{\dagger}(\beta) - u(\beta)\right]|0(\beta)\rangle \\
&= \frac{1}{v(\beta)}\left[\frac{1}{u(\beta)}\,aa^{\dagger} - u(\beta)\right]|0(\beta)\rangle \\
&= \frac{1}{u(\beta)v(\beta)}\left[aa^{\dagger} - u^2(\beta)\right]|0(\beta)\rangle \\
&= \frac{1}{u(\beta)v(\beta)}\left[a^{\dagger}a - v^2(\beta)\right]|0(\beta)\rangle,
\end{aligned}$$

where we have used $[a,a^{\dagger}] = 1$ and $u^2(\beta) = 1 + v^2(\beta)$. Proceeding as before, we find the density matrix associated with this state as

$$\rho_{|1,\tilde{1};\beta\rangle} = \frac{1}{u^2(\beta)v^2(\beta)}\left[a^{\dagger}a - v^2(\beta)\right]\rho_{\beta}\left[a^{\dagger}a - v^2(\beta)\right]. \tag{12.67}$$

Other simple examples are obtained in a similar way:

$$\rho_{|2,\tilde{1};\beta\rangle} = \frac{1}{2v^2(\beta)u^4(\beta)}\left[a^{\dagger 2}a - 2v^2(\beta)a^{\dagger}\right]\rho_{\beta}\left[a^{\dagger}a^2 - 2v^2(\beta)a\right]; \tag{12.68}$$

$$\begin{aligned}
\rho_{|2,\tilde{2};\beta\rangle} = \frac{1}{4v^4(\beta)u^4(\beta)}&\left[a^{\dagger 2}a^2 - 4v^2(\beta)a^{\dagger}a - 2v^2(\beta)\right] \\
&\times\rho_{\beta}\left[a^{\dagger 2}a^2 - 4v^2(\beta)a^{\dagger}a - 2v^2(\beta)\right];
\end{aligned} \tag{12.69}$$

also, the density matrix $\rho_{|1,\tilde{2};\beta\rangle}$ can be obtained from Eq. (12.68) making the replacements $a^{\dagger} \leftrightarrow a$ and $v(\beta) \leftrightarrow u(\beta)$. These examples clearly indicate that all the thermalized Fock states of the type $|n,\tilde{n};\beta\rangle$ have density-matrix representations which are diagonal in the number basis of $\mathcal{H}$; particularly, we find

$$\rho_{|1,\tilde{1};\beta\rangle} = \frac{1}{[1+\bar{n}(\beta)]^2\bar{n}(\beta)}\sum_{r=0}^{\infty}\left(\frac{\bar{n}(\beta)}{1+\bar{n}(\beta)}\right)^{r}[r-\bar{n}(\beta)]^2\,|r\rangle\langle r|\,. \tag{12.70}$$

For a generic thermalized Fock state $|n,\widetilde{m};\beta\rangle = (n!m!)^{-1/2}a^{\dagger n}(\beta)\tilde{a}^{\dagger m}(\beta)|0(\beta)\rangle$, one can proceed by using Eqs. (12.30) and (12.55) and repeatedly applying the commutations relations given by Eq. (12.66). Since an arbitrary normalized state of $\mathcal{H}_T$ can be written as

$$|\Psi,\widetilde{\Phi};\beta\rangle = \sum_{n,m=0}^{\infty} C_{nm}\,|n,\widetilde{m};\beta\rangle, \tag{12.71}$$

where $\sum_{n,m=0}^{\infty}|C_{nm}|^2 = 1$, in principle, one can write down the density matrix associated with any given state of $\mathcal{H}_T$, although this can be a hard task. We shall not provide examples here, leaving for the reader to work out those states he (she) gets interested with.

The general structure of the states of $\mathcal{H}_T$ is such that their density matrices have the form

$$\rho_{_{|\Psi,\widetilde{\Phi};\beta\rangle}} = F(a,a^\dagger;\beta)\rho_\beta F^\dagger(a,a^\dagger;\beta).$$

Conversely, any density matrix of the form

$$\rho = G(a,a^\dagger)\rho_\beta G^\dagger(a,a^\dagger)$$

can be associated with a state of $\mathcal{H}_T$. In fact, the average value of an arbitrary operator A in the mixed state ρ is given by

$$\begin{aligned}\langle A\rangle_\rho &= \mathrm{Tr}\left[G(a,a^\dagger)\rho_\beta G^\dagger(a,a^\dagger)A\right]\\ &= \mathrm{Tr}\left[\rho_\beta G^\dagger(a,a^\dagger)AG(a,a^\dagger)\right]\\ &= \langle 0(\beta)|G^\dagger(a,a^\dagger)AG(a,a^\dagger)|0(\beta)\rangle.\end{aligned}$$

Now, using the relations

$$\begin{aligned}a &= u(\beta)\,a(\beta) + v(\beta)\,\tilde{a}^\dagger(\beta)\,,\\ a^\dagger &= u(\beta)\,a^\dagger(\beta) + v(\beta)\,\tilde{a}(\beta)\,,\end{aligned}$$

we write

$$G(a,a^\dagger) = G'(a(\beta),a^\dagger(\beta),\tilde{a}(\beta),\tilde{a}^\dagger(\beta)).$$

Then we have

$$\langle A\rangle_\rho = \langle 0(\beta)|G'^\dagger AG'|0(\beta)\rangle,$$

which leads to the identification

$$\rho \longleftrightarrow G'(a(\beta),a^\dagger(\beta),\tilde{a}(\beta),\tilde{a}^\dagger(\beta))|0(\beta)\rangle \in \mathcal{H}_T\,.$$

Finally, it is worth to point out that the TFD approach allows us to calculate averages of physical observables of the form $A = A(a,a^\dagger)$ in these thermalized states, which are mixed states, without using their density matrix representations. First, we write the operator $A(a,a^\dagger)$, acting on $\mathcal{H}$, as a function of the thermal and thermal tilde creation and annihilation operators, that is,

$A(a, a^\dagger) = A'(a(\beta), a^\dagger(\beta), \tilde{a}(\beta), \tilde{a}^\dagger(\beta))$. Then, it follows from the definition of the density matrix associated with a given state $|\Psi, \widetilde{\Phi}; \beta\rangle$ that

$$\begin{aligned} \langle A \rangle_{|\Psi, \widetilde{\Phi}; \beta\rangle} &= \mathrm{Tr}\left[\rho_{|\Psi, \widetilde{\Phi}; \beta\rangle} A\right] \\ &= \langle \Psi, \widetilde{\Phi}; \beta \left| A'(a(\beta), a^\dagger(\beta), \tilde{a}(\beta), \tilde{a}^\dagger(\beta)) \right| \Psi, \widetilde{\Phi}; \beta\rangle; \end{aligned} \tag{12.72}$$

since tilde and non-tilde operators commute, the expectation value in the right hand side of the this equation is easily calculated for states in $\mathcal{H}_T$. Such a procedure will be employed in the next chapter where we discuss nonclassical properties of thermalized states of a field mode.

Chapter 13

Nonclassical Properties of Thermal Quantum States

The thermal quantum states introduced in the preceding chapter, elements of the thermal Hilbert space $\mathcal{H}_T$, are all, by construction, mixed states of the physical boson oscillator that incorporate thermal effects. Some of such states, like thermal number states, $|n(\beta)\rangle$, and thermal-tilde number states, $|\widetilde{m}(\beta)\rangle$, correspond to density matrices that are diagonal in the number basis of the physical Hilbert space, $\mathcal{H}$. Nevertheless, some of them present nonclassical features that are fingerprints of the original, non-thermalized, states that have quantum nature. In the present chapter, we discuss some nonclassical properties of these thermal quantum states. We will mainly concentrate on states of $\mathcal{H}_\beta$ and $\widetilde{\mathcal{H}}_\beta$, spaces which are isomorphic to $\mathcal{H}$, establishing comparisons among them. To be definite, we will consider states of a linearly polarized electromagnetic field mode of frequency ω, although the results can be applied to other bosonic fields.

13.1 Photon statistics

One of the quantum characteristics of states of an electromagnetic field mode, not having classical counterpart, is the occurrence of sub-Poissonian photon statistics. Although this property does not appear in all quantum states of a field mode, when it does the state is guaranteed not to have a classical analogue. The nature of the photon statistics of a state is determined by comparing the dispersion of the number operator, $\langle(\Delta N)^2\rangle = \langle N^2\rangle - \langle N\rangle^2$, with the mean number of photons, $\langle N\rangle$, where $N = a^\dagger a$ is the physical number operator. In terms of the Mandel Q-parameter [186], defined by

$$Q = \frac{\langle(\Delta N)^2\rangle - \langle N\rangle}{\langle N\rangle} = \frac{\langle N^2\rangle}{\langle N\rangle} - \langle N\rangle - 1, \tag{13.1}$$

we have: Poissonian states, when $Q = 0$, super-Poissonian states, for $Q > 0$, and sub-Poissonian states [187] when Q belongs to the interval $[-1, 0)$. Coherent states are pure states for which the photon statistics is Poissonian, while the smallest admissible value of Q, -1, occurs for number states where no dispersion in the number of photons exists. The chaotic (thermal) state, on the other hand, is super-

Poissonian. In any case, the photon number distribution of a sub- (or super-) Poissonian state is narrower (broader) than that of coherent states with the same average photon number.

To calculate the Mandel parameter for a given thermal quantum state, we can use directly the density matrix representation of the state to evaluate the mean values appearing in Eq. (13.1). Alternatively, and in a simpler way, we express the physical number operator, and its square, in terms of the thermal creation and annihilation operators and get benefit from the fact that thermal quantum states are pure states of the thermal Hilbert space, $\mathcal{H}_T$. For the number operator, we have

$$\begin{aligned} N &= a^\dagger a \\ &= \left[u(\beta)a^\dagger(\beta) + v(\beta)\tilde{a}(\beta)\right]\left[u(\beta)a(\beta) + v(\beta)\tilde{a}^\dagger(\beta)\right] \\ &= u^2 N(\beta) + v^2\widetilde{N}(\beta) + uv\left[a^\dagger(\beta)\tilde{a}^\dagger(\beta) + \tilde{a}(\beta)a(\beta)\right] + v^2, \end{aligned} \tag{13.2}$$

where $N(\beta) = a^\dagger(\beta)a(\beta)$ and $\widetilde{N}(\beta) = \tilde{a}^\dagger(\beta)\tilde{a}(\beta)$ are the thermal and the thermal-tilde number operators, respectively. Similarly, the square of the number operator is expressed as

$$\begin{aligned} N^2 = {} & u^4 N^2(\beta) + v^4\left(\widetilde{N}(\beta) + 1\right)^2 + u^2v^2\Big(3N(\beta)[\widetilde{N}(\beta) + 1] \\ & + [N(\beta) + 1]\,\widetilde{N}(\beta) + a^2(\beta)\tilde{a}^2(\beta) + a^{\dagger 2}(\beta)\tilde{a}^{\dagger 2}(\beta) + 1\Big) \\ & + u^3v\left([2N(\beta) + 1]\,a(\beta)\tilde{a}(\beta) + [2N(\beta) - 1]\,a^\dagger(\beta)\tilde{a}^\dagger(\beta)\right) \\ & + uv^3\left([2\widetilde{N}(\beta) + 3]a(\beta)\tilde{a}(\beta) + [2\widetilde{N}(\beta) + 1]a^\dagger(\beta)\tilde{a}^\dagger(\beta)\right). \end{aligned} \tag{13.3}$$

Then, the Q-factor for thermal quantum states is determined by calculating expectation values of N and N^2. Let us now consider some examples.

13.1.1 *Thermal states*

We start investigating thermal quantum states belonging to $\mathcal{H}_\beta$. Consider, initially, the thermal number state

$$|n(\beta)\rangle = \frac{1}{\sqrt{n!}}\left[a^\dagger(\beta)\right]^n|0(\beta)\rangle\,.$$

Using $\tilde{a}(\beta)|n(\beta)\rangle = 0$ and remembering that $u^2 = 1 + v^2$, we find

$$\langle N\rangle_{|n(\beta)\rangle} = n + (n+1)\,\bar{n}(\beta) \tag{13.4}$$

and

$$\langle N^2\rangle_{|n(\beta)\rangle} = n^2 + (2n^2 + 3n + 1)\,\bar{n}(\beta) + (n^2 + 3n + 2)\,\bar{n}^2(\beta), \tag{13.5}$$

where

$$\bar{n}(\beta) = v^2(\beta) = \frac{1}{e^{\beta\omega} - 1}$$

is the mean number of photons in the chaotic state, corresponding to $|0(\beta)\rangle$, at temperature β^{-1}. Note that the mean number of physical photons in the state $|n(\beta)\rangle$ is given by n plus a contribution of thermal photons which is linear in $\bar{n}(\beta)$.

Using these expressions, we get the Mandel parameter of the thermal number state as

$$Q_{|n(\beta)\rangle} = \frac{(n+1)\,\bar{n}^2(\beta) - n}{(n+1)\,\bar{n}(\beta) + n}. \tag{13.6}$$

Note that, for $n = 0$, we obtain

$$Q_{|0(\beta)\rangle} = \bar{n}(\beta), \tag{13.7}$$

which is the correct Mandel parameter for the chaotic, thermal, state at temperature β^{-1}. On the other hand, as $\bar{n}(\beta) \to 0$, i.e. as $T = \beta^{-1} \to 0$, we find $Q_{|n\rangle} = -1 + \delta_{n0}$ properly reproducing the Q-factor of the zero-temperature number states. The Mandel parameter of some thermal quantum states are plotted in Fig. 13.1 as a function of $\bar{n}$. From this figure, and directly from Eq. (13.6), we find that the thermal number state with $n \geq 1$ changes from sub-Poissonian to super-Poissonian statistics as the temperature is increased [179]. This transition in the nature of the photon statistics occurs at a critical value

$$\bar{n}_c^{(n)} = \sqrt{\frac{n}{n+1}}\,, \tag{13.8}$$

corresponding to the "critical" temperature (in units of ω)

$$T_c^{(n)} = \left[\ln\left(1 + \sqrt{\frac{n+1}{n}}\right)\right]^{-1};$$

below this value, $Q_{|n(\beta)\rangle} < 0$, while above it we have $Q_{|n(\beta)\rangle} > 0$. This means that the sub-Poissonian character of the number state gradually disappears as the temperature is raised. From Eq. (13.8), we obtain $1/\sqrt{2} \leq \bar{n}_c^{(n)} < 1$ as n varies in $\mathbb{N}^* = \{1, 2, 3, \dots\}$, so that all thermal number states are sub-Poissonian for low temperatures ($\bar{n}(\beta) < 1/\sqrt{2}$) and become super-Poissonian for high temperatures ($\bar{n}(\beta) \geq 1$).

The mean number of photons and the expectation value of N^2 for an arbitrary state of $\mathcal{H}_\beta$,

$$|\Psi(\beta)\rangle = \sum_{n=0}^{\infty} c_n\,|n(\beta)\rangle\,,$$

are given by

$$\langle N\rangle_{|\Psi(\beta)\rangle} = \langle N\rangle_{|\Psi\rangle} + \left(\langle N\rangle_{|\Psi\rangle} + 1\right)\bar{n}(\beta) \tag{13.9}$$

and

$$\begin{aligned}\langle N^2\rangle_{|\Psi(\beta)\rangle} &= \langle N^2\rangle_{|\Psi\rangle} + \left(2\langle N^2\rangle_{|\Psi\rangle} + 3\langle N\rangle_{|\Psi\rangle} + 1\right)\bar{n}(\beta) \\ &\quad + \left(\langle N^2\rangle_{|\Psi\rangle} + 3\langle N\rangle_{|\Psi\rangle} + 2\right)\bar{n}^2(\beta)\,,\end{aligned} \tag{13.10}$$

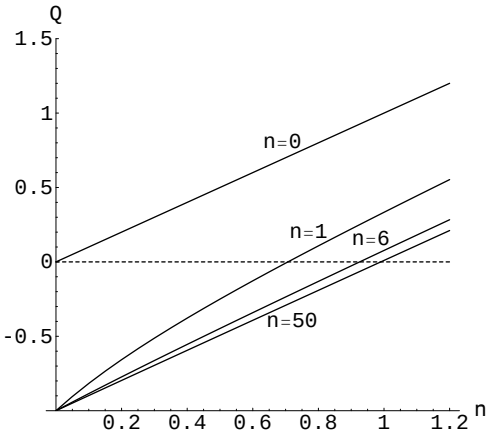


Fig. 13.1 Mandel parameter for some thermal number states.

where $\langle N\rangle_{|\Psi\rangle} = \langle\Psi|N|\Psi\rangle$ and $\langle N^2\rangle_{|\Psi\rangle} = \langle\Psi|N^2|\Psi\rangle$ refer to the corresponding state in $\mathcal{H}$, $|\Psi\rangle = \sum_n c_n|n\rangle$. This is a direct generalization of Eqs. (13.4) and (13.5). The Mandel parameter for $|\Psi(\beta)\rangle$ is then

$$Q_{|\Psi(\beta)\rangle} = \frac{\left[\langle N^2\rangle_{|\Psi\rangle} - \langle N\rangle^2_{|\Psi\rangle}\right][1+\bar{n}(\beta)]^2 + \left[\langle N\rangle_{|\Psi\rangle)} + 1\right]\bar{n}^2(\beta) - \langle N\rangle_{|\Psi\rangle}}{\left[\langle N\rangle_{|\Psi\rangle} + 1\right]\bar{n}(\beta) + \langle N\rangle_{|\Psi\rangle}}. \quad (13.11)$$

Note that, as $\bar{n} \to 0$ ($T \to 0$), $Q_{|\Psi(\beta)\rangle}$ tends to the $Q_{|\Psi\rangle}$, the Mandel parameter of the zero-temperature state $|\Psi\rangle$, as expected; also, Eq. (13.11) reduces to Eq. (13.6) for thermal number states since $|n\rangle$ has vanishing photon number dispersion.

Let us consider some particular examples. For the thermal coherent state $|\alpha(\beta)\rangle$, we find

$$Q_{|\alpha(\beta)\rangle} = \frac{2|\alpha|^2\bar{n}(\beta)[1+\bar{n}(\beta)] + \bar{n}^2(\beta)}{|\alpha|^2[1+\bar{n}(\beta)] + \bar{n}(\beta)}. \quad (13.12)$$

Note that, for $\bar{n}(\beta) \to 0$, $Q_{|\alpha(\beta)\rangle}$ goes to 0 while, for any finite temperature, the thermal coherent state is super-Poissonian. Actually, it follows from the general expression, Eq. (13.11), that the Mandel parameter of an arbitrary state $|\Psi(\beta)\rangle$ increases with $\bar{n}(\beta)$, which is the expected effect of the temperature on photon statistics of the state.

In the case of the thermal displaced number state, $|n(\beta);\alpha\rangle$, we find

$$Q_{|n(\beta);\alpha\rangle} = \frac{(2|\alpha|^2+1)(n+1)\bar{n}^2(\beta) + 2|\alpha|^2(2n+1)\bar{n}(\beta) + (2|\alpha|^2-1)n}{(|\alpha|^2+n)[1+\bar{n}(\beta)] + \bar{n}(\beta)}. \quad (13.13)$$

This expression reduces to the Mandel parameters of the thermal number, Eq. (13.6), and thermal-coherent states, Eq. (13.12), in the limits $\alpha \to 0$ and $n \to 0$, respectively. Also, taking $T \to 0$ we obtain the Mandel parameter of the displaced

number state, namely

$$Q_{|n;\alpha\rangle} = \frac{(2|\alpha|^2 - 1)n}{|\alpha|^2 + n},$$

which is a sub-Poissonian state for $|\alpha| < 1/\sqrt{2}$ irrespective of the value of n. Thus, in this case, raising the temperature leads to a change in the nature of the photon statistics similar to the effect observed for thermal number states. On the other hand, if $|\alpha| \geq 1/\sqrt{2}$, at $T \neq 0$, all thermal displaced number states are super-Poissonian.

Let us now consider elements of $\mathcal{H}_\beta$ that correspond to the thermalization of normalized superpositions of two coherent states belonging to $\mathcal{H}$. When the overlap between the coherent states is negligible, such states are referred to as Schrödinger-cat states since the component states are macroscopically distinguishable. For simplicity, we consider the even (+) and odd (−) coherent states [188], defined in $\mathcal{H}$ by

$$\left|\Psi^{\pm}(\alpha)\right\rangle = \mathcal{N}^{\pm}(\alpha)\ \left(|-\alpha\rangle \pm |\alpha\rangle\right), \tag{13.14}$$

where the normalization constants are

$$\mathcal{N}^{\pm}(\alpha) = \left[2 \pm 2\exp(-2|\alpha|^2)\right]^{-1/2}.$$

Even and odd coherent states are degenerate eigenstates of a^2 with eigenvalue equal to α^2. Without loss of generality, we take $\alpha \in \mathbb{R}$. For these states, we have:

$$\langle N\rangle_{|\Psi^+\rangle} = \alpha^2 \tanh\alpha^2; \tag{13.15}$$

$$\langle N\rangle_{|\Psi^-\rangle} = \alpha^2 \coth\alpha^2, \tag{13.16}$$

and

$$\left\langle N^2\right\rangle_{|\Psi^+\rangle} = \alpha^2 \tanh\alpha^2 + \alpha^4; \tag{13.17}$$

$$\left\langle N^2\right\rangle_{|\Psi^-\rangle} = \alpha^2 \coth\alpha^2 + \alpha^4, \tag{13.18}$$

which lead to

$$Q_{|\Psi^+\rangle} = \alpha^2 \left(\coth\alpha^2 - \tanh\alpha^2\right), \tag{13.19}$$

$$Q_{|\Psi^-\rangle} = -\,Q_{|\Psi^+\rangle}. \tag{13.20}$$

This means that even states have super-Poissonian statistics while odd states are sub-Poissonian [189], for all values of α.

Thermal even and odd coherent states in $\mathcal{H}_\beta$, corresponding to the thermalization of even and odd coherent states (13.14), are given by

$$\left|\Psi^{\pm}(\beta;\alpha)\right\rangle = \mathcal{N}^{\pm}(\alpha)\ \left(|-\alpha(\beta)\rangle \pm |\alpha(\beta)\rangle\right). \tag{13.21}$$

Note that, due to the isomorphism between $\mathcal{H}$ and $\mathcal{H}_\beta$, the normalization constant is the same as that for $|\Psi^{\pm}(\alpha)\rangle$; also, these states are eigenstates of $a^2(\beta)$ with

eigenvalue α^2. For α moderately large, i.e. such that $\langle -\alpha|\alpha\rangle = \exp(-2\alpha^2)$ is small, these states can be referred to as thermal Schrödinger-cat states of the field mode. Using the corresponding mean numbers of photons and expectation values of N^2 of Eqs. (13.15) to (13.18) in Eq. (13.11), we find the Q-parameter for the states $|\Psi^{\pm}(\beta;\alpha)\rangle$. For the even state, we get

$$Q_{|\Psi^-(\beta;\alpha)\rangle} = \frac{[(1+\alpha^4)\coth\alpha^2 + \alpha^2(2-\alpha^2\tanh\alpha^2)]\,\bar{n}^2(\beta)}{(\alpha^2+\coth\alpha^2)\,\bar{n}(\beta)+\alpha^2} + \frac{\alpha^4(\coth\alpha^2-\tanh\alpha^2)(2\bar{n}(\beta)+1)+2\alpha^2\bar{n}(\beta)}{(\alpha^2+\coth\alpha^2)\,\bar{n}(\beta)+\alpha^2}, \qquad (13.22)$$

while, for the odd state, we find

$$Q_{|\Psi^-(\beta;\alpha)\rangle} = \frac{[(1+\alpha^4)\tanh\alpha^2 + \alpha^2(2-\alpha^2\coth\alpha^2)]\,\bar{n}^2(\beta)}{(\alpha^2+\tanh\alpha^2)\,\bar{n}(\beta)+\alpha^2} + \frac{\alpha^4(\tanh\alpha^2-\coth\alpha^2)(2\bar{n}(\beta)+1)+2\alpha^2\bar{n}(\beta)}{(\alpha^2+\tanh\alpha^2)\,\bar{n}(\beta)+\alpha^2}; \qquad (13.23)$$

these expressions transform one into the other with the replacements $\tanh \leftrightarrow \coth$.

The even states, which have $Q > 0$ at $T = 0$, remain super-Poissonian. On the other hand, odd states gradually loose their sub-Poissonian character as the temperature is increased. The Q-parameters for the thermal odd coherent states, at some temperatures, are illustrated in Fig. 13.2. We find that, for all values of α ($\neq 0$), the thermal odd coherent states become super-Poissonian if the temperature is such that $\bar{n}(\beta) \geq \bar{n}_c^{(1)} = 1/\sqrt{2}$; this value reflects, consistently, the fact that $|\Psi^-(\alpha)\rangle \to |1\rangle$ in the limit $\alpha \to 0$.

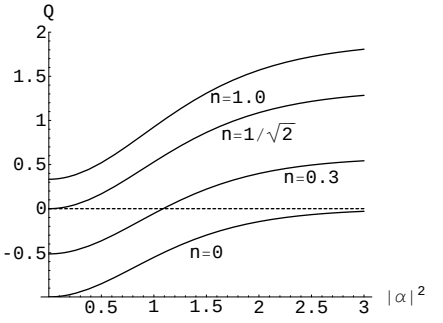


Fig. 13.2 Mandel parameter for thermal odd coherent states, for some values of $\bar{n}(\beta)$.

Many other states of $\mathcal{H}$ are sub-Poissonian; for instance, squeezed coherent states can present sub-Poissonian statistics for some ranges of values of the squeezing and displacing parameters. In all cases, however, the effect of raising the temperature in the corresponding thermal state leads to the change of the nature of the photon statistics at some temperature, as in examples presented above.

13.1.2 *Thermal tilde states*

We now investigate the photon statistics for states in the Hilbert space $\widetilde{\mathcal{H}}_\beta$. Consider, initially, the thermal tilde number state

$$|\widetilde{m}(\beta)\rangle = \frac{1}{\sqrt{m!}}\left[\tilde{a}^\dagger(\beta)\right]^m |0(\beta)\rangle\,.$$

Since $u^2 = 1 + v^2$ and $a(\beta)|\widetilde{m}(\beta)\rangle = 0$, from Eqs. (13.2) and (13.3), we get

$$\langle N\rangle_{|\widetilde{m}(\beta)\rangle} = (m+1)\,\bar{n}(\beta) \tag{13.24}$$

and

$$\langle N^2\rangle_{|\widetilde{m}(\beta)\rangle} = (m+1)\,\bar{n}(\beta) + (m^2+3m+2)\,\bar{n}^2(\beta). \tag{13.25}$$

Then we obtain the Q-parameter for the thermal tilde number states as

$$Q_{|\widetilde{m}(\beta)\rangle} = \bar{n}(\beta)\ \ , \quad \forall\, m \in \mathbb{N}\,. \tag{13.26}$$

In words, all thermal tilde number state have the same super-Poissonian photon statistics as that of the chaotic, thermal, state ρ_β.

Now consider a general thermal tilde state,

$$|\widetilde{\Psi}(\beta)\rangle = \sum_{m=0}^{\infty} c_m\,|\widetilde{m}(\beta)\rangle\ .$$

The mean number of photons and the expectation value of N^2, in this case, are

$$\langle N\rangle_{|\tilde{\Psi}(\beta)\rangle} = (\langle N\rangle_{|\Psi\rangle} + 1)\,\bar{n}(\beta) \tag{13.27}$$

and

$$\langle N^2\rangle_{|\Psi(\beta)\rangle} = \left(\langle N\rangle_{|\Psi\rangle} + 1\right)\bar{n}(\beta) + \left(\langle N^2\rangle_{|\Psi\rangle} + 3\langle N\rangle_{|\Psi\rangle} + 2\right)\bar{n}^2(\beta)\,, \tag{13.28}$$

where $\langle N\rangle_{|\Psi\rangle}$ and $\langle N^2\rangle_{|\Psi\rangle}$ refer to the state $|\Psi\rangle = \sum_n c_n|n\rangle$, as before. Inserting Eqs. (13.27) and (13.28) into Eq. (13.1) we obtain the Mandel parameter for the state $|\widetilde{\Psi}(\beta)\rangle$,

$$Q_{|\tilde{\Psi}(\beta)\rangle} = \left(\frac{\langle N^2\rangle_{|\Psi\rangle} - \langle N\rangle^2_{|\Psi\rangle}}{\langle N\rangle_{|\Psi\rangle} + 1} + 1\right)\bar{n}(\beta). \tag{13.29}$$

Note that all thermal tilde states have a positive Q-parameter for $T \neq 0$, which is equal to the Mandel parameter of the thermal vacuum $|0(\beta)\rangle$ multiplied by a factor greater than 1. In particular, for a thermal tilde coherent state $|\widetilde{\alpha}(\beta)\rangle$, we have

$$Q_{|\tilde{\alpha}(\beta)\rangle} = \left(1 + \frac{|\alpha|^2}{1+|\alpha|^2}\right)\bar{n}(\beta). \tag{13.30}$$

Other examples can be readily worked out. Therefore we find that all thermal tilde states are super-Poissonian irrespective of the nature of the photon statistics of the original, non-thermalized, state.

13.2 Quadrature squeezing

We now turn the discussion to another important nonclassical feature which may be present in quantum states of a field mode, which is the reduction of the quantum noise of a field quadrature below the vacuum value. The field-quadrature operators, acting on $\mathcal{H}$, are defined as

$$X_1 = \frac{1}{2}\left(a + a^\dagger\right) \tag{13.31}$$

and

$$X_2 = \frac{1}{2i}\left(a - a^\dagger\right). \tag{13.32}$$

They correspond to position and momentum operators of a boson oscillator and satisfy the commutation relation

$$[X_1, X_2] = \frac{i}{2}.$$

Therefore, their variances, $\langle(\Delta X_j)^2\rangle = \langle X_j^2\rangle - \langle X_j\rangle^2$, fulfill the Heisenberg uncertainty relation

$$\sqrt{\langle(\Delta X_1)^2\rangle}\,\sqrt{\langle(\Delta X_2)^2\rangle} \geq \frac{1}{4}. \tag{13.33}$$

This quantum mechanical requirement must be respected for all states of the system, irrespective of the nature of the state, whether pure or mixed.

For coherent states $|\alpha\rangle$, including the vacuum $|0\rangle$, we have

$$\sqrt{\langle(\Delta X_1)^2\rangle_{|\alpha\rangle}} = \sqrt{\langle(\Delta X_2)^2\rangle_{|\alpha\rangle}} = \frac{1}{2}$$

and the equality in Eq. (13.33) holds. These states are minimum uncertainty states but not the only ones. Consider the squeezed vacuum state

$$\left|re^{i\varphi}, 0\right\rangle = \exp\left(\frac{1}{2}re^{-i\varphi}a^2 - \frac{1}{2}re^{i\varphi}a^{\dagger 2}\right)|0\rangle\,; \tag{13.34}$$

for this state, we have

$$\langle(\Delta X_j)^2\rangle_{|re^{i\varphi},0\rangle} = \frac{1}{4}\left[\cosh^2 r + \sinh^2 r + (-1)^j 2\sinh r\cosh r\cos\varphi\right]. \tag{13.35}$$

Taking $\varphi = 0$, we get

$$\langle(\Delta X_1)^2\rangle_{|r,0\rangle} = \frac{1}{4}e^{-2r}\ ,\ \ \langle(\Delta X_2)^2\rangle_{|r,0\rangle} = \frac{1}{4}e^{2r},$$

while, for $\varphi = \pi$, we have the same values but with X_1 exchanged with X_2. Thus the squeezed vacuum states $|r, 0\rangle$ and $|-r, 0\rangle$ are also minimum uncertainty states. However, for these states, one of the quadratures presents less quantum noise than for the vacuum state or a coherent state; that is, fluctuations in that quadrature are squeezed while in the other they are augmented to preserve the uncertainty relation. Naturally, this does not happen for all the squeezed vacuum states; for example, when $\varphi = \pi/2$ none of the quadrature variances are squeezed at all.

Also, by varying the parameters r and φ, we easily find squeezed vacuum states presenting quadrature squeezing without equalizing the uncertainty relation. This kind of analysis can be extended for squeezed coherent states.

Quadrature squeezing is a quantum property which is not restricted to states obtained by applying the squeezing operator to other state. In the case of the even and odd coherent states, Eq. (13.14), for example, we find

$$\langle(\Delta X_1)^2\rangle_{|\Psi^{\pm}(\alpha)\rangle} = \frac{1}{4} + \frac{\alpha^2}{1 \pm \exp(-2\alpha^2)}, \tag{13.36}$$

$$\langle(\Delta X_2)^2\rangle_{|\Psi^{\pm}(\alpha)\rangle} = \frac{1}{4} \mp \frac{\alpha^2 \exp(-2\alpha^2)}{1 \pm \exp(-2\alpha^2)}; \tag{13.37}$$

this shows that, while odd states do not present reduced fluctuations in the quadratures, even coherent states, with α not too large, have the X_2 quadrature squeezed. Another example is the Yurke-Stoler state [190],

$$|\Psi_i(\alpha)\rangle = \frac{1}{\sqrt{2}}\left(i|-\alpha\rangle + |\alpha\rangle\right), \tag{13.38}$$

for which (taking $\alpha \in \mathbb{R}$)

$$\langle(\Delta X_1)^2\rangle_{|\Psi_i(\alpha)\rangle} = \frac{1}{4} + \alpha^2,$$

$$\langle(\Delta X_2)^2\rangle_{|\Psi_i(\alpha)\rangle} = \frac{1}{4} - \alpha^2 \exp(-4\alpha^2);$$

in this case, the X_2 quadrature is squeezed for all values of α.

Let us now consider thermalized states of the field mode. The variances of the quadrature operators for thermalized states are more easily calculated if the the operators X_j and X_j^2, $j = 1, 2$, are written in terms of thermal creation and annihilation operators. We have

$$X_1 = \frac{1}{2}\left\{u(\beta)\left[a^{\dagger}(\beta) + a(\beta)\right] + v(\beta)\left[\widetilde{a}^{\dagger}(\beta) + \widetilde{a}(\beta)\right]\right\}; \tag{13.39}$$

$$X_2 = \frac{1}{2i}\left\{u(\beta)\left[a(\beta) - a^{\dagger}(\beta)\right] - v(\beta)\left[\widetilde{a}(\beta) - \widetilde{a}^{\dagger}(\beta)\right]\right\}, \tag{13.40}$$

and

$$\begin{aligned} X_1^2 = \frac{1}{4}\Big\{ & u^2(\beta)\left[2N(\beta) + 1 + a^{\dagger 2}(\beta) + a^2(\beta)\right] \\ & + v^2(\beta)\left[2\widetilde{N}(\beta) + 1 + \widetilde{a}^{\dagger 2}(\beta) + \widetilde{a}^2(\beta)\right] \\ & + 2u(\beta)v(\beta)\left[a^{\dagger}(\beta)\widetilde{a}^{\dagger}(\beta) + a^{\dagger}(\beta)\widetilde{a}(\beta) + a(\beta)\widetilde{a}^{\dagger}(\beta) + a(\beta)\widetilde{a}(\beta)\right]\Big\}; \end{aligned} \tag{13.41}$$

$$\begin{aligned} X_2^2 = \frac{1}{4}\Big\{ & u^2(\beta)\left[2N(\beta) + 1 - a^{\dagger 2}(\beta) - a^2(\beta)\right] \\ & + v^2(\beta)\left[2\widetilde{N}(\beta) + 1 - \widetilde{a}^{\dagger 2}(\beta) - \widetilde{a}^2(\beta)\right] \\ & + 2u(\beta)v(\beta)\left[\widetilde{a}^{\dagger}(\beta) - a^{\dagger}(\beta)\widetilde{a}(\beta) - a(\beta)\widetilde{a}^{\dagger}(\beta) + a(\beta)\widetilde{a}(\beta)\right]\Big\}, \end{aligned} \tag{13.42}$$

where, again, $N(\beta) = a^\dagger(\beta)a(\beta)$ and $\widetilde{N}(\beta) = \widetilde{a}^\dagger(\beta)\widetilde{a}(\beta)$.

Let us analyze the occurrence of quadrature squeezing in thermal states. In this case, from the isomorphism between $\mathcal{H}_\beta$ and $\mathcal{H}$, we immediately get, for a generic state $|\Psi(\beta)\rangle$,

$$\langle X_j \rangle_{|\Psi(\beta)\rangle} = u(\beta)\, \langle X_j \rangle_{|\Psi\rangle} \tag{13.43}$$

and

$$\langle X_j^2 \rangle_{|\Psi(\beta)\rangle} = u^2(\beta)\, \langle X_j^2 \rangle_{|\Psi\rangle} + \frac{1}{4} v^2(\beta), \tag{13.44}$$

with $j = 1, 2$, where $|\Psi\rangle$ is the corresponding state in $\mathcal{H}$. These equations lead to, for both quadratures,

$$\langle (\Delta X_j)^2 \rangle_{|\Psi(\beta)\rangle} = [1 + \bar{n}(\beta)]\, \langle (\Delta X_j)^2 \rangle_{|\Psi\rangle} + \frac{1}{4}\bar{n}(\beta)\,,\ j = 1, 2\,. \tag{13.45}$$

Note that the effect of temperature is the same on both quadratures although the variances are not equal in the general case. The quadrature variances in the state $|\Psi(\beta)\rangle$ reduce to those of the state $|\Psi\rangle$ in the limit $T \to 0$. On the other hand, as $\bar{n}(\beta)$ increases from 0, the quadrature variances also increase; therefore, if a state $|\Psi\rangle$ presents squeezing in one of its quadratures at $T = 0$, by raising the temperature the Heisenberg limit is reached and the squeezing effect disappears. Let us look at a typical example.

Consider the thermal Yurke-Stoler state, defined by

$$|\Psi_i(\beta; \alpha)\rangle = \frac{1}{\sqrt{2}} \left(i|-\alpha(\beta)\rangle + |\alpha(\beta)\rangle \right); \tag{13.46}$$

in this case, we find

$$\langle (\Delta X_2)^2 \rangle_{|\Psi_i(\beta;\alpha)\rangle} = [1 + \bar{n}(\beta)] \left[\frac{1}{4} - \alpha^2 \exp(-4\alpha^2) \right] + \frac{1}{4}\bar{n}(\beta). \tag{13.47}$$

The square of the variance of the X_2 quadrature for this state is plotted in Fig. 13.3 as a function of $|\alpha|^2$, for some values of $\bar{n}(\beta)$. We find that the quadrature squeezing, which occurs for all values of α at $T = 0$, gradually disappears as the temperature is increased. Also, the minimum value of $S_2(|\alpha|^2; \bar{n}(\beta)) = \langle (\Delta X_2)^2 \rangle_{|\Psi_i(\beta;\alpha)\rangle} - 0.25$, with respect to variations of $|\alpha|^2$ (for fixed $\bar{n}(\beta)$) which occurs at $|\alpha|^2 = 0.25$, reaches 0 for $\bar{n}(\beta) = 0.2254$; this means that, for $T \gtrsim 0.59\omega$ no quadrature squeezing exists for any thermal Yurke-Stoler state. Other examples can be worked out in the same way, leading to similar results.

Consider now states pertaining to $\widetilde{\mathcal{H}}_\beta$. For an arbitrary state $|\widetilde{\Psi}(\beta)\rangle$, we find

$$\langle X_j \rangle_{|\tilde{\Psi}(\beta)\rangle} = (-1)^{j-1} v(\beta)\, \langle X_j \rangle_{|\tilde{\Psi}\rangle} \tag{13.48}$$

and

$$\langle X_j^2 \rangle_{|\tilde{\Psi}(\beta)\rangle} = v^2(\beta)\, \langle X_j^2 \rangle_{|\tilde{\Psi}\rangle} + \frac{1}{4} u^2(\beta), \tag{13.49}$$

with $j = 1, 2$. These expressions lead to, for both quadratures,

$$\langle (\Delta X_j)^2 \rangle_{|\tilde{\Psi}(\beta)\rangle} = \bar{n}(\beta) \langle (\Delta X_j)^2 \rangle_{|\tilde{\Psi}\rangle} + \frac{1}{4} \left[\bar{n}(\beta) + 1 \right]\,,\ j = 1, 2\,. \tag{13.50}$$

We find that $\langle (\Delta X_j)^2 \rangle > 0.25$ for any value of T (no matter how small it is), so that quadrature squeezing does not appear for thermal tilde states, irrespective of the occurrence of this effect in the state $|\Psi\rangle$. Therefore, the thermal tilde states do not present any of the nonclassical features we have discussed so far.

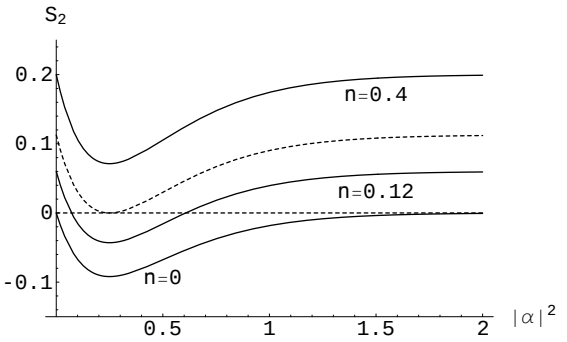


Fig. 13.3 Plot of $S_2 = \langle(\Delta X_2)^2\rangle - 0.25$ for the thermal Yurke-Stoler state, for some values of $\bar{n}(\beta)$. The dotted line corresponds to the value $\bar{n}(\beta) = 0.2254$.

13.3 Atomic population inversion

In some experiments in cavity quantum electrodynamics, the population of atomic states is monitored as a function of time. For the case of a two-level (Rydberg) atom interacting with a cavity-field mode, as described by the single-photon Jaynes-Cummings model [180] in the rotating wave approximation, the atom-field Hamiltonian is given by

$$H = \frac{\omega_0}{2}\,\sigma_3 + \omega\, a^\dagger a + \lambda\left(\sigma_+\, a \,+\, \sigma_-\, a^\dagger\right) \;, \tag{13.51}$$

where ω_0 is the frequency of the transition between the ground and excited atomic states, $\omega_0 = E_{|e\rangle} - E_{|g\rangle}$, ω is the field-mode frequency and λ is the coupling parameter. In the above equation, σ_3, σ_+ and σ_- are the Pauli matrices,

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \;\;,\;\; \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \;\;,\;\; \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \;,$$

with σ_+ and σ_- corresponding to the raising and lowering operators in the atomic two-level basis, respectively. For a general state of the field mode, described by the density matrix $\rho_{\rm F}$, the time evolution of the atomic population inversion is

$$\begin{aligned} W(t) &= \mathrm{Tr}\,\left[\rho_{\rm AF}(t)\,\sigma_3\right] \\ &= \mathrm{Tr}\,\left[e^{-iHt}\,\{|\psi_{\rm A}(0)\rangle\,\langle\psi_{\rm A}(0)|\otimes\rho_{\rm F}(0)\}\;e^{iHt}\,\sigma_3\right] \;, \end{aligned} \tag{13.52}$$

where $|\psi_{\rm A}\rangle$ represents a pure atomic state.

When the initial atomic state is an arbitrary superposition of the ground, $|g\rangle$, and excited, $|e\rangle$, states

$$|\psi_{\rm A}(0)\rangle = c_g\,|g\rangle + c_e\,|e\rangle \;\;,$$

the atomic population inversion [191, 192] is given by

$$W_\delta(t) = |c_e|^2 \left\{ 1 - 2 \sum_{l=0}^{\infty} \frac{l+1}{\nu(l)+1} \sin^2 \left(\lambda t \sqrt{\nu(l)+1} \right) \langle l| \rho_{\rm F}(0) |l\rangle \right\}$$
$$- |c_g|^2 \left\{ 1 - 2 \sum_{l=0}^{\infty} \frac{l}{\nu(l)} \sin^2 \left(\lambda t \sqrt{\nu(l)} \right) \langle l| \rho_{\rm F}(0) |l\rangle \right\}$$
$$+ 2 |c_e| |c_g| \sum_{l=0}^{\infty} \sqrt{l+1} \left[\sin(\phi+\gamma) \frac{\sin \left(2\lambda t \sqrt{\nu(l)+1} \right)}{\sqrt{\nu(l)+1}} \right.$$
$$\left. + \delta \cos(\phi+\gamma) \frac{\sin^2 \left(\lambda t \sqrt{\nu(l)+1} \right)}{\nu(l)+1} \right] |\langle l| \rho_{\rm F}(0) |l+1\rangle| \,. \qquad (13.53)$$

Here

$$\nu(l) = l + \frac{\delta^2}{4} \,,$$

the detuning parameter is

$$\delta = \frac{\omega_0 - \omega}{\lambda} \,,$$

and the phases ϕ and γ are defined by

$$c_e \, c_g^* = |c_e| \, |c_g| \, \exp(-i\phi)$$

and

$$\langle l| \rho_{\rm F}(0) |l+1\rangle = |\langle l| \rho_{\rm F}(0) |l+1\rangle| \exp(-i\gamma) \,.$$

Note that the last term in Eq. (13.53) does not appear when one deals with a mixture of number states but it is relevant for treating pure states; in fact, for pure states, this general expression reduces to that obtained in [193].

Considering the resonant case, $\delta = 0$, and the initial state of the atom being the excited state $|e\rangle$, the expression for the atomic population inversion becomes much simpler than Eq. (13.53),

$$W_0(t) = \sum_{l=0}^{\infty} \cos \left(2\lambda t \sqrt{l+1} \right) \langle l| \hat{\rho}_{\rm F}(0) |l\rangle \,. \qquad (13.54)$$

For simplicity, we shall consider this case in the analysis of some examples, without loosing the relevant physical aspects. For the number state $|n\rangle$, we have

$$W_0^{|n\rangle}(t) = \cos \left(2\lambda t \sqrt{n+1} \right) , \qquad (13.55)$$

which is periodic and similar to the behavior obtained with the semiclassical Rabi model. On the other hand, for a coherent state $|\alpha\rangle$, we get

$$W_0^{|\alpha\rangle}(t) = e^{-|\alpha|^2} \sum_{l=0}^{\infty} \frac{|\alpha|^{2l}}{l!} \cos \left(2\lambda t \sqrt{l+1} \right) . \qquad (13.56)$$

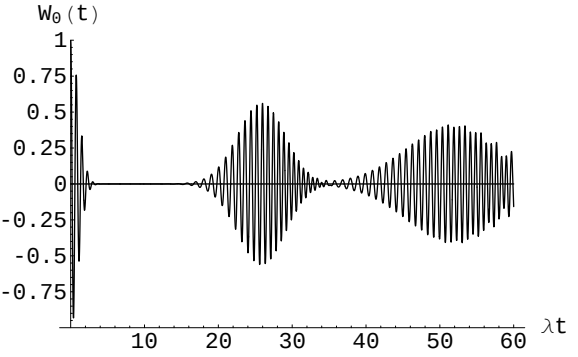


Fig. 13.4 Atomic population inversion for the field in a coherent state with $|\alpha| = 4$, at zero detuning with the atom initially at the excited level.

The atomic population inversion for the field mode in a coherent state [194] is shown in Fig. 13.4. We clearly find that collapses and revivals of the Rabi oscillations in a non-periodic pattern is quite different from the semiclassical case where the oscillations have constant amplitude. This happens for the field in the most-classical pure state, the coherent state, distinctly from the number state; this somewhat counterintuitive aspect is a feature of the quantum model.

Consider now the field mode in a thermal number state $|n(\beta)\rangle$. Using the number basis expansion of $\rho_{|n(\beta)\rangle}$, Eq. (12.34), we find

$$W_0^{|n(\beta)\rangle}(t) = \frac{1}{(1+\bar{n})^n} \sum_{l=0}^{\infty} \frac{(n+l)!}{n!\, l!} P_l^B(\bar{n}) \cos\left(2\lambda t \sqrt{n+l+1}\right) , \tag{13.57}$$

where we have introduced the notation

$$P_l^B(\bar{n}) = \frac{1}{1+\bar{n}} \left(\frac{\bar{n}}{1+\bar{n}}\right)^l \tag{13.58}$$

for the Bose-Einstein distribution. Since

$$\lim_{\bar{n}\to 0} P_l^B(\bar{n}) = \delta_{l0} ,$$

for $\bar{n} \to 0$, Eq. (13.57) reduces to the inversion for the number state given above. On the other hand, taking $n = 0$ one obtains the atomic population inversion for the field in a thermal vacuum state

$$W_0^{|0(\beta)\rangle}(t) = \sum_{l=0}^{\infty} P_l^B(\bar{n}) \cos\left(2\lambda t \sqrt{l+1}\right) . \tag{13.59}$$

The atomic inversion, when the field is in a chaotic (thermal) state, is illustrated in Fig. 13.5 for the mean number of thermal photons fixed as $\bar{n}(\beta) = 16$; the pattern shows a chaotic behavior very distinct from that of the coherent state with the same mean number of photons.

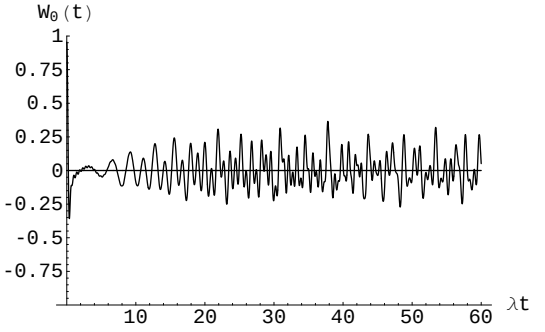


Fig. 13.5 Atomic population inversion for the field in thermal vacuum state with $\bar{n}(\beta) = 16$, at zero detuning with the atom initially at the excited level.

The atomic population inversion, in the case of the thermal number state with $n = 1$, is illustrated in Figs. 13.6(a)–13.6(d) for some values of $\bar{n}$. It is seen that, from a nearly regular oscillatory behavior at low T, similar to that of the number state $|1\rangle$, one gets a more chaotic inversion pattern, like that of the thermal (ρ_β) state [194], at a moderate temperature, and a collapse and revival configuration as the temperature is increased further. For larger n, we get a more marked behavior with collapses and revivals of the atomic population inversion appearing at lower temperatures and being greatly enhanced at high temperatures. This interesting feature of the thermal number state is illustrated in Figs. 13.6(e)–13.6(h), where the atomic inversion is plotted as a function of the rescaled time λt for $n = 5$ and some values of $\bar{n}(\beta)$.

It follows from the discussion of the nature of the photon statistics and of the atomic population inversion made above that nonclassical properties of the thermal number states gradually disappear as the temperature is increased; it looks as though $|n(\beta)\rangle$ evolves continuously from being quantum to becoming classical as the temperature is raised from zero.

Let us now consider the atomic population inversion for a two-level atom interacting with a field mode in the thermal tilde number state. Using the number-basis representation of $\rho_{|\tilde{m}(\beta)\rangle}$, Eq. (12.59), we find

$$W_0^{|\tilde{m}(\beta)\rangle}(t) = \frac{1}{(1+\bar{n})^m} \sum_{l=0}^{\infty} \frac{(m+l)!}{m!\, l!} P_l^B(\bar{n}) \cos\left(2\lambda t\sqrt{l+1}\right) , \tag{13.60}$$

where $P_l^B(\bar{n})$ is given by Eq. (13.58). For $\bar{n} \to 0$, we obtain the atomic population inversion when the field is in the vacuum state and the atom initially in the excited state $|e\rangle$,

$$W_0^{|0\rangle} = \cos(2\lambda t),$$

associated with the spontaneous emission and reabsorption of photons by the atom. The behavior of $W_0^{|\tilde{m}(\beta)\rangle}(t)$ as temperature is varied is shown in Fig. 13.7 for two

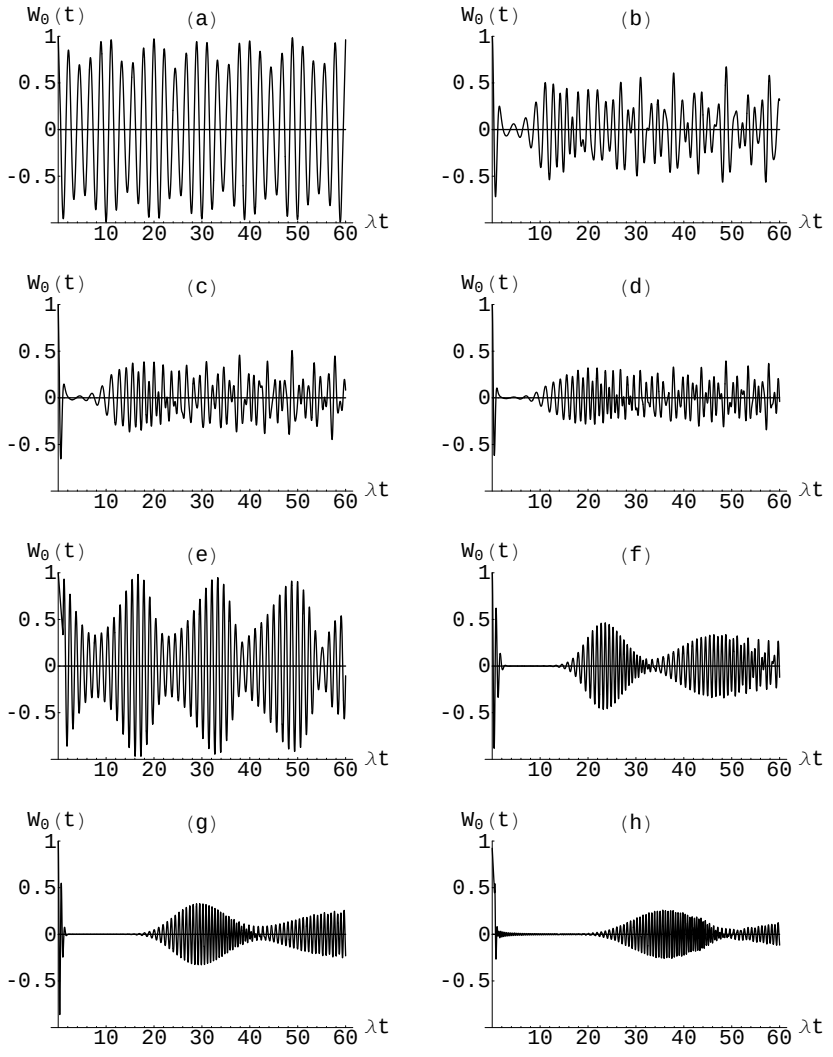


Fig. 13.6 Atomic population inversion for the field the thermal number states $|1(\beta)\rangle$ (a)–(d) and $|5(\beta)\rangle$ (e)–(h), at zero detuning with the atom initially at the excited level. The values of $\bar{n}(\beta)$ are: (a) and (e) 0.1; (b) and (f) 1.5; (c) and (g) 3.0; and (d) and (h) 5.0.

cases, $m = 1$ and $m = 5$. Comparison with the plots of the inversion for the thermal number states $|1(\beta)\rangle$ and $|5(\beta)\rangle$ (Fig. 13.6) shows that differences when the temperature is low but essentially the same behavior of collapses and revivals for large T.

On general grounds, and as indicated by the examples discussed above, one

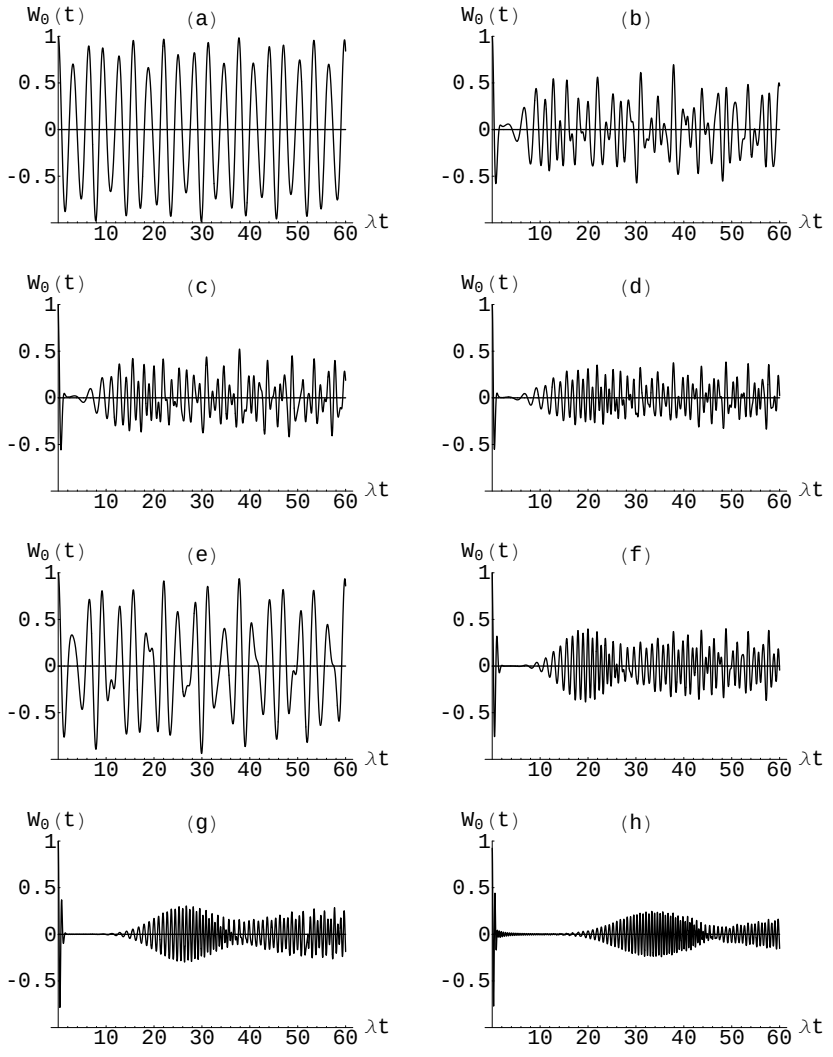


Fig. 13.7 Atomic population inversion for the field in thermal tilde number state $|\tilde{1}(\beta)\rangle$ (a)–(d) and $|\tilde{5}(\beta)\rangle$ (e)–(h), at zero detuning with the atom initially at the excited level. The values of $\bar{n}(\beta)$ are: (a) and (e) 0.1; (b) and (f) 1.5; (c) and (g) 3.0; and (d) and (h) 5.0.

expects that quantum characteristics of the thermalized states tend to disappear as the temperature is raised. But the question whether a thermalized state, like the thermal number state, becomes a classical state above a certain temperature cannot be answered by analyzing few nonclassical properties. To properly address this point, one should investigate the representation of the state in phase space with

increasing temperatures.

13.4 Phase space representation

The basic representations of a field-mode state in phase space are the P-, Q- and Wigner functions. These are linear representations of the corresponding density matrix, ρ, defined as two-dimensional Fourier transforms of the normally, anti-normally and symmetrically ordered characteristic functions,

$$\chi_N(\eta) = \mathrm{Tr}[\rho\, e^{\eta \hat{a}^\dagger} e^{-\eta^* \hat{a}}]\,,$$
$$\chi_A(\eta) = \mathrm{Tr}[\rho\, e^{-\eta^* \hat{a}} e^{\eta \hat{a}^\dagger}]\,,$$
$$\chi(\eta) = \mathrm{Tr}[\rho\, e^{\eta \hat{a}^\dagger - \eta^* \hat{a}}]\,,$$

respectively:

$$P(\gamma) = \frac{1}{\pi^2} \int d^2\eta \exp\left(\gamma\eta^* - \gamma^*\eta\right)\, \chi_N(\eta)\,, \tag{13.61}$$

$$Q(\gamma) = \frac{1}{\pi^2} \int d^2\eta \exp\left(\gamma\eta^* - \gamma^*\eta\right)\, \chi_A(\eta)\,, \tag{13.62}$$

$$W(\gamma) = \frac{1}{\pi^2} \int d^2\eta \exp\left(\gamma\eta^* - \gamma^*\eta\right)\, \chi(\eta)\,, \tag{13.63}$$

where γ and η are complex numbers and $d^2\eta = d\mathrm{Re}(\eta) d\mathrm{Im}(\eta)$ [174].

The P representation, introduced by Glauber and Sudarshan [195, 196], is the diagonal representation of the density matrix in the coherent basis and is also defined by

$$\rho = \int d^2\gamma\, P(\gamma)\, |\gamma\rangle\, \langle\gamma|$$

where $\gamma = x + iy$ and $d^2\gamma = dxdy$, while the Q-function corresponds to the diagonal matrix elements of ρ in the coherent basis, namely

$$Q(\gamma) = \frac{1}{\pi} \langle\gamma|\, \rho\, |\gamma\rangle\ .$$

On the other hand, the Wigner function is a coordinate-momentum representation which can be alternatively defined by

$$W(x,y) = \frac{1}{\pi} \int < x - z/2|\ \rho\ |x + z/2 > e^{-i\,y\ z} dz,$$

as presented in Chapter 3.

Distinctly from the P-function, which is usually highly singular, the Q-function is always a positive regular function. The Wigner function is also regular, but it is not a true probability distribution in phase space for a quantum state since, even being regular, it may assume negative values. Both the Q-and the Wigner functions are Gaussian convolutions of the P- function,

$$W(\gamma) = \frac{2}{\pi} \int \mathrm{d}^2\eta\, P(\eta)\, e^{-2|\eta-\gamma|^2}\,,$$
$$Q(\gamma) = \frac{1}{\pi} \int \mathrm{d}^2\eta\, P(\eta)\, e^{-|\eta-\gamma|^2}\,,$$

which accounts for their rather smoother behaviors.

Now consider the case of mixed states whose density matrices can be written in the form

$$\rho = \sum_{j=0}^{\infty} p_j \, |\psi_j\rangle \, \langle\psi_j| \tag{13.64}$$

with $\sum_{j=0}^{\infty} p_j = 1$, where $|\psi_j\rangle$ are normalized pure state of the field mode. The linearity of the P-, Q- and Wigner representations assures that these functions, for mixed states of the type presented in Eq. (13.64), are expressed in terms of the corresponding functions of the constituent pure states as

$$P(\gamma) = \sum_{j=0}^{\infty} p_j \, P_{|\psi_j\rangle}(\gamma) \, , \tag{13.65}$$

$$Q(\gamma) = \sum_{j=0}^{\infty} p_j \, Q_{|\psi_j\rangle}(\gamma) \, , \tag{13.66}$$

$$W(\gamma) = \sum_{j=0}^{\infty} p_j \, W_{|\psi_j\rangle}(\gamma) \, , \tag{13.67}$$

with $P_{|\psi_j\rangle}(\gamma)$, $Q_{|\psi_j\rangle}(\gamma)$ and $W_{|\psi_j\rangle}(\gamma)$ denoting the P- , Q- and Wigner functions of the state $|\psi_j\rangle$, respectively. Here we consider particularly the case where $|\psi_j\rangle = |j\rangle$ is a number state.

We now use these observations to find the phase space representation of thermal states focusing, particularly, on thermal number states. Since the P-function is a more complicated object, we concentrate on the Q- and Wigner functions.

13.4.1 *Q-function of the thermal number state*

For a single number state $|n\rangle$, the Q-function is given by

$$Q_{|n\rangle}(\gamma) = \frac{1}{\pi} \, |\langle n, |\, \gamma\rangle|^2 = \frac{1}{\pi} \, \exp\left(-|\gamma^2|\right) \, \frac{|\gamma^2|^n}{n!} \, , \tag{13.68}$$

where $\gamma = x + iy$. Note that $Q_{|n\rangle}(0,0) = 0$, for all $n \neq 0$. Now, it follows from Eqs. (12.34) and (13.66) that the Q-function of the thermal number state $|n(\beta)\rangle$ is given by

$$Q_{|n(\beta)\rangle}(x,y) = \frac{1}{\pi} \, \exp\left[-(x^2+y^2)\right] \, \frac{1}{(1+\bar{n})^n} \sum_{r=0}^{\infty} \frac{(n+r)!}{n!\, r!} P_r^B(\bar{n}) \, \frac{(x^2+y^2)^{n+r}}{(n+r)!} \, . \tag{13.69}$$

where P_r^B is given by Eq. (13.58). Note that, for $n = 0$, the above equation reduces to the Q-function of the chaotic, thermal, state

$$Q_{|0(\beta)\rangle}(x,y) = \frac{1}{\pi} \frac{1}{1+\bar{n}} \, \exp\left(-\frac{x^2+y^2}{1+\bar{n}}\right) \, , \tag{13.70}$$

which becomes the Gaussian Q-function of the vacuum state as $\bar{n}(\beta) \to 0$; the temperature effect on the vacuum state is manifested in the broadening of this Gaussian function.

On the other hand, the Q-function of a number state $|n\rangle$ (with $n \neq 0$) is a Gaussian with a crater dug symmetrically in it, reaching zero at the origin. As the temperature is increased ($\bar{n}$ grows), the Q-function of the thermal number state preserves the form of a non-active volcano, but with the mountain becoming broader and losing height, as illustrated in Fig. 13.8. Since the Q-function is everywhere positive, vanishing only at the origin, for all values of T, it is not a good representation to show any eventual change in the nature of the thermal number state as the temperature is varied; this may not be the case of the Wigner quasi-probability distribution.

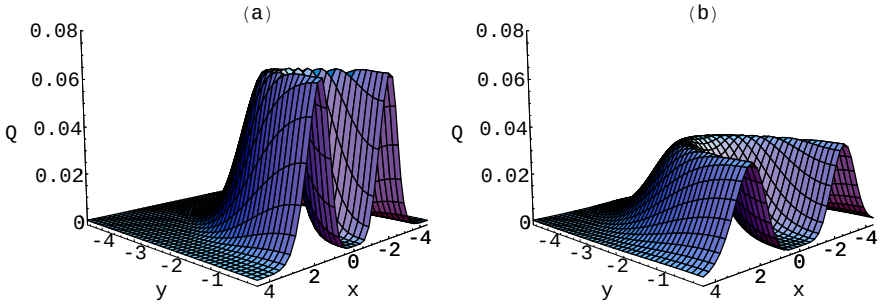


Fig. 13.8 Q-function for the thermal number state $|3(\beta)\rangle$ for two values of $\bar{n}(\beta)$: (a) 0.1, (b) 1.0.

13.4.2 *Wigner function of the thermal number state*

The Wigner function of the number state [174], $|n\rangle$, is given by

$$W_{|n\rangle}(\gamma) = \frac{2}{\pi} \exp\left(-2|\gamma|^2\right) (-1)^n L_n(4|\gamma|^2) \,, \tag{13.71}$$

where $L_n(z)$ stands for the Laguerre polynomial. Therefore, it follows from Eqs. (12.34) and (13.67) that the Wigner function of the thermal number state is

$$W_{|n(\beta)\rangle}(x,y) = \frac{2}{\pi} \exp\left[-2(x^2+y^2)\right] \frac{1}{(1+\bar{n})^n} \times \sum_{r=0}^{\infty} \frac{(n+r)!}{n!\, r!} P_r^B(\bar{n}) (-1)^{n+r} L_{n+r}\left[4(x^2+y^2)\right] \tag{13.72}$$

Naturally, when $n = 0$, Eq. (13.72) becomes the Wigner function of the chaotic, thermal, state

$$W_{|0(\beta)\rangle}(x,y) = \frac{1}{\pi} \frac{2}{1+2\bar{n}} \exp\left(-\frac{2\left(x^2+y^2\right)}{1+2\bar{n}}\right) \,, \tag{13.73}$$

having a Gaussian form which reduces to that of the vacuum state as $\bar{n} \to 0$.

Both Q- and Wigner functions of the thermal number state are symmetric around the origin, since they are mixtures of number states which have random phases. For $n \neq 0$, the Wigner function varies gradually, as the temperature is increased, from the shape of an active volcano, characteristic of a number state, to that of a non-active one, similar to the form of the Q-function, as illustrated in Fig. 13.9. Apparently, for a given $n \neq 0$, the thermal number state changes its nature from being a quantum state at low temperatures, the Wigner function possessing negative values, to becoming classical for high values of $\bar{n}$. However, a detailed analysis of the crater of the volcano shows that the Wigner function never becomes nonnegative and thus the thermal number state does not reduce exactly to a nonclassical state as the temperature grows. This leads to the question about the nonclassical depth of the thermal number state, the point addressed in the next section.

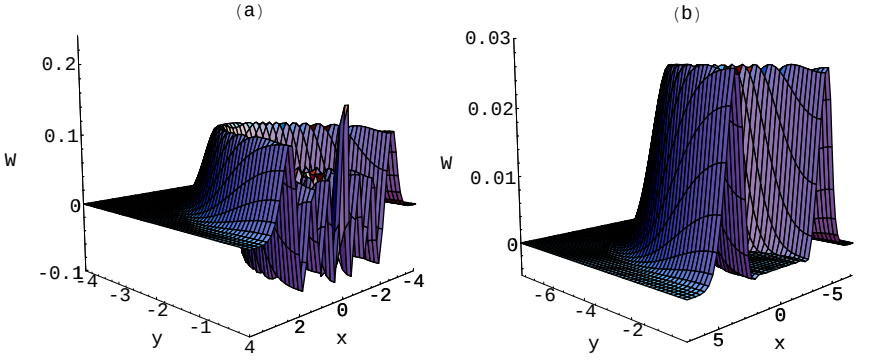


Fig. 13.9 Wigner function of the state $|6(\beta)\rangle$ for two values of $\bar{n}(\beta)$: (a) 0.1 and (b) 1.5.

13.4.3 *R-representation and nonclassical depth of the thermal number state*

To discuss the nonclassical depth of the thermal number state, we consider the Lee procedure [197] and introduce the one-parameter representation

$$R(\gamma; s) = \frac{1}{\pi s} \int \mathrm{d}^2\eta \, P(\eta) \, e^{-|\eta-\gamma|^2/s}, \tag{13.74}$$

where $\gamma = x + iy$. The function $R(\gamma; s)$ interpolates between P-, W- and Q-functions, reducing to them for the values $s = 0, 1/2, 1$ respectively. This one-parameter representation is a simplified version of the complex-parameter representation earlier introduced by Cahill and Glauber [198]. The nonclassical depth of a

given state is defined as the minimum (s_m) among the values of s for which the R-function becomes strictly nonnegative. Naturally, $0 \leq s_m \leq 1$ with 0 being the classical value, associated with coherent states for example, and 1 corresponding to the maximum degree of nonclassicality, as for a number state.

For a number state $|n\rangle$, we have

$$R_{|n\rangle}(\gamma; s) = \frac{1}{\pi s} \exp\left(-\frac{|\gamma^2|}{s}\right) \left[-\frac{(1-s)}{s}\right]^n L_n\left(\frac{|\gamma|^2}{s(1-s)}\right). \tag{13.75}$$

Since the R-representation is linear in the density matrix, using Eq. (12.34), we obtain the R-function for the thermal number state $|n(\beta)\rangle$ as

$$R_{|n(\beta)\rangle}(x, y; s) = \frac{1}{\pi s} \exp\left[-\frac{(x^2+y^2)}{s}\right] \frac{1}{(1+\bar{n})^n} \times \sum_{r=0}^{\infty} \frac{(n+r)!}{n!\, r!} P_r^B(\bar{n}) \left[-\frac{(1-s)}{s}\right]^{n+r} L_{n+r}\left[\frac{(x^2+y^2)}{s(1-s)}\right]. \tag{13.76}$$

The value of this function at the origin when $1/2 < s < 1$,

$$R_{|n(\beta)\rangle}(0, 0; s) = \frac{1}{\pi}(-1)^n \frac{(1-s)^n}{(s+\bar{n})^{n+1}}\ , \tag{13.77}$$

shows that, for n odd, the R-function has a negative value at origin for s in this range; thus, $s_m = 1$ and the thermal number state with n odd is as nonclassical as possible. When n is even, $R_{|n(\beta)\rangle}(0, 0; s)$ is positive and one has to analyze the minimum value of the R-function. As illustrated in Fig. 13.10, where profiles of R-functions along the x-axis are plotted for a specific thermal number state, the minimum value of R (for n even) tends to zero as s approaches 1 but remains negative for all $s < 1$, implying that the thermal number state is always as nonclassical as possible within the measure discussed. In this way, it is clear that the thermal number state satisfies the Lee's theorem [199] by which a state with density operator not containing the vacuum component, $|0\rangle\langle 0|$, possesses the maximum degree of nonclassicality. Analyzing how a given R-function changes as the temperature is increased, it is found that its minimum value tends to zero but it is negative for all $s < 1$, as occurs with the Wigner function ($s = 1/2$) illustrated in Fig. 13.9. It may be stated that the quantum fingerprint of the number state remains in the thermal number state and cannot be completely erased by increasing the temperature.

13.4.4 *Phase space representations of the thermal tilde number state*

A thermal tilde number state, $|\widetilde{m}(\beta)\rangle$, is represented by a density matrix that is also diagonal in the number basis of $\mathcal{H}$. Thus, from the linearity of the R-representation and the R-function for the number state $|n\rangle$, Eq. (13.75), we find the R-function

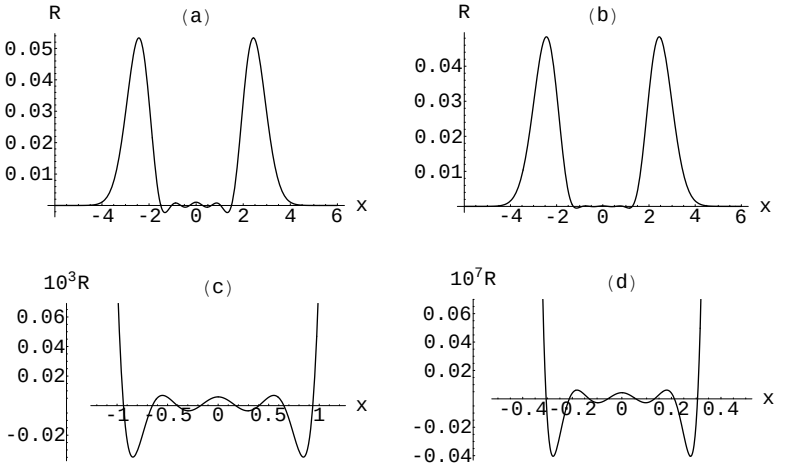


Fig. 13.10 Profiles along the x-axis of some R-functions for the thermal number state $|4(\beta)\rangle$ with $\bar{n}(\beta) = 0.5$: (a) s = 0.7; (b) s = 0.8; (c) s = 0.9; (d) s = 0.99.

for the thermal tilde number state $|\widetilde{m}(\beta)\rangle$ as

$$R_{|\widetilde{m}(\beta)\rangle}(x,y;s) = \frac{1}{\pi s}\exp\left[-\frac{(x^2+y^2)}{s}\right]\frac{1}{(1+\bar{n})^m} \times \sum_{r=0}^{\infty}\frac{(m+r)!}{m!\,r!}P_r^B(\bar{n})\left[-\frac{(1-s)}{s}\right]^r L_r\left[\frac{(x^2+y^2)}{s(1-s)}\right]. \tag{13.78}$$

Taking the limit $s \to 1$ in this expression, and using

$$\lim_{s\to 1}\left[-\frac{(1-s)}{s}\right]^r L_r\left[\frac{z}{s(1-s)}\right] = \frac{z^r}{r!},$$

we obtain the Q-function for $|\widetilde{m}(\beta)\rangle$ as

$$Q_{|\widetilde{m}(\beta)\rangle}(x,y) = \frac{1}{\pi}\,\exp\left[-(x^2+y^2)\right]\frac{1}{(1+\bar{n})^n}\sum_{r=0}^{\infty}\frac{(n+r)!}{n!\,r!}P_r^B(\bar{n})\,\frac{(x^2+y^2)^r}{r!}\,. \tag{13.79}$$

This function is plotted in Fig. 13.11 for a given thermal tilde number state at two distinct temperature. We find that, for low temperatures, the Q-function has a nearly Gaussian shape that resembles that of the vacuum state of $\mathcal{H}$,

$$Q_{|0\rangle} = \frac{1}{\pi}\exp[-(x^2+y^2)],$$

which is the proper limit of Eq. (13.79) as $\bar{n}(\beta) \to 0$. Note that, distinctly of the case of the thermal number state, the Q-function of $|\widetilde{m}(\beta)\rangle$ does not vanish at the origin or on any other point at a finite distance from the origin.

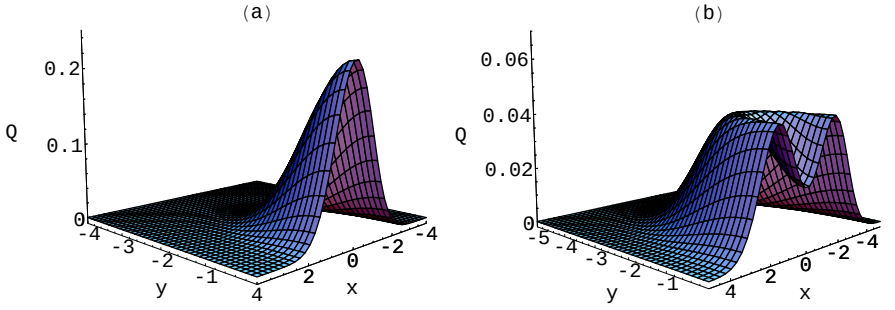


Fig. 13.11 Q-function for the thermal tilde number state $|\tilde{3}(\beta)\rangle$ for two values of $\bar{n}(\beta)$: (a) 0.1, (b) 1.0.

Now fixing $s = 1/2$ in Eq. (13.78), we get the Wigner function of the thermal tilde number state $|\widetilde{m}(\beta)\rangle$ as

$$W_{|\widetilde{m}(\beta)\rangle}(x,y) = \frac{2}{\pi}\exp\left[-2(x^2+y^2)\right]\frac{1}{(1+\bar{n})^m} \times \sum_{r=0}^{\infty}\frac{(m+r)!}{m!\,r!}P_r^B(\bar{n})\,(-1)^r\,L_r\left[4(x^2+y^2)\right]. \tag{13.80}$$

In Fig. 13.12, we illustrate the Wigner function of the state $|\tilde{6}(\beta)\rangle$, for two distinct values of the temperature.

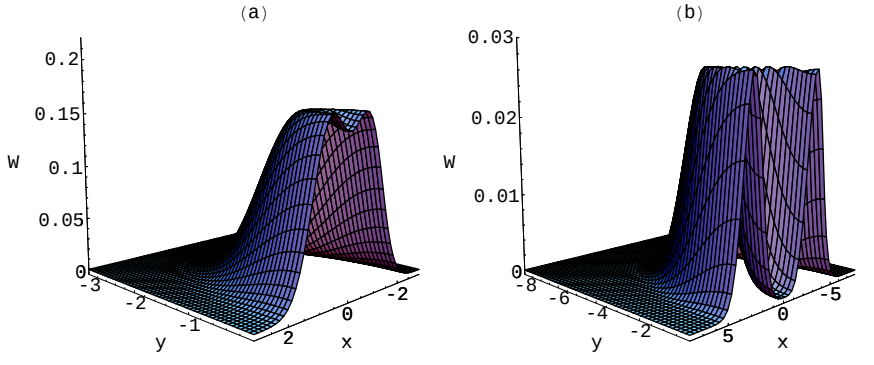


Fig. 13.12 Wigner function of the state $|\tilde{6}(\beta)\rangle$ for two values of $\bar{n}(\beta)$: (a) 0.12 and (b) 1.5.

Comparison between these figures clearly shows that the thermal tilde number state has a much more classical behavior than the thermal number state; its Wigner function does not assume negative values. Actually, its R-function is non-negative

even for s smaller than (but close to) 0.5; this can be verified by plotting profiles of the type shown in Fig. 13.10.

The discussion of phase-space representations can also be made, along these lines, for other thermalized states of a field mode. In particular, for simple states of the type $|n, \tilde{n}; \beta\rangle$, which have diagonal density matrices in the number basis and have R-functions that are symmetric around the origin, one can look at the competition between the tilde and non-tilde parts to establish the degree of non-classicality of the state. We leave such analysis to the interested reader. In the next chapter we move on to another relevant aspect for quantum optics and discuss the amount of entanglement of states of bipartite systems constructed with inspiration from TFD.

Chapter 14

$SU(2)$ and $SU(1,1)$ Systems: Entanglement

Considering states of systems with $SU(2)$ and $SU(1,1)$ symmetry, the TFD approach is applied to spin 1/2 systems and bipartite entangled states. This analysis of entangled states constructed with the inspiration of TFD is the main goal of the present chapter.

We study the nature of the entanglement for boson and fermion states. We first investigate two-mode squeezed states in the case of bosons, then we construct the fermionic version, to show that such states are maximally entangled, for both bosons and fermions. For the case of fermions, the situation is more intricate, demanding coherent fermion state and density operator, which is achieved by using Grassmann variables. Hence the problem of constructing entangled states, using squeezed states, can be put in a succinct form. We start by deriving some properties of the two-mode squeezed-vacuum state and its generalization, the Caves-Schumaker states [200]. These results will be used later to prove the property of maximum entanglement of boson squeezed states; then the fermion counterpart of the boson squeezed-vacuum and the Caves-Schumaker states are introduced and some properties, like the maximum entanglement, are analyzed.

14.1 Maximum entanglement

Quantum mechanics gives rise to the notion of entangled states, which are states of two or more systems correlated with each other, but without a classical analog. Indeed, this entanglement may have non-local features. Bell [201, 202] was the first to present a way to analyze entangled states, by comparing such correlations to the classical correlated states, that are defined via classical probability distributions. The appearance of entangled states is a consequence of the direct-product structure of the Hilbert space of multipartite systems and the superposition principle of quantum mechanics.

A recent interest in entangled states arose since they are essential for teleporting quantum states, from one locus to another, which is a basic ingredient in the theory of quantum computers [203, 204]. In order to progress with such a program of quan-

tum communication, the measure of entanglement is a crucial aspect of the theory that has to be fully developed; and this has been discussed in the literature in different ways [205–211]. On the other hand, the ideal conditions for teleporting require specific entangled states characterized by a maximum entanglement [212, 213], a characteristic feature that can be present not only in boson systems, but also for fermions.

The notion of maximum entanglement of a bipartite system, say (A, B), described by a pure state $|\psi(A, B)\rangle$ is analyzed. Let us introduce the reduced density operator, ρ_A, by

$$\rho_A = \mathrm{Tr}_B(|\psi(A, B)\rangle\langle\psi(A, B)|), \tag{14.1}$$

where Tr_B stands for the trace over the variables of the subsystem B. A measure of entanglement of the pure state $|\psi(A, B)\rangle$ is defined by the von Neumann entropy associated with the reduced density operator [212, 213],

$$S(\rho_A) = -\mathrm{Tr}\,(\rho_A \ln \rho_A)\,. \tag{14.2}$$

The condition for a maximum entanglement of A and B, that is, the condition for $|\,\psi(A, B)\rangle$ to be a maximally entangled state, is that $S(\rho_A)$ be a maximum. Note that, for a product state of the type $|\Phi(A)\rangle \otimes |\Phi(B)\rangle$, the reduced density operator corresponds to a pure state of the subsystem and, therefore, its von Neumann entropy vanishes.

Since $S(\rho_A)$ is a homogeneous function of first degree in its dependency on E_A, the energy of the sub-system A, we require $\delta S(E_A) = 0$ under the constraints

$$E_A = \langle H_A \rangle = \mathrm{Tr}\rho_A H_A, \quad \mathrm{Tr}\rho_A = 1, \tag{14.3}$$

where H_A is the Hamiltonian of system A. Following methods similar to those of statistical mechanics, as presented in Chapter 2, we derive a constraint equation for ρ_A,

$$\alpha_0 - 1 + \alpha_1 H_A + \ln \rho_A = 0, \tag{14.4}$$

where α_0 and α_1 are Lagrange multipliers associated with given constraints. Using Eq. (14.4) we get a Gibbs-like density operator,

$$\rho_A = \frac{1}{Z} \exp(\alpha_1 H_A), \tag{14.5}$$

where $Z = \exp(1 - \alpha_0)$. Multiplying Eq. (14.4) by ρ_A, taking the trace and using Eqs. (14.3) and (14.5), we derive

$$\ln Z + \alpha_1 E_A + S = 0.$$

For convenience, let us write $\alpha_1 = -1/\tau$, then we have $\tau \ln Z = E_A - \tau S$. The function $F(\tau) = \tau \ln Z$ describes the Legendre transform of S since we assume that $\tau = \partial E/\partial S$. Here τ is an intensive parameter describing the fact that E_A, given by Eq. (14.3), is constant in the state described by ρ_A. Although fluctuations can exist, these are not a result for any heat bath (or ensemble of states) but rather *a*

consequence of the entanglement of the states A and B. We thus have a prescription for a bipartite pure state $|\psi(A,B)\rangle$ to be maximally entangled, under the energy constraint: its corresponding reduced density matrix, as defined in Eq. (14.1), is explicitly given by Eq. (14.5), such that

$$Z = \mathrm{Tr}\exp(-\tau H_A). \tag{14.6}$$

This provides the maximum entangled state. In this way we show in the following that, using the scheme of TFD for the $SU(1,1)$ and $SU(2)$ symmetries, we can explicitly construct examples of maximally entangled states, such that the measurement of the entanglement is given by Eq. (14.2).

14.2 Maximally entangled states and $SU(1,1)$ symmetry

Let us consider a two boson oscillators described by creation, $a^\dagger$ and $b^\dagger$, and annihilation, a and b, operators satisfying the algebraic relations

$$[b, b^\dagger] = [a, a^\dagger] = 1, \tag{14.7}$$

$$[a, b] = [a, b^\dagger] = [a^\dagger, b] = [a^\dagger, b^\dagger] = 0. \tag{14.8}$$

Following the TFD approach, we construct a two-mode linear canonical transformation presenting an $SU(1,1)$ symmetry. First, define the following operators

$$S_+ = a^\dagger b^\dagger,$$
$$S_- = ab,$$
$$S_0 = \frac{1}{2}(a^\dagger a + bb^\dagger),$$

which satisfy the $su(1,1)$ algebra, namely

$$[S_0, S_\pm] = S_\pm,$$
$$[S_+, S_-] = -S_0.$$

Now, introduce a canonical transformation

$$U(\gamma) = \exp[\gamma(S_+ - S_-)],$$

where γ is a parameter to be specified later. The canonical nature of $U(\gamma)$ maintains the invariance of the algebra specified by Eqs. (14.7) and (14.8) for the transformed operators, which are given by

$$a(\gamma) = U(\gamma)a^\dagger U(\gamma),$$
$$a^\dagger(\gamma) = U(\gamma)a^\dagger U(\gamma),$$
$$b(\gamma) = U(\gamma)b^\dagger U(\gamma),$$
$$b^\dagger(\gamma) = U(\gamma)b^\dagger U(\gamma).$$

Consider the two-mode vacuum

$$|0_a, 0_b\rangle = |0_a\rangle \otimes |0_b\rangle,$$

such that $a|0_a\rangle = b|0_b\rangle = 0$. Applying the transformation $U(\gamma)$, we have

$$|0(\gamma)\rangle = \exp[\gamma(S_+ - S_-)] \mid 0_a, 0_b\rangle, \tag{14.9}$$

Here we use the notation $|0(\gamma)\rangle = |\psi(A,B)\rangle$ for the transformed vacuum in order to emphasize that we are dealing with a bipartite system, with A and B referring to the degrees of freedom associated with the boson operators $a^\dagger, a$ and $b^\dagger, b$ respectively. For convenience we write Eq. (14.9) as

$$\begin{aligned}|\psi(A,B)\rangle &= e^{\tanh\gamma a^\dagger b^\dagger} e^{-\ln\cosh\gamma(bb^\dagger + a^\dagger a)} e^{\tanh(-ba)}|0_a,0_b\rangle \\ &= \exp(-\ln\cosh\gamma)\sum_m(-\tanh\gamma)^m\frac{1}{m!}(a^\dagger b^\dagger)^m|0_a,0_b\rangle. \end{aligned}\tag{14.10}$$

Using this expression, we show that the state $|\psi(A,B)\rangle$ is a maximally entangled state.

Consider the density matrix corresponding to the state $|\psi(A,B)\rangle$, $\rho(A,B) = |\psi(A,B)\rangle\langle\psi(A,B)|$, and take the trace in the B variables; the resulting reduced density matrix is then

$$\begin{aligned}\rho_A &= \mathrm{Tr}_B[|\psi(A,B)\rangle\langle\psi(A,B)|] \\ &= \frac{1}{(\cosh\gamma)^2}\sum_{m,n}\sum_l \frac{1}{m!n!}(-\tanh\gamma)^{m+n}(a^\dagger)^n|0_a\rangle\langle 0_a|a^m\langle l|(b^\dagger)^n|0_b\rangle\langle 0_b|b^m|l\rangle \\ &= \frac{1}{(\cosh\gamma)^2}\sum_{m=0}^{\infty}(-\tanh\gamma)^{2m}|m\rangle\langle m|.\end{aligned}$$

Define the parameter τ such that

$$\begin{aligned}\cosh\gamma(\tau) &= \frac{1}{\sqrt{1-e^{-\tau w}}} \\ \tanh\gamma(\tau) &= e^{-\tau w/2};\end{aligned}$$

with this parametrization, ρ_A is written as

$$\rho_A = (1-e^{-\tau w})\sum_{m=0}^{\infty} e^{-\tau w m}|m\rangle\langle m|.$$

This expression can be cast in the canonical-Gibbs ensemble form by defining

$$H_A = wa^\dagger a$$

and

$$Z(\tau) = Tre^{-\tau H_A} = (1-e^{-\tau w})^{-1}.$$

Then we have

$$\rho_A = \frac{1}{Z(\tau)}e^{-\tau H_A},$$

showing that the state $|\psi(A,B)\rangle = \exp[\gamma(S_+ - S_-)]|0_a,0_b\rangle$, is a maximally entangled state with the symmetry $SU(1,1)$.

14.3 Maximally entangled states and $SU(2)$ symmetry

In order to construct bipartite states of two systems A and B of maximum entanglement, with an $SU(2)$ symmetry, we use the two-boson Schwinger representation for the $su(2)$ Lie algebra, developed before in Chapter 6.

The two bosons, with annihilation operators b_1 and b_2, are such that these operators commute among themselves and also with the boson annihilation operators a_1 and a_2, giving rise to the doubling of the $su(2)$ algebra, i.e.

$$[S_0, S_\pm] = \pm S_\pm, \tag{14.11}$$

$$[S_+, S_-] = 2S_0, \tag{14.12}$$

$$[\widetilde{S}_0, \widetilde{S}_\pm] = \pm \widetilde{S}_\pm, \tag{14.13}$$

$$[\widetilde{S}_+, \widetilde{S}_-] = 2\widetilde{S}_0, \tag{14.14}$$

such that the tilde operators $\widetilde{S}_-$, $\widetilde{S}_+$ and $\widetilde{S}_0$ commute with the non-tilde operators and are now given by

$$\widetilde{S}_+ = b_1^\dagger b_2 \tag{14.15}$$

$$\widetilde{S}_- = b_2^\dagger b_1 \tag{14.16}$$

$$\widetilde{S}_0 = \frac{1}{2}(b_1^\dagger b_1 - b_2^\dagger b_2). \tag{14.17}$$

The non-tilde operators are

$$S_+ = a_1^\dagger a_2$$

$$S_- = a_2^\dagger a_1$$

$$S_0 = \frac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2).$$

It is important to point out that tilde operators here do not refer to the TFD operators. Instead, these mimic TFD operators to underline the $SU(2)$ symmetry.

Consider the state $|\psi(A,B)\rangle$ given by

$$\begin{aligned} |\psi(A,B)\rangle &= \exp[\gamma(S_+\widetilde{S}_+ + S_-\widetilde{S}_-)]|0_a, 0_b\rangle, \\ &= \exp[\gamma(a_1^\dagger b_1^\dagger a_2 b_2 - a_2^\dagger b_2 \dagger a_1 b_1)]|0_a, 0_b\rangle \\ &= (\cos\gamma + \sin\gamma a_1^\dagger b_1^\dagger a_2 b_2)|0_a, 0_b\rangle, \end{aligned} \tag{14.18}$$

where A represents the degrees of freedom described by the operators S; B represents the other system described by the operators $\widetilde{S}$, and $|0_a, 0_b\rangle = |0_a\rangle \otimes |0_b\rangle = |0,1\rangle_a \otimes |0,1\rangle_b \equiv |0\rangle_{a_1}|1\rangle_{a_2}|0\rangle_{b_1}|1\rangle_{b_2}$ (see Chapter 6). The quantity γ is an arbitrary constant to be specified. Consider $\rho(A,B) = |\psi(A,B)\rangle\langle\psi(A,B)|$, and take the trace in the B variables, that is

$$\begin{aligned} \rho_A &= Tr_B|\psi(A,B)\rangle\langle\psi(A,B)| \\ &= \sum_{m,n}{}^{(b)}\langle m|_{b_1}\langle n|_{b_1}(\cos\gamma + \sin\gamma a_1^\dagger b_1^\dagger a_2 b_2)|0\rangle_{a_1}|1\rangle_{a_2}|0\rangle_{b_1}|1\rangle_{b_2}\langle 1|_{b_2}\langle 0|_{b_1}\langle 0|_{a_2}\langle 1|_{a_1} \\ &\times (\cos\gamma + \sin\gamma a_1^\dagger b_1^\dagger a_2 b_2)^\dagger |n\rangle_{b_1}|m\rangle_{b_2}, \end{aligned}$$

where the indices in the states, as b_2 in $|1\rangle_{b_2}$ or $\langle 1|_{b_2}$, are used to specify the action of the different operators, so that $|1\rangle_{b_2} = b_2^\dagger\,|0\rangle_{b_2}$, and so on. With some algebraic manipulations we get

$$\rho_A = \cos^2\gamma|0\rangle_{a_1}|1\rangle_{a_2}\langle 1|_{a_2}\langle 0|_{a_1} + \sin^2\gamma|1\rangle_{a_1}|0\rangle_{a_2}\langle 0|_{a_2}\langle 1|_{a_1}. \tag{14.19}$$

In the case of spin 1/2, we have

$$|0\rangle_{a_1}|1\rangle_{a_2} = |s = 1/2, m = -1/2\rangle \equiv |-1/2\rangle,$$

and

$$|1\rangle_{a_1}|0\rangle_{a_2} = |s = 1/2, m = 1/2\rangle \equiv |1/2\rangle.$$

Defining

$$\cos\gamma = \frac{1}{\sqrt{1+e^{-\tau\omega}}}\ ,\ \ \sin\gamma = \frac{e^{-\tau\omega/2}}{\sqrt{1+e^{-\tau\omega}}}\,,$$

ρ_A is written as

$$\rho_A = \frac{1}{Z}e^{-\tau\omega S_0}\,|1/2\rangle\,\langle 1/2| + \frac{1}{Z}e^{-\tau\omega S_0}\,|-1/2\rangle\,\langle -1/2|\,,$$

since the eigenvalues of S_0 are $\pm\frac{1}{2}$. As $\mathrm{Tr}\rho_A = 1$, then $Z = e^{-\tau\omega/2} + e^{\tau\omega/2}$. Then we have

$$\begin{aligned}\rho_A &= \frac{1}{Z}\sum_{m=1/2,-1/2} e^{-\tau\omega S_0}|m\rangle\langle m| \\ &= \frac{1}{Z}e^{-\tau\omega S_0}\sum_{m=1/2,-1/2}|m\rangle\langle m| = \frac{1}{Z}e^{-\tau H_A},\end{aligned}$$

where $H_A = \omega S_0$. Therefore the state given by Eq. (14.18) is a maximally entangled state. The generalization for any value of spin is straightforward.

14.4 Entanglement of a system with fixed spin

In the last section $|\psi(A = S, B = \tilde{S}; \gamma)\rangle$ was used to describe a maximally entangled state. If we consider an arbitrary spin value, corresponding to arbitrary values of the number operators n_1 and n_2, $|\psi(A = S, B = \tilde{S}; \gamma)\rangle$ is a maximally entangled state of two systems, each one with two bosons. However, for the system of two (defined) spin 1/2 particles, for instance, we have the eingenvalues of the number operator as $n_1 = 0, 1$ and $n_2 = 0, 1$, which no longer correspond to the spectrum of bosonic number operators, but rather to fermionic-like ones. In such a case the bosonic algebra does not describe physical bosons but works as auxiliary variables to treat the entanglement of two spin systems. Accordingly, since we define a fixed (not arbitrary) value for the spin, we have to analyze more closely the consequences of that, with the Schwinger representation which is usually introduced for arbitrary spin.

Returning to the Schwinger bosonic representation, imposing the conditions on the spectrum of n_1 $(= 0, 1)$ and n_2 $(= 0, 1)$, and defining s with a fixed value, then we are lead to a situation of redefining the algebra of the auxiliary operators a_1 and a_2. Summarizing first our results, originally operators a_1 and a_2, and their hermitian adjoint operators, $a_1^\dagger$ and $a_2^\dagger$, satisfy the bosonic algebra

$$[a_1, a_1^\dagger] = [a_2, a_2^\dagger] = 1, \tag{14.20}$$

$$[a_1, a_2] = [a_1, a_2^\dagger] = [a_1^\dagger, a_2] = [a_1^\dagger, a_2^\dagger] = 0. \tag{14.21}$$

In addition, for the spin 1/2, we have the subsidiary conditions (allowing the fixed value for the spin),

$$[a_1, a_1^\dagger]_+ = [a_2, a_2^\dagger]_+ = 1, \tag{14.22}$$

$$[a_1, a_2]_+ = [a_1, a_2^\dagger]_+ = [a_1^\dagger, a_2]_+ = [a_1^\dagger, a_2^\dagger]_+ = 0, \tag{14.23}$$

where $[,]_+$ stands for the anticommutator. A solution that fulfills all these conditions, Eqs. (14.20)–(14.23), is found by assuming the algebra for the operators a_i and $a_i^\dagger$, $(i = 1, 2)$ to be

$$a_i a_i^\dagger = 1, \tag{14.24}$$

$$[N_i, a_i^\dagger] = a_i^\dagger, \tag{14.25}$$

$$[N_i, a_i] = -a_i, \tag{14.26}$$

with $a_i a_i = a_i^\dagger a_i^\dagger = 0$ and $N_i = a_i^\dagger a_i$. Indeed it is a simple matter to show that in this case the eigenvalues of the number operators are $n_i = 0, 1,\ i = 1, 2$.

For the case of spin 1, we consider the basic algebra given by Eqs. (14.24)–(14.26) with N_i given by

$$N_i = a_i^\dagger a_i + a_i^\dagger a_i^\dagger a_i a_i,$$

such that $a_i^\dagger a_i^\dagger a_i^\dagger = a_i a_i a_i = 0$, that is third and higher order monomials of $a_i^\dagger$ and a_i are zero. In this case we derive $n_i = 0, 1, 2$, (see Chapter 6) and we find $s = 1$ and $m = -1, 0, 1$.

This procedure can be generalized for an arbitrary but fixed value of spin. That is, for a spin s, such that $n_i = 2s$, we consider Eqs. (14.24)–(14.26) supplemented by a proper definition of N_i, which reads

$$N_i = \sum_{j=1}^{2s} (a_i^\dagger)^j (a_i)^j. \tag{14.27}$$

For the particular situation in which $s \to \infty$, we will find the approach of infinite statistics proposed by Greenberg [214, 215].

In short, we have explored the similarity with the usual definition of entropy in statistical mechanics to construct maximally entangled states using the approach of TFD. As TFD is a thermal formalism founded on algebraic bases (duplication of the usual Hilbert space and Bogoliubov transformations), it has been used as a compass to give the proper direction to build maximum entangled states with a well-defined

symmetry. We have studied the case of two bosons with $SU(1,1)$ symmetry and four bosons (actually two systems, each one with two bosons) with $SU(2)$ symmetry. Still in the case of $SU(2)$ symmetry, the entanglement of two systems with fixed value of spin ia considered, using a modified version of the two-boson Schwinger representation for the $su(2)$ Lie algebra.

The usual way to describe fixed value of spin using boson operators was proposed by Holstein and Primakof [218]. However such a method works if we are interested in describing a system with spin via one bosonic operator. But this has not been the case here, since it needed two operators associated to each spin to introduce the state of maximum entanglement through TFD. Obviously for a finite spectrum, the pair of Schwinger operators loses the bosonic characteristic, giving rise to a new algebra.

14.5 Entanglement of two-boson squeezed states

Let us consider a two-boson system specified by the operators a and b obeying the algebra $[a, a^\dagger] = [b, b^\dagger] = 1$, $[a, b] = 0$. Initially, we restate the results presented in Sec. 14.2 with the language of squeezed states. In general, we can consider this in terms of two independent electromagnetic field modes. We define two unitary displacement operators, one for each mode,

$$D_a(\xi) = \exp[\xi a^\dagger - \xi^* a], \tag{14.28}$$

$$D_b(\eta) = \exp[\eta b^\dagger - \eta^* b], \tag{14.29}$$

and the two-mode squeezing operator

$$S_{ab}(\gamma) = \exp[\gamma(a^\dagger b^\dagger - ab)], \tag{14.30}$$

with γ a real non-negative number for simplicity. From now on, we use the subscript a and b referring to the subsystems (the field modes) A and B of the bipartite system (A, B).

The operator $S_{ab}(\gamma)$ engenders a rotation in the two-mode space, similar to that of the Bogoliubov transformation in TFD; thus, using the standard TFD procedure (see Chapters 5 and 6), we get

$$\begin{aligned}
a(\gamma) &= S_{ab}(\gamma) a S_{ab}^\dagger(\gamma) = u(\gamma) a - v(\gamma) b^\dagger, \\
a^\dagger(\gamma) &= S_{ab}(\gamma) a^\dagger S_{ab}^\dagger(\gamma) = u(\gamma) a^\dagger - v(\gamma) b, \\
b(\gamma) &= S_{ab}(\gamma) b S_{ab}^\dagger(\gamma) = u(\gamma) b - v(\gamma) a^\dagger, \\
b^\dagger(\gamma) &= S_{ab}(\gamma) b^\dagger S_{ab}^\dagger(\gamma) = u(\gamma) b^\dagger - v(\gamma) a,
\end{aligned}$$

where $u(\gamma) = \cosh(\gamma)$ and $v(\gamma) = \sinh(\gamma)$.

Let us first consider the two-mode squeezed vacuum (TMSV) defined by

$$|\gamma\rangle_{ab} = S_{ab}(\gamma)|0\rangle_{ab}, \tag{14.31}$$

where

$$|0\rangle_{ab} = |0\rangle_a \otimes 0\rangle_b \equiv |0\rangle_a |0\rangle_b \tag{14.32}$$

is the two-mode vacuum with $a|0\rangle_a = b|0\rangle_b = 0$. For the two-mode squeezed state, we have

$$a(\gamma)|\gamma\rangle_{ab} = b(\gamma)|\gamma\rangle_{ab} = 0, \tag{14.33}$$

so that it has the same structure as the thermal vacuum used to introduce TFD. Another important result is that $S_{ab}(\gamma)$ is a canonical transformation, i.e.

$$[a(\gamma), a^\dagger(\gamma)] = [b(\gamma), b^\dagger(\gamma)] = 1\,, \quad [a(\gamma), b(\gamma)] = 0\,.$$

Using the operator identity

$$\exp[\gamma(A+B)] = \exp[(\tanh\gamma)B]\,\exp[(\ln\cosh\gamma)C]\,\exp[(\tanh\gamma)A],$$

with $A = -ab$, $B = a^\dagger b^\dagger$ and $C = [A, B] = -a^\dagger a - bb^\dagger$, the TMSV is written as

$$|\gamma\rangle_{ab} = \frac{1}{\cosh\gamma}\exp[(\tanh\gamma)a^\dagger b^\dagger]\,|0\rangle_{ab}.$$

Introducing the change of parametrization by taking $\tanh\gamma = \exp(-\tau/2)$, and defining

$$Z(\tau) = [1 - \exp(-\tau)]^{-1} = \mathrm{Tr}\exp[-\tau a^\dagger a],$$

we find

$$|\gamma\rangle_{ab} = \frac{1}{\sqrt{Z(\tau)}}\sum_{n=0}^{\infty} e^{-\tau n/2}|n\rangle_a |n\rangle_b. \tag{14.34}$$

Therefore, the TMSV $|\gamma\rangle_{ab}$ is written as

$$|\gamma\rangle_{ab} = \sqrt{f_a(\tau)}\sum_{n=0}^{\infty}|n\rangle_a|n\rangle_b, \tag{14.35}$$

where

$$f_a(\tau) = \frac{1}{Z(\tau)}\exp(-\tau a^\dagger a). \tag{14.36}$$

This form makes it easy to show that the TMSV is a maximally entangled state; however, we use it to prove a more general result.

Consider two-mode squeezed coherent states, also referred to as Caves-Schumaker (CS) states, which are defined as a result of the action of the two-mode squeezing operator on a two-mode coherent state, i.e.

$$|\xi, \eta, \gamma\rangle\rangle = S_{ab}(\gamma)D_a(\xi)D_b(\eta)|0\rangle_{ab}. \tag{14.37}$$

It can be shown that, with an appropriate choice of parameters, this state coincides with a two-mode displaced squeezed vacuum, that is

$$|\xi, \eta, \gamma\rangle\rangle = |\bar{\xi}, \bar{\eta}, \gamma\rangle,$$

with

$$|\bar{\xi},\bar{\eta},\gamma\rangle = D_a(\bar{\xi})D_b(\bar{\eta})S_{ab}(\gamma)|0\rangle_{ab}. \tag{14.38}$$

The new parameters, $\bar{\xi}$ and $\bar{\eta}$, are related with the former ones by

$$\begin{pmatrix} \bar{\xi} \\ \bar{\eta}^* \end{pmatrix} = \mathcal{B}_B(\gamma) \begin{pmatrix} \xi \\ \eta^* \end{pmatrix}; \tag{14.39}$$

where $\mathcal{B}_B(\gamma)$ is the matrix form associated with $S_{ab}(\gamma)$ given by

$$\mathcal{B}_B(\gamma) = \begin{pmatrix} u(\gamma) & -v(\gamma) \\ -v(\gamma) & u(\gamma) \end{pmatrix}. \tag{14.40}$$

Note that, for $\xi = \eta = 0$, the CS state reduces to the TMSV, $|\gamma\rangle_{ab} = S_{ab}(\gamma)|0\rangle$. We explore these results to show that the state $|\xi,\eta,\gamma\rangle\rangle$ leads to a well-defined Gibbs-like density matrix.

To do so, we calculate the reduced density matrix, say $\rho_a = \mathrm{Tr}_b\rho_{ab}$, associated with the density operator describing the CS state, taking $\rho_{ab} = |\xi,\eta,\gamma\rangle\langle\gamma,\eta,\xi|$. Using the notation,

$$|r\rangle_b = \frac{1}{\sqrt{n!}}(b^\dagger)^r|0\rangle_b$$

(similarly for mode a) to represent the number states, we write the matrix elements of ρ_a as

$$\begin{aligned}\langle s|\rho_a|t\rangle &= \sum_r {}_a\langle s|_b\langle r|\rho_{ab}|r\rangle_b|t\rangle_a \\ &= \sum_{r,m,n} {}_a\langle s|D_a(\xi)\sqrt{f_a(\tau)}|n\rangle_{ab}\langle r|D_b(\eta)|n\rangle_b \\ &\quad \times {}_b\langle m|D_b(\eta)^\dagger|r\rangle_{ba}\langle m|\sqrt{f_a(\tau)}D_a(\xi)^\dagger|t\rangle_a.\end{aligned}$$

Changing the order of the matrix elements in the b mode, and using the completeness relation, we obtain

$$\langle s|\rho_a|t\rangle = \langle s|D_a(\xi)f_a(\tau)D_a(\xi)^\dagger|t\rangle.$$

Thus, we get

$$\rho_a = D_a(\xi)f_a(\tau)D_a^\dagger(\xi) = \frac{1}{Z(\tau)}\exp\left[-\tau a^\dagger(\xi)a(\xi)\right], \tag{14.41}$$

where

$$a(\xi) = D_a(\xi)aD_a^\dagger(\xi)$$

is the displaced annihilation operator of mode a. Therefore, ρ_a is a Gibbs-like density matrix. In particular, for $\xi = 0$, we find $\rho_a = f_a(\tau)$ showing that the TMSV, $|\gamma\rangle_{ab}$, also generates a Gibbs-like reduced density matrix.

Using the displaced Fock basis, $\{D_a(\xi)|n\rangle_a\}$, we show that the reduced von Neumann entropy for a CS state is

$$\mathcal{S}(\tau) = \frac{\tau}{e^\tau - 1} - \log\left(1 - e^{-\tau}\right). \tag{14.42}$$

Thus, all CS states, with the same (fixed) squeezing parameter, have the same amount of entanglement independent of the displacement parameters. Among them, the one having the smallest energy is the TMSV ($\xi = 0$); its reduced energy, $\mathcal{E}_a = \mathrm{Tr}(\rho_a a^\dagger a)$, is given by

$$\mathcal{E}(\tau) = \frac{1}{e^\tau - 1}.$$

Since both actions of displacing and squeezing the vacuum lead to states with greater energy, the TMSV is the maximum entangled state when the energy is fixed.

Let us now analyze comparatively the amount of entanglement of the TMSV. Consider the state

$$|\Psi\rangle_{ab}^{(N)} = \frac{1}{N}\sum_{n=0}^{N-1} |n\rangle_a |n\rangle_b$$

which has reduced energy and entropy given by

$$\mathcal{E}'(N) = (N-1)/2,$$
$$\mathcal{S}'(N) = \log N.$$

This state has the greatest amount of entanglement among all pure states belonging to the finite (N^2) dimensional subspace spanned by $\{|0\rangle_a |0\rangle_b, |0\rangle_a |1\rangle_b, \ldots, |N-1\rangle_a |N-1\rangle_b\}$, corresponding to equal occupation probability. Naturally, as $N \to \infty$, both energy and amount of entanglement of $|\Psi\rangle_{ab}^{(N)}$ goes to ∞.

Now, take another parametrization of the TMSV by writing

$$\tau = \log(\chi + 1) - \log(\chi - 1);$$

the limiting cases of zero and infinite squeezing correspond to $\chi = 1$ ($\gamma = 0,\ \tau = \infty$) and $\chi = \infty$ ($\gamma = \infty,\ \tau = 0$), respectively. The reduced energy and the amount of entanglement of the TMSV are then written as

$$\mathcal{E}(\chi) = \frac{\chi - 1}{2}$$
$$\mathcal{S}(\chi) = \frac{1}{2}\left[(\chi+1)\log(\chi+1) - (\chi-1)\log(\chi-1) - 2\log 2\right].$$

We find that both $\mathcal{E}(\chi)$ and $\mathcal{S}(\chi)$ go to ∞ as $\chi \to \infty$, with $\mathcal{S}(\chi) \sim \log\chi$ in this limit. In Fig. 14.1, we plot the difference between $\mathcal{S}(\chi)$ and $\log\chi$, showing explicitly that the TMSV has an amount of entanglement greater than that of the state $|\Psi\rangle_{ab}^{(N)}$ with the same energy, for all $N \geq 2$. This comparison emphasizes the fact that the maximum entanglement states, that we discussed, are under the energy constraint.

14.6 Coherent fermion states and density matrix operators

The experimental tools of laser cooling, magnetic and magneto-optic traps have advanced tremendously [219, 220]. This leads to the production of a degenerate

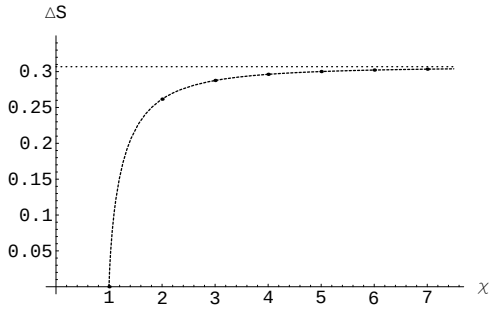


Fig. 14.1 Plot of $\Delta\mathcal{S} = \mathcal{S}(\chi) - \log\chi$ as a function of χ. The dots on the curve indicate the values of the difference $\mathcal{S}(N) - \mathcal{S}'(N)$.

Fermi gas as well as condensates of rare isotopes, a fact that has been achieved through the technique called sympathetic cooling [220]. Due to the nature of the Fermi gas, it is not possible to cool it to very low temperatures by itself. However, if it is mixed with a Bose condensate, then that would produce a degenerate Fermi gas, and recent experiments have pointed out such a possibility [221–224]. In fact such a gas has been employed to form Fermi molecular gas using the Feshbach resonances. These experiments have formed a ^6Li degenerate Fermi gas. Then by introducing a magnetic field and ramping it over the Feshbach resonances, molecular ($^6Li_2$) gas is formed. The probability of formation varies from $\sim 50\%$ to $\sim 80\%$, which is to be compared with the Boson case where the molecule formation probability is $\sim 100\%$. These results suggest that a careful study of the Fermi coherent state and Fermi density operators is needed. Some of these concepts have been introduced for fermion systems [225–227, 78]. Cahill and Glauber [228] have introduced P-function, Q-function and Wigner function for fermions; all of them are described as a counterpart of the bosonic systems and are made possible through the use of Grassmann variables.

A coherent fermion state [225, 226, 228] can be defined by introducing a displacement-like operator $D(\xi)$, where ξ is a Grassmann variable, trying to reproduce formally the basic results of the boson case. This is accomplished in the following way. Consider two Grassmann numbers ξ and η; as we discussed in Chapter 3 we have $\{\xi, \eta\} = \xi\eta + \eta\xi = 0$, and $\{\xi, a\} = \{\xi, a^\dagger\} = 0$, where the fermion operators a and $a^\dagger$ satisfy the anticommutation relation $\{a, a^\dagger\} = 1$. (In this section, without risk, we keep the same notation for the creation and annihilation operators as that for bosons.) The complex conjugation is taken as an antilinear mapping $* : \xi \to \xi^*$ such that, for a general expression involving Grassmann numbers and the operators a and $a^\dagger$, with $c \in \mathbb{C}$, we have

$$(\xi_i\xi_j^* + c\eta_i\eta_j)^* = \xi_j\xi_i^* + c^*\eta_j^*\eta_i^* ,$$
$$(a_i\xi_j a_k^\dagger\eta_l^*)^\dagger = (\eta_l^*\xi_j a_i a_k^\dagger)^\dagger = a_k a_i^\dagger\xi_j^*\eta_l .$$

The Grassmann variable ξ is considered independent of ξ^*.

The fermion displacement operator is defined by

$$D_a(\xi) = \exp(a^\dagger \xi - \xi^* a), \tag{14.43}$$

such that

$$D_a(\xi) a D_a^\dagger(\xi) = a - \xi,$$

with the coherent state given by

$$|\xi\rangle = D_a(\xi)|0\rangle_a,$$

such that $a|\xi\rangle = \xi|\xi\rangle$. Then we prove that the dual coherent state is given by $\langle\xi| = \langle 0|D_a^\dagger(\xi)$, with $D_a^\dagger(\xi) = D_a^{-1}(\xi)$. As a consequence

$$\langle\xi|\eta\rangle = \exp\left(\xi^*\eta - \frac{1}{2}\xi^*\xi - \frac{1}{2}\eta^*\eta\right)$$

and $\langle\xi|D_a^\dagger(\xi) = \langle\xi|\xi^*$. In terms of the number basis, the state $|\xi\rangle$ is written as

$$|\xi\rangle = e^{-\xi^*\xi/2}\sum_{n=0}^{1}(-\xi)^n|n\rangle \tag{14.44}$$

and, then, we have $\langle n|\xi\rangle = \exp(-\xi^*\xi/2)(\xi)^n$.

The integration is defined, as usual, by $\int d\xi = 0$ and $\int d\xi\xi = 1$. Note that, in particular, we have $\int d\xi^*\xi^* = 1$, resulting in $(d\xi)^* = -d\xi^*$, and

$$\int d\xi^* d\xi\, \xi\xi^* = 1\,,$$

$$\int d\xi^* d\xi\, |\xi\rangle\langle\xi| = \int d^2\xi\, |\xi\rangle\langle\xi| = 1$$

Cahill and Glauber [228] introduced the following coherent fermion state representation for a density operator, i.e.

$$\rho = \int d^2\xi\, P(\xi)\, |-\xi\rangle\langle\xi|,$$

where $P(\xi)$ is the corresponding P-function. Notice that the density operator

$$\rho_\xi = |-\xi\rangle\langle\xi|. \tag{14.45}$$

possesses the expected properties to be taken as representing the coherent state $|\xi\rangle$. First, it is normalized, $\mathrm{Tr}\rho_\xi = 1$. This property can be proved from the matrix representation of ρ_ξ, by calculating $\langle m|\rho_\xi|n\rangle = \exp(\xi\xi^*)(-\xi)^m(\xi^*)^n$, giving rise to

$$\rho_\xi = \begin{pmatrix} 1-\xi^*\xi & \xi^* \\ -\xi & \xi^*\xi \end{pmatrix}.$$

Secondly, $\mathrm{Tr}(\rho_\xi a^\dagger a) = \xi^*\xi$, which is similar to the boson case. Observe that ρ_ξ, although not being hermitian, is introduced in such way that $\rho^\dagger = \rho$ [228].

Using the properties described above, we can prove that the displaced fermion number state is given by

$$D_a(\xi)|n\rangle = (a^\dagger - \xi^*)^n|\xi\rangle,$$

with $n = 0, 1$. Another property useful for calculations but reflecting also the nature of ρ_ξ is given by

$$\langle m|\rho_\xi|n\rangle = (-1)^{m(n+1)}\langle\xi|n\rangle\langle m|\xi\rangle, \tag{14.46}$$

where $\langle m|\rho_\xi|n\rangle = \langle m|-\xi\rangle\langle\xi|n\rangle$. For $m = n$ we have $\langle n|-\xi\rangle\langle\xi|n\rangle = \langle\xi|n\rangle\langle n|\xi\rangle$. The usefulness of this result is apparent in proving that $\mathrm{Tr}\rho_\xi = 1$.

14.7 Entanglement of two-mode squeezed fermion states

Let us now consider a two-fermion system, specified by the operators a and b satisfying the algebra $\{a, a^\dagger\} = \{b, b^\dagger\} = 1$, with all other anti-commutation relations being zero. A fermionic two-mode squeezed vacuum state is defined by

$$|\gamma\rangle_{ab} = S_{ab}(\gamma)|0\rangle_{ab}, \tag{14.47}$$

where

$$S_{ab}(\gamma) = \exp[\gamma(a^\dagger b^\dagger - ab)]$$

and γ is taken as a real number, for simplicity. Similarly to the bosonic case, some useful formulas can be derived using $S_{ab}(\gamma)$:

$$a(\gamma) = S_{ab}(\gamma) a S^\dagger_{ab}(\gamma) = u(\gamma)a - v(\gamma)b^\dagger,$$
$$b(\gamma) = S_{ab}(\gamma) b S^\dagger_{ab}(\gamma) = u(\gamma)b + v(\gamma)a^\dagger,$$

and the corresponding ones for $a^\dagger(\gamma)$ and $b^\dagger(\gamma)$; now, however, $u(\gamma) = \cos(\gamma)$ and $v(\gamma) = \sin(\gamma)$. Thus, for the fermion two-mode squeezed vacuum state $|\gamma\rangle_{ab}$, we have $a(\gamma)|\gamma\rangle_{ab} = b(\gamma)|\gamma\rangle_{ab} = 0$, since $a|0\rangle_a = b|0\rangle_b = 0$.

The squeezing operator $S_{ab}(\gamma)$ is a canonical transformation, in the sense that, the anti-commutation relations are preserved,

$$\{a(\gamma), a(\gamma)^\dagger\} = \{b(\gamma), b(\gamma)^\dagger\} = 1\ ,\ \ \{a(\gamma), b(\gamma)\} = 0\,.$$

The matrix form $\mathcal{B}_F(\gamma)$ associated with $S_{ab}(\gamma)$ is

$$\mathcal{B}_F(\gamma) = \begin{pmatrix} u(\gamma) & v(\gamma) \\ -v(\gamma) & u(\gamma) \end{pmatrix}. \tag{14.48}$$

The vector $|\gamma\rangle_{ab}$ can be written as a TFD state. To see that let us write

$$|\gamma\rangle_{ab} = [1 - \gamma(ba - a^\dagger b^\dagger) + \frac{\gamma^2}{2!}(ba - a^\dagger b^\dagger)^2 + ...]|0\rangle_{ab}. \tag{14.49}$$

Using the property

$$(ba - a^\dagger b^\dagger)^{2n}|0\rangle_{ab} = (-1)^n|0\rangle_{ab}\,,$$

and introducing the following reparametrization

$$u(\gamma) = \cos\gamma = \frac{1}{\sqrt{1 + e^{-\tau}}}$$
$$v(\gamma) = \sin\gamma = \frac{1}{\sqrt{1 + e^{\tau}}},$$

we obtain

$$|\gamma\rangle_{ab} = \left(\cos\gamma + \sin\gamma\, a^\dagger b^\dagger\right)|0\rangle_{ab}$$
$$\frac{1}{\sqrt{1 + e^{-\tau}}}\,(1 + e^{-\tau/2} a^\dagger b^\dagger)|0\rangle_{ab}. \tag{14.50}$$

Defining $Z(\tau) = 1 + e^{-\tau}$, we get

$$|\gamma\rangle_{ab} = \frac{1}{\sqrt{Z(\tau)}}\, e^{-\tau N/2}\, (|0\rangle_a|0\rangle_b + |1\rangle_a|1\rangle_b)\,, \tag{14.51}$$

where $N = a^\dagger a$, the fermion number operator for the mode a, is such that $N|n\rangle_a = n|n\rangle_a$. Therefore, we obtain

$$|\gamma\rangle_{ab} = \sqrt{f_a(\tau)}\, \sum_{n=0}^{1} |n\rangle_a|n\rangle_b,$$

with

$$f_a(\tau) = \frac{1}{Z(\tau)}\, \exp(-\tau a^\dagger a).$$

With these results, we can prove the following statement. Given the two fermion displacement operators,

$$D_a(\xi) = \exp(a^\dagger \xi - \xi^* a),$$
$$D_b(\eta) = \exp(b^\dagger \eta - \eta^* b),$$

where ξ and η are Grassmann numbers, then

$$S_{ab}(\gamma) D_a(\xi) D_b(\eta) = D_a(\bar{\xi}) D_b(\bar{\eta}) S_{ab}(\gamma) \tag{14.52}$$

where

$$\begin{pmatrix} \bar{\xi} \\ \bar{\eta}^* \end{pmatrix} = \mathcal{B}_F(\gamma) \begin{pmatrix} \xi \\ \eta^* \end{pmatrix}. \tag{14.53}$$

Thus, the fermion version of the CS state, defined by

$$|\xi, \eta; \gamma\rangle\rangle_{ab} = S_{ab}(\gamma) D_a(\xi) D_b(\eta) |0\rangle_{ab},$$

is related to the state

$$|\xi, \eta; \gamma\rangle_{ab} = D_a(\xi) D_b(\eta) S_{ab}(\gamma) |0\rangle_{ab}$$

by the transformation given in Eqs. (14.52) and (14.53). As in the bosonic case, when $\xi = \eta = 0$ we have the two-fermion squeezed vacuum state $|\gamma\rangle_{ab} = S_{ab}(\gamma)|0\rangle_{ab}$.

Now we turn our attention to the nature of the entanglement in squeezed fermion states. Considering the states $|\xi, \eta; \gamma\rangle$ and inspired by the definition of the density operator given in Eq. (14.45), we introduce the following density matrix, associated with the CS state,

$$\rho_{ab} = |-\xi, -\eta, \gamma\rangle\langle\gamma, \eta, \xi|. \tag{14.54}$$

Performing the trace in the mode b and using the properties derived before, we can prove that

$$\rho_a = D_a(\xi) f_a(\tau) D_a(\xi)^\dagger,$$

similar to the boson case. Then we find that the state $|\xi, \eta, \gamma\rangle$ has reduced density operator in the form of a Gibbs-like density. The reduced entropy is thus maximal.

However, in the fermionic case, the CS states are not in general physical states [228] since they involve Grassmann variables. The two-fermion squeezed vacuum state $|\gamma\rangle_{ab}$, corresponding to the CS state with $\xi = \eta = 0$, is nevertheless physical and maximally entangled.

It is worth mentioning that, in the case of fermions, there is another class of physical states having maximum entanglement for a given value of the reduced energy. In fact, one can show that the state

$$|\gamma\rangle'_{ab} = \frac{1}{\sqrt{Z(\tau)}} \left(|0\rangle_a |1\rangle_b + e^{-\tau/2} |1\rangle_a |0\rangle_b \right) \tag{14.55}$$

has a reduced density operator, ρ'_a, identical to the reduced density operator ρ_a, associated with the state $|\gamma\rangle_{ab}$; therefore, these states have identical reduced energy and entropy to those of the two-fermion squeezed vacuum and are also maximally entangled states.

Summarizing, in this chapter we have analyzed some classes of two-mode boson and fermion states, looking for explicit realization of maximum entangled states with fixed energy. We have studied the case of squeezed two-mode boson states, and then, constructed the fermion version, to show that such states, in both cases, are maximum entangled. For achieving these results we have demonstrated some relations involving the squeezed boson states, which are then extended to the case of fermions. The calculations for fermions are performed with a generalization of the fermion density operator introduced by Cahill and Glauber [228].

PART IV

Compactified Fields

Chapter 15

Compactified Fields

Considering a topology of the type $\Gamma^d_D = \mathbb{S}^{1_1} \times ... \times \mathbb{S}^{1_d} \times \mathbb{R}^{D-d}$, fields compactified in space and time are studied. In the analysis, a Bogoliubov transformation is introduced which accounts simultaneously for spatial compactification and thermal effects. Such a Bogoliubov transformation provides a generalization of the thermofield dynamics [95–97, 106, 231]. In the same context the generalization of the Matsubara formalism is analyzed. For both cases the Feynman rules are stated and these results are the basic tool for applications discussed in the following chapters.

The formulation of the quantum field theory on curved space time is, for long, one of the most intricate and still not fully solved problem in physics. Its importance lies in the fact that several physical systems are described within such a formalism. In particular, we find the class of systems defined on flat spaces, with non-trivial topologies. This is the case of space-time considered as a simply or non-simply connected D-dimensional manifold with topology of type Γ^d_D. The topological structure of the space-time does not modify local field equations written in the Minkowski space. However, the topology imposes modifications on boundary conditions over fields and Green functions [232, 233]. The physical manifestation of this type of topology includes, for example, vacuum energy fluctuations, giving rise to the Casimir effect, or in phase transitions, the dependence of the critical temperature on the parameters of compactification. In the later case, there is, in the literature, an experimental interest in the analysis of the dependence of the critical temperature of superconductors on spatial boundaries such as films, wires and grains [234–236]. In the case of the Casimir effect, as was first analyzed [237], the vacuum fluctuations of the electromagnetic field confined between two conducting plates with separation L give rise to an attractive force between the plates. The effect has been applied to different geometries, fields and physical boundary conditions [238–241] with interest in different areas such as the confinement in particle physics and cosmological models.

In another context, this type of topology Γ^d_D emerges in quantum field theory at finite temperature, as we have pointed out in Chapter 8. In this case we have $\Gamma^1_4 = \mathbb{S}^1 \times \mathbb{R}^3$, where the dimension of compactification is the time axis, and the circumference $\mathbb{S}^1$ has length $\beta = 1/T$, where T is the temperature. The formal-

ism of the quantum field theory at finite temperature can be extended for space coordinates. One aspect still to be understood in this case is how to derive this prescription from a topological level, such that one can take into account boundary conditions other than those imposed by the KMS condition. This is one of the central aspects to be considered in the present chapter. For this a purpose, we start with purely topological elements and consider the ingredients of the imaginary time formalism and the thermofield dynamics to describe a quantum field theory in Γ_D^d. A physical consequence of such a procedure is that the compactification is interpreted as a process with condensation of the field in the vacuum.

15.1 Compactification and topology

Consider a D dimensional Minkowski space, as a simply or non-simply connected flat space-time, but with a topology Γ_D^d where d is the number of compactified dimensions. Taking initially the scalar field, the Green function satisfies the D-dimensional Klein-Gordon equation

$$(\Box + m^2)G(x;\beta) = \delta(x). \tag{15.1}$$

The topology Γ_D^d does not change the local properties of the system. This implies that locally the Minkowski space, as well as the differential equation describing the evolution of the system, are the same. However, the topology imposes modifications on boundary conditions to be fulfilled by the field and the respective Green function.

15.1.1 *Compactification of one space dimension*

To start we take $d = 1$ and $D = 4$, with $\mathbb{S}^1$ standing for the compactification in one spatial dimension, say x^1, and with the length of the circumference $\mathbb{S}^1$ being L_1. For this Γ_4^1 topology, the Green function satisfies the periodic boundary condition,

$$G(x^0, x^1, x^2, x^3) \equiv G(x^0, x^1 + L_1, x^2, x^3) = G(x + L_1 n_1), \tag{15.2}$$

where $n_1 = (n_1^\mu) = (0, 1, 0, 0)$ is a space-like vector. Note that $x^1 = 0$ is identified with $x^1 = L_1$ due to the topology, such that $0 \leq x^1 \leq L_1$; the other space-axis variables run in the interval $(-\infty, +\infty)$. A solution for Eq. (15.1), respecting Eq. (15.2), is obtained by analyzing the Fourier expansion of the Green function, resulting in

$$G(x - y; L_1) = \frac{1}{L_1} \sum_{n=-\infty}^{\infty} \frac{1}{(2\pi)^3} \int dp_0 dp_2 dp_3 e^{-ip_n(x-y)} G(p_n; L_1), \tag{15.3}$$

where

$$p_n = (p_0, p_{1n}, p_2, p_3), \quad p_{1n} = \frac{2\pi n}{L_1},$$

and

$$G(p_n; L_1) = \frac{-1}{p_n^2 - m^2}. \tag{15.4}$$

In addition, we write,

$$G(p_n; L_1) = \int_0^{L_1} dx^1 \int dx^0 dx^2 dx^3 e^{ip_n(x-y)} G(x-y; L_1). \tag{15.5}$$

This solution is useful to treat perturbative theories, as shown by Birrel and Ford [232]. However, it would be interesting to separate the divergent contribution of the flat space-time from terms describing the topological effect in the expression for $G(x-y; L_1)$. In this case, we can investigate and treat the divergent contributions arising from the free space-time, and analyze the limits as, for instance, $L_1 \to \infty$, resulting in a $3+1$ flat space-time, or $L_1 \to 0$, a $2+1$ flat space-time. This is accomplished here, following some adaptation of the Dolan and Jackiw calculations to separate the effect of temperature in the Green function for the scalar field [60]. The method is based on finding the Fourier transform (the integral Fourier representation) of $G(x-y; L_1)$.

We write $G(x-y; L_1)$ as

$$G(x-y; L_1) = \theta(x^1 - y^1) G^{>}(x-y; L_1) + \theta(y^1 - x^1) G^{<}(x-y; L_1). \tag{15.6}$$

From Eq. (15.2), we have

$$G^{<}(x; L_1) \mid_{x^1=0} = G^{>}(x; L_1) \mid_{x^1=L_1}. \tag{15.7}$$

Using this form, Eq.(15.5) reads

$$G(p_n; L_1) = \int_0^{L_1} dx^1 \int dx^0 dx^2 dx^3 e^{ip_n x} G^{>}(x; L_1). \tag{15.8}$$

The integral Fourier transform of $G(x-y; L_1)$, denoted by $\overline{G}(p; L_1)$, is

$$\overline{G}(p; L_1) = \overline{G}^{(1)}(p; L_1) + \overline{G}^{(2)}(p; L_1), \tag{15.9}$$

where

$$\overline{G}^{(1)}(p; L_1) = \int d^4x e^{ipx} \theta(x^1) G^{>}(x; L_1), \tag{15.10}$$

$$\overline{G}^{(2)}(p; L_1) = \int d^4x e^{ipx} \theta(-x^1) G^{<}(x; L_1). \tag{15.11}$$

Writing

$$G^{>}(x; L_1) = \int \frac{d^4p}{(2\pi)^4} e^{-ipx} \overline{G}^{>}(p; L_1) \tag{15.12}$$

and using the integral representation of the step function,

$$\int dk^1 \frac{e^{-ik^1 x^1}}{k^1 + p^1 + i\varepsilon} = (-2\pi i) e^{ip^1 x^1} \theta(x^1),$$

in Eq. (15.10), we derive

$$\overline{G}^{(1)}(p; L_1) = i \int \frac{dk^1}{2\pi} \frac{\overline{G}^{>}(p_0, k_1, p_2, p_3; L_1)}{k^1 - p^1 + i\varepsilon}. \tag{15.13}$$

With

$$G^{<}(x;L_1)=\int\frac{d^4p}{(2\pi)^4}e^{-ipx}\overline{G}^{<}(p;L_1),$$

and the integral representation of the step function,

$$\int dk^1\frac{e^{-ik^1x^1}}{k^1+p^1-i\varepsilon}=2\pi i e^{ip^1x^1}\theta(-x^1),$$

in Eq. (15.11.), we derive

$$\overline{G}^{(2)}(p;L_1)=-i\int\frac{dk^1}{2\pi}\frac{\overline{G}^{<}(p_0,k_1,p_2,p_3;L_1)}{k^1-p^1-i\varepsilon}. \tag{15.14}$$

Substituting Eqs. (15.13) and (15.14) in Eq. (15.9), we get

$$\overline{G}(p;L_1)=i\int\frac{dk^1}{2\pi}\left[\frac{\overline{G}^{>}(p_0,k_1,p_2,p_3;L_1)}{k^1-p^1+i\varepsilon}-\frac{\overline{G}^{<}(p_0,k_1,p_2,p_3;L_1)}{k^1-p^1-i\varepsilon}\right] \tag{15.15}$$

Now we show how the periodicity condition is written in momentum space. From Eq. (15.7) we have

$$\begin{aligned}G^{<}(x^0,x^1,x^2,x^3;L_1)&=G^{>}(x^0,x^1+L_1,x^2,x^3;L_1)\\&=e^{L_1\partial_1}G^{>}(x^0,x^1,x^2,x^3;L_1).\end{aligned}$$

Considering the Fourier transform of $G^{<}(x,L_1)$, we get

$$\begin{aligned}\overline{G}^{<}(p;L_1)&=\int d^4pe^{ipx}G^{<}(x;L_1)\\&=\int d^4pe^{ipx}e^{L_1\partial_1}G^{>}(x;L_1).\end{aligned}$$

Using Eq. (15.12) in this expression, we find

$$\overline{G}^{<}(p;L_1)=e^{iL_1p^1}\overline{G}^{>}(p;L_1). \tag{15.16}$$

Defining

$$f_{L_1}(p^1)=\frac{1}{e^{iL_1p^1}-1},$$

we write

$$\overline{G}^{>}(p;L_1)=f_{L_1}(p_1)A(p;L_1) \tag{15.17}$$

$$\overline{G}^{<}(p;L_1)=[f_{L_1}(p_1)+1]A(p;L_1), \tag{15.18}$$

that, using Eq. (15.16), gives

$$A(p;L_1)=\overline{G}^{<}(p;L_1)-\overline{G}^{>}(p;L_1).$$

With these results, Eq. (15.15) reads

$$\begin{aligned}\overline{G}(p;L_1)=i\int\frac{dk^1}{2\pi}\Bigg[&\frac{f_{L_1}(k^1)A(p_0,k_1,p_2,p_3;L_1)}{k^1-p^1+i\varepsilon}\\&-\frac{[f_{L_1}(k^1)+1]A(p_0,k_1,p_2,p_3;L_1)}{k^1-p^1-i\varepsilon}\Bigg].\end{aligned} \tag{15.19}$$

We do not have as yet an explicit expression for $A(p;L_1)$. To determine this function, we use the fact that we know $G(p_n;L_1)$, according to Eq. (15.4). Combining Eqs. (15.8) and (15.12) we have

$$G(p_n;L_1)=\int_0^{L_1}dx^1\int dx^0dx^2dx^3e^{p_nx}\int\frac{d^4k}{(2\pi)^4}e^{-ikx}\overline{G}^{>}(k;L_1).$$

Using Eq. (15.17) and the integral

$$\int_0^{L_1}dx^1e^{-i(p_n^1-k^1)x^1}=\frac{1}{f_{L_1}(k^1)}\frac{i}{p_n^1-k^1},$$

we obtain

$$G(p_n;L_1)=i\int\frac{dk^1}{2\pi}\frac{A(p_0,k_1,p_2,p_3;L_1)}{p_n^1-k^1},$$

where $A(p)$ is the spectral function associated with the momentum p^1.

We consider the analytic continuation of $G(p_n;L_1)$ to take p_n^1 to a continuum variable, p^1. The only possible analytical continuation of $G(p_n;L_1)$ without essential singularity at $p\to\infty$ is the function

$$\mathcal{G}_0(p)=i\int\frac{dk^1}{2\pi}\frac{A(p_0,k_1,p_2,p_3)}{p^1-k^1},$$

where, by definition,

$$\mathcal{G}_0(p)=\frac{-1}{p^2-m^2}. \tag{15.20}$$

Using this result, we calculate $A(p)$ by showing that

$$\begin{aligned}\mathcal{G}(p;\varepsilon)&=\mathcal{G}_0(p_0,p^1+i\varepsilon,p^2,p^3)-\mathcal{G}_0(p_0,p^1-i\varepsilon,p^2,p^3)\\&=i\int\frac{dk^1}{2\pi}A(p_0,k_1,p_2,p_3)\left[\frac{1}{p^1-k^1+i\varepsilon}-\frac{1}{p^1-k^1-i\varepsilon}\right]\\&=i\int\frac{dk^1}{2\pi}A(p_0,k_1,p_2,p_3)(-2\pi i)\delta(p^1-k^1).\end{aligned}$$

where we have used

$$\delta(x)=\lim_{\varepsilon\to0}\frac{1}{2\pi i}\left[\frac{1}{x-i\varepsilon}-\frac{1}{x+i\varepsilon}\right].$$

It results in

$$A(p)=\mathcal{G}_0(p_0,p^1+i\varepsilon,p^2,p^3)-\mathcal{G}_0(p_0,p^1-i\varepsilon,p^2,p^3)$$

describing a discontinuity of $\mathcal{G}_0(p)$ across the real axis p^1.

As $\mathcal{G}_0(p)$ is given in Eq. (15.20), we find the spectral function

$$\begin{aligned}A(p)=&\frac{-1}{(p^0)^2-(p^1+i\varepsilon)^2+(p^2)^2-(p^3)^2-m^2}\\&+\frac{1}{(p^0)^2-(p^1-i\varepsilon)^2+(p^2)^2-(p^3)^2-m^2},\end{aligned}$$

resulting in

$$A(p) = -2\pi i\delta(p^2 - m^2). \tag{15.21}$$

Then the spectral function ensures the mass-shell condition.

Using Eq. (15.21) and the identity

$$\delta(x^2 - y^2) = \frac{1}{2|y|}\left[\delta(x + y) + \delta(x - y)\right],$$

Eq. (15.19) reads

$$\overline{G}(p; L_1) = G_0(p) + v_B^2(p^1; L_1)[G_0(p) - G_0^*(p)],$$

where

$$G_0(p) = \frac{-1}{p^2 - m^2 + i\varepsilon}$$

and

$$v_B^2(p^1; L_1) = f_{L_1}(p^1) = \sum_{l=1}^{\infty} e^{-ilL_1p^1}.$$

The subscript B in $v_B^2(p^1, \beta)$ is to emphasize the boson nature of the field. As a final result we find

$$G(x - y; L_1) = \int \frac{d^4p}{(2\pi)^4} e^{-ip(x-y)}\{G_0(p) + v^2(p^1, L_1)[G_0(p) - G_0^*(p)]\}, \tag{15.22}$$

where

$$G_0(p) - G_0^*(p) = 2\pi i\delta(p^2 - m^2) = -A(p).$$

One basic and important result in this representation is that the content of the flat space is given in a separated term involving only $G_0(p)$, while the topological effect is present in the term with $v_B^2(p^1, L_1)$, describing the effect of compactification. This feature will play an important role in calculating Casimir effect.

15.1.2 *Compactification of time dimension*

In quantum field theory at finite temperature we have the KMS condition, that for boson operators, reads

$$\langle A_H(t)B_H(t')\rangle_\beta = \langle B_H(t')A_H(t + i\beta)\rangle_\beta.$$

An immediate consequence of the KMS condition is that the Green function is also periodic, i.e.

$$G(x - y; \beta) = G(x - y - i\beta n_0; \beta), \tag{15.23}$$

where n_0 is a time-like vector given by $(n_0^\mu) = (1, 0, 0, 0)$. With a Wick rotation, such that $t \to i\tau$, the KMS condition assures that $G(x - y, \beta)$ is a solution of the Euclidian Klein-Gordon equation with $\Box = -(\partial_\tau^2 + \nabla)$ under the periodic boundary condition, with period β.

As a result of the periodicity, the Fourier representation for $G(x,\beta)$ is written as

$$G(x-y;\beta)=\frac{1}{\beta}\sum_{n=-\infty}^{\infty}\int\frac{d^3p}{(2\pi)^3}\,\frac{e^{-ip_n(x-y)}}{p^2+m^2+i\varepsilon}, \tag{15.24}$$

with $p_n=(p_n^0,p^1,p^2,p^3)$, and $p_n^0=2\pi n/\beta$ being the Matsubara frequency. Therefore, the effect of temperature introduced by the Matsubara formalism corresponds to taking the $T=0$ Euclidian theory written in a topology $\mathbb{S}^1\times\mathbb{R}^3$, where the circumference $\mathbb{S}^1$ has perimeter β. This is the content of the KMS condition. Therefore, the integral Fourier representation of $G(x-y;\beta)$ is calculated following the same steps used for the compactification of one-space dimension, using the energy spectral function given by [60, 243]

$$A(p)=\mathcal{G}_0(p_0+i\varepsilon,\mathbf{p})-\mathcal{G}_0(p_0-i\varepsilon,\mathbf{p}).$$

The final result is

$$G(x-y;\beta)=\int\frac{d^4p}{(2\pi)^4}e^{-ip(x-y)}G_0(p;\beta), \tag{15.25}$$

where

$$\begin{aligned}G_0(p;\beta)&=G_0(p)+v_B^2(p_0;\beta)[G_0(p)-G_0^*(p)]\\&=G_0(p)+2\pi i v_B^2(p_0;\beta)\delta(p^2-m^2)\end{aligned} \tag{15.26}$$

and

$$v_B^2(p_0;\beta)=\sum_{n=1}^{\infty}e^{-n\beta|p_0|}=\frac{1}{e^{\beta|p_0|}-1}=n(\beta). \tag{15.27}$$

15.1.3 *Compactification of space and time*

We consider now the topology $\Gamma_4^2=\mathbb{S}^1\times\mathbb{S}^1\times\mathbb{R}^2$, treating a boson field in two compactified dimensions in the directions x^0 and x^1. This is equivalent to imposing on the Green function periodic boundary conditions along two directions. In the x^1-axis, the compactification is in a circumference of length L_1; and in the Euclidian x^0-axis, the compactification is in a circumference of length β. In this case, the series-integral Fourier expansion of the Green function is

$$\begin{aligned}G(x-y;\beta,L_1)=&\frac{1}{L_1}\sum_{l=-\infty}^{\infty}\frac{1}{\beta}\sum_{n=-\infty}^{\infty}\frac{1}{(2\pi)^2}\\&\times\int dp_2dp_3e^{-ip_{nl}(x-y)}G(p_{nl};\beta,L_1),\end{aligned} \tag{15.28}$$

where

$$p_{nl}=(p_n^0,p_l^1,p^2,p^3),$$

with

$$p_n^0=\frac{2\pi n}{\beta};\quad p_l^1=\frac{2\pi l}{L_1}$$

and

$$G(p_{nl};\beta,L_1)=\frac{-1}{p_{nl}^2-m^2}. \tag{15.29}$$

In order to find the integral Fourier representation of $G(x-y;\beta;L_1)$, we proceed by first treating the sum in l. We write Eq. (15.28) as

$$G(x-y;\beta,L_1)=\frac{1}{\beta}\sum_{n=-\infty}^{\infty}G_n(x-y;L_1), \tag{15.30}$$

where

$$G_n(x-y;L_1)=\frac{1}{(2\pi)^2}\frac{1}{L_1}\sum_{l=-\infty}^{\infty}\int dp_2dp_3e^{-ip_{nl}(x-y)}G(p_{nl};L_1).$$

Therefore, following the same steps as for the case of $G(x-y;L_1)$, we obtain

$$G_n(x-y;L_1)=\frac{1}{(2\pi)^3}\int dp_1dp_2dp_3e^{-ip_n(x-y)}\overline{G}(p_n,L_1),$$

where

$$\overline{G}(p_n,L_1)=\ G_0(p_n)+v_B^2(p^1,L_1)[G_0(p_n)-G_0^*(p_n)]\ .$$

Using this result in Eq. (15.30), and following the steps for the case of time confinement, we derive

$$\begin{aligned}G(x-y;\beta,L_1)=\int\frac{d^4p}{(2\pi)^4}e^{-ip(x-y)}\{&\overline{G}(p;L_1)\\&+v_B^2(p_0;\beta)[\overline{G}(p;L_1)-\overline{G}^*(p;L_1)]\},\end{aligned}$$

that can be written as

$$\begin{aligned}G(x-y;\beta,L_1)=\int\frac{d^4p}{(2\pi)^4}e^{-ip(x-y)}\{&G_0(p)\\&+v_B^2(p_0,p_1;\beta,L_1)[G_0(p)-G_0^*(p)]\},\end{aligned}$$

where

$$v_B^2(k_0,k_1;\beta,L_1)=v_B^2(p_0;\beta)+v_B^2(p_1;L_1)+2v_B^2(p_0;\beta)v_B^2(p_1;L_1), \tag{15.31}$$

Observe that

$$\begin{aligned}v_B^2(k_0;\beta)&=\lim_{L_1\to\infty}v_B^2(k_0,k_1;\beta,L_1),\\v_B^2(k_1;L_1)&=\lim_{\beta\to\infty}v_B^2(k_0,k_1;\beta,L_1).\end{aligned}$$

The same procedure can be carried out for fermion fields. In this case, we impose anti-periodic boundary conditions for fields and Green functions. Physically, these conditions mean that, for the time axis, we reproduce the KMS boundary conditions, and so the compactification describes the temperature. For the space components, anti-periodicity for fermions is equivalent to the bag-model boundary conditions,

stating that fermion currents do not cross the bag boundary. This condition is convenient to treat phenomenological or effective models for quark confinement.

Taking the topology $\mathbb{S}^1 \times \mathbb{S}^1 \times \mathbb{R}^2$, the result after compactifications is

$$S(x-y;\beta,L_1) = \int \frac{d^4p}{(2\pi)^4} e^{-ip(x-y)} \{S_0(p) + v_F^2(p_0,p_1;\beta,L_1)[S_0(p) - S_0^*(p)]\},$$

where

$$v_F^2(p_0,p_1;\beta,L_1) = v_F^2(p_0;\beta) + v_F^2(p_1;L_1) + 2v_F^2(p_0;\beta)v_F^2(p_1;L_1), \tag{15.32}$$

with $v_F^2(p_0;\beta)$ and $v_F^2(p_1;L_1)$ given by

$$v_F^2(p_0;\beta) = \sum_{l_0=1}^{\infty} (-1)^{l_0+1} e^{-l_0\beta p_0} = \frac{1}{1+e^{\beta p_0}}$$

$$v_F^2(p_1;L_1) = \sum_{l_1=1}^{\infty} (-1)^{l_1+1} e^{-il_1 L_1 p^1}.$$

Again it is important to note that

$$v_F^2(p_0;\beta) = \lim_{L_1\to\infty} v_F^2(p_0,p_1;\beta,L_1),$$
$$v_F^2(p_1;L_1) = \lim_{\beta\to\infty} v_F^2(p_0,p_1;\beta,L_1).$$

Explicitly we have

$$v^2(p_0,p_1;\beta,L_1) = \sum_{l_0=1}^{\infty} (-1)^{l_0+1} e^{-\beta p_0 l_0} + \sum_{l_1=1}^{\infty} (-1)^{l_1+1} e^{-iL_1 p^1 l_1} + 2 \sum_{l_0,l_1=1}^{\infty} (-1)^{l_0+l_1+2} e^{-\beta p_0 l_0 - iL_1 p^1 l_1}. \tag{15.33}$$

15.1.4 *Compactification in d-dimensions*

The results derived for bosons and fermions in two compactified dimensions can be generalized to a D-dimensional manifold and the topology $\Gamma_D^d = \mathbb{S}^{1_1} \times ... \times \mathbb{S}^{1_d} \times \mathbb{R}^{D-d}$. To treat this general case, we distinguish the time variable and take $d = 1 + N$, N being the number of compactified space coordinates. Then writing $\alpha = (\alpha_0, \alpha_1, \alpha_2, ..., \alpha_N)$, for the set of compactification parameters, and $k_{(\alpha)} = (k_0, ..., k_N)$, we obtain

$$v_\xi^2(k_{(\alpha)};\alpha) = \sum_{s=1}^{N+1} \sum_{\{\sigma_s\}} \left(\prod_{n=1}^{s} f(\alpha_{\sigma_n}) \right) 2^{s-1} \times \sum_{l_{\sigma_1},...,l_{\sigma_s}=1}^{\infty} (-\xi)^{s+\sum_{r=1}^{s} l_{\sigma_r}} \exp\{-\sum_{j=1}^{s} \alpha_{\sigma_j} l_{\sigma_j} k_{\sigma_j}\}, \tag{15.34}$$

where $f(\alpha_j) = 0$ for $\alpha_j = 0$, $f(\alpha_j) = 1$ otherwise and $\{\sigma_s\}$ denotes the set of all combinations with s elements, $\{\sigma_1, \sigma_2, ...\sigma_s\}$, of the first $N+1$ natural numbers $\{0, 1, 2, ..., N\}$, that is all subsets containing s elements, which we choose to write in an ordered form, $\sigma_1 < \sigma_2 < \cdots < \sigma_s$. Here $v_\xi^2(k_{(\alpha)}, \alpha)$ stands for both boson ($\xi = -1$) and fermion ($\xi = +1$) fields.

The Green function for bosons and fermions are, respectively, given by

$$G(x-y;\alpha) = \int \frac{d^4k}{(2\pi)^4} e^{-ik(x-y)} \{G_0(k) + v_B^2(k_\alpha;\alpha)[G_0(k) - G_0^*(k)]\}, \tag{15.35}$$

and

$$S(x-y;\alpha) = \int \frac{d^4k}{(2\pi)^4} e^{-ik(x-y)} \{S_0(k) + v_F^2(k_\alpha;\alpha)[S_0(k) - S_0^*(k)]\}. \tag{15.36}$$

Since there is no risk of confusion, we are using the notation:

$$v_-^2(k_{(\alpha)};\alpha) = v_B^2(k_\alpha;\alpha),$$
$$v_+^2(k_{(\alpha)};\alpha) = v_F^2(k_\alpha;\alpha).$$

These results are similar to the case of the TFD propagator. This points to the way to construct a field theory in a topology Γ_D^d.

15.2 Generalized Bogoliubov transformation

Since the structure of $G(x-y;\alpha)$ is similar to the propagator in quantum field theory for bosons at finite temperature, we use $v_B(k_\alpha;\alpha)$ to introduce a Bogoliubov transformation following the algebraic rules of TFD. Define $u(k_\alpha;\alpha)$ by

$$u^2(k_\alpha;\alpha) - v^2(k_\alpha;\alpha) = 1,$$

and

$$B(k_\alpha;\alpha) = \begin{pmatrix} u(k_\alpha;\alpha) & -v(k_\alpha;\alpha) \\ -v(k_\alpha;\alpha) & u(k_\alpha;\alpha) \end{pmatrix}. \tag{15.37}$$

We have dropped the subscript of B for simplicity. We write a doubled Green function as

$$G_0^{ab}(x-y;\alpha) = \int \frac{d^4k}{(2\pi)^4} e^{-ik(x-y)}\ G_0^{ab}(k;\alpha), \tag{15.38}$$

where

$$G_0^{ab}(k;\alpha) = B^{(ac)}(k_\alpha;\alpha) G_0^{(cd)}(k) B^{\dagger(db)}(k_\alpha;\alpha),$$

with

$$\left(G_0^{(cd)}(k)\right) = \begin{pmatrix} G_0(k) & 0 \\ 0 & -G_0^*(k) \end{pmatrix}.$$

In terms of components we have

$$G_0^{11}(k;\alpha) = G_0(k) + \ v^2(k_\alpha;\alpha)[G_0(k) - G_0^*(k)], \tag{15.39}$$

$$G_0^{12}(k;\alpha) = G_0^{21}(k;\alpha) = \ v(k_\alpha;\alpha)u(k_\alpha;\alpha)[G_0(k) - G_0^*(k)], \tag{15.40}$$

$$G_0^{22}(k;\alpha) = -G_0^*(k) - v^2(k_\alpha;\alpha)[G_0(k) - G_0^*(k)]. \tag{15.41}$$

This Green function is a generalization of the TFD Green function, since here $v^2(k_\alpha,\alpha)$ describes space and time compactification. Therefore the doubled structure of TFD is used to introduce the canonical form of $G_0^{ab}(x-y;\alpha)$ in terms of quantum fields. The doubling is defined by the tilde conjugations rules.

In order to introduce the unitary transformation equivalent to the matrix B, a new parametrization is defined in terms of the parameter $\theta(k_\alpha;\alpha)$ as

$$u(k_\alpha;\alpha) = \cosh\theta(k_\alpha;\alpha),$$
$$v(k_\alpha;\alpha) = \sinh\theta(k_\alpha;\alpha).$$

Using $\theta(k_\alpha;\alpha)$, the Bogoliubov transformation applied to all modes is written in the form

$$\begin{aligned} U(\alpha) &= \exp\left\{\sum_k \theta(k_\alpha;\alpha)[a^\dagger(k)\tilde{a}^\dagger(k) - a(k)\tilde{a}(k)]\right\} \\ &= \prod_k U(k;\alpha), \end{aligned} \tag{15.42}$$

where

$$U(k_\alpha;\alpha) = \exp\{\theta(k_\alpha;\alpha)[a^\dagger(k)\tilde{a}^\dagger(k) - a(k)\tilde{a}(k)]\}.$$

The k in the sum and the product of the above equation is to be taken in the continuum limit. Since $U(\alpha)$ has the same form as in the case of standard TFD, all results derived for fields follow along the same lines. We show here only some results, in order to emphasize the d-compactification and that there is no need of Gibbs ensemble in the analysis.

Using the boson creation and annihilation operators, $a^\dagger(k)$ and $a(k)$, we introduce the α-operators by

$$\begin{aligned} a(k;\alpha) &= U(k_\alpha;\alpha)a(k)U^{-1}(k_\alpha;\alpha) \\ &= u(k_\alpha;\alpha)a(k) - v(k_\alpha;\alpha)\,\tilde{a}^\dagger(k). \end{aligned}$$

The inverse is

$$a(k) = u(k_\alpha;\alpha)a(k;\alpha) + v(k_\alpha;\alpha)\,\tilde{a}^\dagger(k;\alpha),$$

such that the other operators $a^\dagger(k), \tilde{a}(k)$ and $\tilde{a}^\dagger(k)$ can be obtained by applying the hermitian or the tilde conjugation rules. Commutation relations for modes read,

$$[a(k;\alpha), a^\dagger(k';\alpha)] = (2\pi)^3 2k_0\delta(\mathbf{k}-\mathbf{k}'), \tag{15.43}$$

$$[\tilde{a}(k;\alpha), \tilde{a}^\dagger(k';\alpha)] = (2\pi)^3 2k_0\delta(\mathbf{k}-\mathbf{k}'), \tag{15.44}$$

with all other commutation relations being zero.

The Hilbert space is constructed from the α-vacuum, $|0(\alpha)\rangle = U(\alpha)|0,\tilde{0}\rangle$, where $|0,\tilde{0}\rangle = \bigotimes_k |0,\tilde{0}\rangle_k$ and $|0,\tilde{0}\rangle_k$ is the vacuum for the mode k. The α-vacuum is such that

$$a(k;\alpha)|0(\alpha)\rangle = \tilde{a}(k;\alpha)|0(\alpha)\rangle = 0$$

and $\langle 0(\alpha)|0(\alpha)\rangle = 1$. The basis vectors are given in the form

$$[a^\dagger(k_1;\alpha)]^{m_1}\cdots[a^\dagger(k_M;\alpha)]^{m_M}[\tilde{a}^\dagger(k_1;\alpha)]^{n_1}\cdots[\tilde{a}^\dagger(k_N;\alpha)]^{n_N}|0(\alpha)\rangle, \tag{15.45}$$

where $n_i, m_j = 0, 1, 2, ...$, with N and M being indices for an arbitrary mode.

Considering one mode for simplicity, we write $|0(\alpha)\rangle$ in terms of $u(\alpha)$ and $v(\alpha)$,

$$\begin{aligned}|0(\alpha)\rangle &= \frac{1}{u(\alpha)}\exp[\frac{v(\alpha)}{u(\alpha)}a^\dagger\tilde{a}^\dagger]|0,\tilde{0}\rangle \\ &= \frac{1}{u(\alpha)}\sum_n\left(\frac{v(\alpha)}{u(\alpha)}\right)^n|n,\tilde{n}\rangle.\end{aligned} \tag{15.46}$$

Defining

$$\rho_{nn}^{1/2} = \frac{1}{u(\alpha)}\left(\frac{v(\alpha)}{u(\alpha)}\right)^n,$$

we write

$$|0(\alpha)\rangle = \sum_n \rho_{nn}^{1/2}|n,\tilde{n}\rangle,$$

which is, for arbitrary compactification, the counterpart of TFD. As a consequence, the average of an observable A, a non-tilde operator, is given by

$$\langle 0(\alpha)|A|0(\alpha)\rangle = \sum_n \rho_{nn}A_{nn} = Tr(\rho A),$$

where the matrix ρ is

$$\rho = \frac{1}{u^2(\alpha)}\left(\frac{v(\alpha)}{u(\alpha)}\right)^{2a^\dagger a}.$$

Notice that this result is a generalization of TFD in the sense that if we consider, as an example, $\mathbb{S}^1\times\mathbb{R}^3$, compactified in the time axis, then $\rho = e^{-\beta H}/Z$, where H is the Hamiltonian for the free boson system and $Z(\beta) = u^2(\beta)$. In the next section we use the Bogoliubov transformation in order to introduce α-dependent fields.

15.3 Field theory

We define for bosons

$$\begin{aligned}\phi(x;\alpha) &= U(\alpha)\phi(x)U^{-1}(\alpha), \\ \widetilde{\phi}(x;\alpha) &= U(\alpha)\widetilde{\phi}(x)U^{-1}(\alpha).\end{aligned}$$

Using a Bogoliubov transformation for each of the infinite modes, we have

$$\phi(x;\alpha) = \int \frac{d^3k}{(2\pi)^3}\frac{1}{2k_0}\,[a(k;\alpha)e^{-ikx} + a^\dagger(k;\alpha)e^{ikx}]$$

and

$$\widetilde{\phi}(x;\alpha) = \int \frac{d^3k}{(2\pi)^3}\frac{1}{2k_0}\,[\tilde{a}(k;\alpha)e^{ikx} + \tilde{a}^\dagger(k;\alpha)e^{-ikx}].$$

Let us calculate the propagator, using the α-vacuum. The α-propagator for real scalar field, as calculated in the last section, is given by

$$G(x-y;\alpha) = -i\langle 0(\alpha)|T[\phi(x)\phi(y)]|0(\alpha)\rangle. \tag{15.47}$$

Following standard TFD calculations, we obtain

$$G(x-y;\alpha) = \int \frac{d^4k}{(2\pi)^4}e^{-ik(x-y)}G(k;\alpha), \tag{15.48}$$

where

$$G(k;\alpha) = G_0(k) + v^2(k_\alpha;\alpha)[G_0(k) - G_0^*(k)], \tag{15.49}$$

as in Eq. (15.35).

We can also show that $G(x-y;\alpha)$ can be calculated by using the α-field operators, that is,

$$G(x-y;\alpha) = -i\langle\tilde{0},0|T[\phi(x,\alpha)\phi(y,\alpha)]|0,\tilde{0}\rangle.$$

This is a motivation to write this field theory in terms of α-field operators; that is, the Lagrangian density for the Klein-Gordon field giving rise to the α-propagator is

$$\widehat{\mathcal{L}} = \mathcal{L} - \widetilde{\mathcal{L}} = \frac{1}{2}\partial_\mu\phi(x;\alpha)\partial^\mu\phi(x;\alpha) - \frac{1}{2}m^2\phi^2(x;\alpha)$$
$$-\frac{1}{2}\partial_\mu\widetilde{\phi}(x;\alpha)\partial^\mu\widetilde{\phi}(x;\alpha) + \frac{1}{2}m^2\widetilde{\phi}^2(x;\alpha).$$

Similar structures can be introduced for the compactification of fermion fields. In this case, the Lagrangian density of the Dirac field is

$$\widehat{\mathcal{L}} = \frac{1}{2}\overline{\psi}(x;\alpha)[\gamma\cdot i\overleftrightarrow{\partial} - m]\psi(x;\alpha)$$
$$-\frac{1}{2}\widetilde{\overline{\psi}}(x;\alpha)[-\gamma^*\cdot i\overleftrightarrow{\partial} - m]\widetilde{\psi}(x;\alpha),$$

where $\gamma^* = (\gamma^T)^\dagger$. In this expression, the fields $\psi(x;\alpha)$ and $\widetilde{\overline{\psi}}(x;\alpha)$ are expanded in modes by

$$\psi(x;\alpha) = \int \frac{d^3k}{(2\pi)^3}\frac{m}{k_0}\sum_{\zeta=1}^{2}[b_\zeta(k_\alpha;\alpha)u^{(\zeta)}(k)e^{-ikx} + d_\zeta^\dagger(k_\alpha;\alpha)v^{(\zeta)}(k)e^{ikx}],$$

$$\widetilde{\overline{\psi}}(x;\alpha) = \int \frac{d^3k}{(2\pi)^3}\frac{m}{k_0}\sum_{\zeta=1}^{2}[\tilde{b}_\zeta^\dagger(k_\alpha;\alpha)\overline{u}^{*(\zeta)}(k)e^{-ikx} + \tilde{d}_\zeta(k_\alpha;\alpha)\overline{v}^{*(\zeta)}(k)e^{ikx}].$$

As a consequence of anti-commutation relations for these fields, we obtain

$$\{b_\zeta(k_\alpha;\alpha),b^\dagger_\varkappa(k'_\alpha;\alpha)\} = \{d_\zeta(k_\alpha;\alpha),d^\dagger_\varkappa(k'_\alpha;\alpha)\} = (2\pi)^3\frac{k_0}{m}\delta(\mathbf{k}-\mathbf{k}')\delta_{\zeta\varkappa},$$
$$\{\tilde{b}_\zeta(k_\alpha;\alpha),\tilde{b}^\dagger_\varkappa(k'_\alpha;\alpha)\} = \{\tilde{d}_\zeta(k_\alpha;\alpha),\tilde{d}^\dagger_\varkappa(k'_\alpha;\alpha)\} = (2\pi)^3\frac{k_0}{m}\delta(\mathbf{k}-\mathbf{k}')\delta_{\zeta\varkappa}.$$

with all other anti-commutation relations being zero.

The Bogoliubov transformation is

$$\begin{aligned} U(\alpha) &= \exp\sum_k\{\theta_b(k_\alpha;\alpha)[b^\dagger(k)\tilde{b}^\dagger(k) - b(k)\tilde{b}(k)] \\ &\quad +\theta_d(k_\alpha;\alpha)[d^\dagger(k)\tilde{d}^\dagger(k) - d(k)\tilde{d}(k)]\} \\ &= \prod_k U_b(k_\alpha;\alpha)U_d(k_\alpha;\alpha), \end{aligned}$$

with

$$U_b(k;\alpha) = \exp\{\theta_b(k_\alpha;\alpha)[b^\dagger(k)\tilde{b}^\dagger(k) - b(k)\tilde{b}(k)]\},$$
$$U_d(k;\alpha) = \exp\{\theta_d(k_\alpha;\alpha)[d^\dagger(k)\tilde{d}^\dagger(k) - d(k)\tilde{d}(k)]\},$$

where θ_b and θ_d are defined by

$$\cos\theta_b(k_\alpha;\alpha) = v_b(k_\alpha;\alpha),$$
$$\cos\theta_d(k_\alpha;\alpha) = v_d(k_\alpha;\alpha),$$

while $v_b(k_\alpha;\alpha)$ and $v_d(k_\alpha;\alpha)$ are given in Eq. (15.34), with $\xi = +1$. In the case of the compactification of the time axis, we have

$$v_b^2(k_0;\beta) = \frac{1}{e^{\beta(w_k-\mu_b)}+1},$$
$$v_d^2(k_0;\beta) = \frac{1}{e^{\beta(w_k+\mu_d)}+1},$$

μ_b and μ_d being the chemical potentials for particles and anti-particles, respectively, and $v_b(k;\beta)$ and $v_d(k;\beta)$ fulfilling the relations: $v_b^2(k;\beta)+u_b^2(k;\beta)=1$ and $v_d^2(k;\beta)+u_d^2(k;\beta)=1$. The Bogoliubov transformation in the form of 2×2 matrix for particles (b) and anti-particles (d) is

$$B_{b,d}(k_\alpha;\alpha) = \begin{pmatrix} u_{b,d}(k_\alpha;\alpha) & v_{b,d}(k_\alpha;\alpha) \\ -v_{b,d}(k_\alpha;\alpha) & u_{b,d}(k_\alpha;\alpha)\end{pmatrix}. \tag{15.50}$$

The Hilbert space is built from the α-vacuum, $|0(\alpha)\rangle = U(\alpha)|0,\tilde{0}\rangle$, where

$$|0,\tilde{0}\rangle = \bigotimes_k |0,\tilde{0}\rangle_k$$

and $|0,\tilde{0}\rangle_k$ is the vacuum for the mode k considering particles and anti-particles. The α-vacuum is such that

$$b(k_\alpha;\alpha)|0(\alpha)\rangle = \tilde{b}(k_\alpha;\alpha)|0(\alpha)\rangle = 0,$$
$$d(k_\alpha;\alpha)|0(\alpha)\rangle = \tilde{d}(k_\alpha;\alpha)|0(\alpha)\rangle = 0,$$

and $\langle 0(\alpha)|0(\alpha)\rangle = 1$. Basis vectors are given in the form

$$[b^\dagger(k_{1\alpha};\alpha)]^{n1}\cdots[d^\dagger(k_{M\alpha};\alpha)]^{n_M}[\tilde{b}^\dagger(k_{1\alpha};\alpha)]^{n_1}\cdots[\tilde{d}^\dagger(k_{N\alpha};\alpha)]^{n_N}|0(\alpha)\rangle,$$

where now $n_i, m_i = 0, 1$.

The fermion α-operators are written in terms of non α-operators by

$$\begin{aligned} b(k_\alpha;\alpha) &= U(\alpha)b(k)U^{-1}(\alpha) = U(k,\alpha)b(k)U^{-1}(k,\alpha) \\ &= u_b(k_\alpha;\alpha)b(k) - v_b(k_\alpha;\alpha)\tilde{b}^\dagger(k), \\ d(k;\alpha) &= U(\alpha)d(k)U^{-1}(\alpha) = U(k_\alpha;\alpha)d(k)U^{-1}(k_\alpha;\alpha) \\ &= u_d(k_\alpha;\alpha)d(k) - v_d(k_\alpha;\alpha)\tilde{d}^\dagger(k). \end{aligned}$$

The inverse formulas are

$$\begin{aligned} b(k) &= u_b(k_\alpha;\alpha)b(k_\alpha;\alpha) + v_b(k_\alpha;\alpha)\tilde{b}^\dagger(k_\alpha;\alpha), \\ d(k) &= u_d(k_\alpha;\alpha)d(k_\alpha;\alpha) + v_d(k_\alpha;\alpha)\tilde{d}^\dagger(k_\alpha;\alpha). \end{aligned}$$

Here each operator, b or d, carries a spin index that is suppressed.

The α-Green function for the Dirac field is defined by

$$S(x-y;\alpha) = -i\langle 0(\alpha)|T[\psi(x)\overline{\psi}(y)]|0(\alpha)\rangle, \tag{15.51}$$

resulting in Eq. (15.36).

15.4 Feynman rules

We have presented a formalism to consider the quantum field theory in a flat manifold with topology $(\mathbb{S}^1)^d \times \mathbb{R}^{D-d}$, such that the fields and the Green functions fulfill periodic (bosons) or antiperiodic(fermions) boundary conditions. The result of the topological analysis is a generalization of thermofield dynamics and the Matsubara formalism. Let us collect the main results, emphasizing the Feynman rules.

(i) *α-fields*

In this case we have the generalization of TFD but using the same algebraic methods. That is the Hilbert space of TFD, $\mathcal{H}_T$, is denoted by $\mathcal{H}_\alpha$ to emphasize that we have a generalized (α-dependent) Bogoliubov transformation acting on the doubled Hilbert space $\mathcal{H}\otimes\widetilde{\mathcal{H}}$, giving rise to a theory of compactified field in a topology $(\mathbb{S}^1)^d \times \mathbb{R}^{D-d}$. Interacting fields in TFD theory are described by exploring the algebraic properties of the Bogoliubov transformation. Hence for α-fields the perturbative theory is the same as for TFD. Considering the $(1,1)$-component for the generating function, the diagrams are the same as for the $\alpha = 0$ (flat space) theory. The Feynman rules are defined by taking the $\alpha = 0$ (flat space) theory and substituting the α-dependent n-point functions. For the Klein-Gordon field, for instance, the Feynman rules in momentum space are obtained by the substitution

$$G_0(p) \to G_0(p;\alpha).$$

(ii) *Generalized Matsubara formalism*
In the case of the imaginary-time (Matsubara) formalism, the perturbative theory is the same as for the $\alpha = 0$ (flat space) theory. The Feynman rules in the momentum space are modified by taking, for each compactified dimension, the integrals in momentum space replaced by sums as

$$\int dp^i \to \frac{1}{L_i} \sum_{l_i=-\infty}^{\infty}$$

with

$$p_i \to p_{l_i} = \frac{2\pi l_i}{L_i},$$

for bosons, and

$$p_i \to p_{l_i} = \frac{2\pi (l_i + \frac{1}{2})}{L_i},$$

for fermions.

In the above rules, i runs over the compactified dimensions.

Finally it is important to clarify the meaning of the Bogoliubov transformation. Since it is used to define the α-vacuum, $|0(\alpha)\rangle$, this state can be interpreted as a condensate for the observable operators. This is the case since $a|0(\alpha)\rangle \neq 0$. In this language, the $a(\alpha)$ and $a^\dagger(\alpha)$ are the annihilation and creation operators of quasi-particles. The pair that gives rise to the quasi-particles are the operator a and $\tilde{a}$, since, for instance in the case of bosons we have $a(\alpha) = u(\alpha)a - v(\alpha)\tilde{a}^\dagger$. In terms of these quasi-particles, the field operator $\phi(x;\alpha)$ leads to the Green function $G(x-y;\alpha) = -i\langle \tilde{0}, 0|T[\phi(x,\alpha)\phi(y,\alpha)]|0,\tilde{0}\rangle$. As a consequence, the effect of compactification in the topology Γ_D^d is described by a process of condensation of the field in vacuum.

In the following chapters, we use this approach to study the Casimir effect, superconducting systems in compactified space dimensions and the Gross-Neveu model. In these applications, the effect of space as well as time compactification plays a dominant role.

Chapter 16

Casimir Effect for the Electromagnetic Field

The Casimir effect [237] was discovered while studying vacuum fluctuations of the electromagnetic field confined between two conductor plates with separation a, defined by the Dirichlet boundary conditions. The effect was an attractive force between the plates given by the negative pressure $P = -\pi^2/240a^4$. It has been generalized to different fields defined in space-time manifolds with non-trivial topologies and geometries [238–242, 244–263, 98, 264–266]. The Casimir force was measured with a precision of few percents [251, 267, 268] only at the end of 1990's; raising interest, in particular, in the context of microelectronics and nanotechnologies as a practical tool for switching devices [269]. The Casimir force is strictly a quantum effect, in fact an effect from the vacuum, that has manifestation at the level of mesoscopic systems.

The effect of temperature was first studied by Lifshitz [270, 271] who presented an alternative derivation for the Casimir force, including an analysis of the dielectric material between the plates. Actually, the effect of temperature on the interaction between the conducting parallel plates may be significant for separations greater than $3\mu m$ [272]. Brown and Maclay [273] treated the effect of temperature using the imaginary time-formalism and the image-method, deriving expressions for the energy-momentum tensor for the electromagnetic field. As a result the Casimir effect appears from the propagator by summing an infinite set of images [241, 273].

In this chapter we address the Casimir effect using the method of compactified fields based on the generalized Bogoliubov transformation. Two points are worth emphasizing. The calculations are carried out in a covariant way presenting the propagator with a separation of the flat space contribution and the effect of compactification. For practical purposes, these aspects are interesting when associated with the renormalization scheme. As a physical consequence, due to the Bogoliubov transformation, the Casimir effect is interpreted as a vacuum condensation effect of the electromagnetic field. For convenience the presentation is carried out in the canonical formalism.

16.1 The vacuum state of the electromagnetic field

The Lagrangian density for the free electromagnetic field is

$$\mathcal{L} = -\frac{1}{4} F^{\mu\nu} F_{\ \mu\nu},$$

where

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu.$$

The vector potential, A_μ, satisfies the equation

$$(g^{\mu\nu}\Box - \partial^\mu \partial\nu) A_\nu(x) = 0.$$

Let us discuss briefly the quantization of the electromagnetic field in the canonical formalism, using the Coulomb gauge.

The momentum conjugate to A_ν is

$$\pi^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_0 A_\mu)},$$

resulting in $\pi^0 = 0$ and $\pi^i = \partial^0 A^i - \partial^i A^0$. We can get consistency working in the Coulomb gauge, with $A^0 = 0$ and $\nabla \cdot \mathbf{A} = 0$; imposing a constraint among the three components of $\mathbf{A}$. It follows that $\pi = \partial^0 \mathbf{A}$ and the equation of motion reads $\Box A_\nu(x) = 0$. In this gauge, as we do not keep the Lorentz covariance, it is convenient to take the Fourier series of $\mathbf{A}$ and π , that is

$$\mathbf{A}(\mathbf{x}, t) = \frac{1}{V} \sum_{\mathbf{k},\lambda} e^{i\mathbf{k}\cdot\mathbf{x}} \epsilon_{\mathbf{k}}^{(\lambda)} q_{\mathbf{k}}^{(\lambda)}(t),$$

where $\epsilon_{\mathbf{k}}^{(\lambda)}$ are three unit vectors. The 3-momentum density is then

$$\pi(\mathbf{x}, t) = \frac{1}{V} \sum_{\mathbf{k},\lambda} e^{i\mathbf{k}\cdot\mathbf{x}} \epsilon_{\mathbf{k}}^{(\lambda)} p_{\mathbf{k}}^{(\lambda)}(t),$$

where $p_{\mathbf{k}}^{(\lambda)}(t) = \partial^0 q_{\mathbf{k}}^{(\lambda)}(t)$. The Hermicity of the field implies that

$$\epsilon_{-\mathbf{k}}^{(\lambda)} q_{-\mathbf{k}}^{(\lambda)}(t) = \epsilon_{\mathbf{k}}^{(\lambda)} q_{\mathbf{k}}^{(\lambda)\dagger}(t), \quad \epsilon_{\mathbf{k}}^{(\lambda)} p_{-\mathbf{k}}^{(\lambda)}(t) = \epsilon_{-\mathbf{k}}^{(\lambda)} p_{\mathbf{k}}^{(\lambda)\dagger}(t).$$

The vectors $\epsilon_{\mathbf{k}}^{(\lambda)}$ are assumed to form an orthonormal basis, that is, $\epsilon_{\mathbf{k}}^{(\lambda)} \cdot \epsilon_{\mathbf{k}}^{(\lambda')} = \delta_{\lambda\lambda'}$, and due to the gauge, $\epsilon_{\mathbf{k}}^{(\lambda)} \cdot \mathbf{k} = 0$. We specify the notation for the index λ in the relations above, by defining:

$$\epsilon_{\mathbf{k}}^{(\lambda)}, \lambda = 1, 2; \quad \epsilon_{\mathbf{k}}^{(3)} = \frac{\mathbf{k}}{|\mathbf{k}|},$$

where $\epsilon_{\mathbf{k}}^{(3)}$ is the longitudinal direction for the propagation of $\mathbf{A}(\mathbf{x}, t)$. Therefore, $\mathbf{A}(\mathbf{x}, t)$ is in the plane defined by the two *polarization vectors*, $\epsilon_{\mathbf{k}}^{(1)}$ and $\epsilon_{\mathbf{k}}^{(2)}$. This is the *polarization plane*, which is perpendicular to the propagation direction $\epsilon_{\mathbf{k}}^{(3)}$.

Keeping in mind these results, the non-null commutation relations are defined by

$$[A_i(\mathbf{x},t),\pi_j(\mathbf{x}',t)] = i[\delta_{ij} - \frac{1}{\nabla^2}\partial_i\partial_j]\delta(\mathbf{x}-\mathbf{x}'). \tag{16.1}$$

The second term in this relation ensures that there is no photon with longitudinal polarization. In terms of $q_{\mathbf{k}}^{(\lambda)}(t)$ and $p_{\mathbf{k}}^{(\lambda)}(t)$, the non-null commutation relations read

$$[q_{\mathbf{k}}^{(\lambda)}(t), p_{\mathbf{k}'}^{(\lambda')}(t)] = i\delta_{\lambda\lambda'}\delta_{\mathbf{k},\mathbf{k}'}. \tag{16.2}$$

With these operators, the energy of the electromagnetic field is written as

$$\begin{aligned} H &= \frac{1}{2}\int_V d^3x(\pi^2 + \mathbf{A}\cdot\nabla^2\mathbf{A}) \\ &= \frac{1}{2}\sum_{\mathbf{k},\lambda}\left(p_{\mathbf{k}}^{(\lambda)\dagger}p_{\mathbf{k}}^{(\lambda)} + \omega_k^2 q_{\mathbf{k}}^{(\lambda)\dagger}q_{\mathbf{k}}^{(\lambda)}\right), \end{aligned}$$

where we have used $\omega_k^2 = \mathbf{k}^2$. The Hamiltonian describes a collection of quantum oscillators. Then we introduce the operator

$$a_{\mathbf{k}}^{(\lambda)} = \sqrt{\frac{1}{2}\omega_k}\left(q_{\mathbf{k}}^{(\lambda)} + \frac{i}{\omega_k}p_{\mathbf{k}'}^{(\lambda')\dagger}\right).$$

From Eq. (16.2) we derive

$$[a_{\mathbf{k}}^{(\lambda)}, a_{\mathbf{k}'}^{(\lambda')\dagger}] = \delta_{\lambda\lambda'}\delta_{\mathbf{k},\mathbf{k}'},$$

showing that $a_{\mathbf{k}}^{(\lambda)}(t)$ and $a_{\mathbf{k}'}^{(\lambda)\dagger}$ are the annihilation and the creation operators of photons with momentum $\mathbf{k}$ and polarization λ.

The Hamiltonian reads

$$H = \sum_{\mathbf{k},\lambda}\omega_k(n_k^\lambda + \frac{1}{2}), \tag{16.3}$$

where $n_k^\lambda = a_{\mathbf{k}}^{(\lambda)\dagger}a_{\mathbf{k}}^{(\lambda)}$ is the number operator. In this expression, the term independent of n_k^λ,

$$H_{vac} = \sum_{\mathbf{k}}\omega_k,$$

corresponds to the energy of the fundamental state, being called the *vacuum energy* (observe that we have summed over the two polarization states). When the theory is formulated in the flat, without boundary, space-time, this energy provides an infinite contribution to the average of H in the vacuum state. In this case, as proved by Takahashi [274] for massive particles, the term H_{vac} is subtracted out by imposition of the Lorentz symmetry; then we perform the normal ordering. The same procedure is assumed valid for non-massive particles, as is the case of photons. The physical consequence is that, in flat space-time, the vacuum state energy is zero, as a consequence of symmetry. The situation is more involved, however, with

non-trivial space-times, considering boundary conditions, non-trivial geometries or topologies, etc. In this case, the Takahashi theorem does not work anymore. Since the back-ground manifold for the theory has changed, there are implications in the energy spectrum, resulting in particular, to modifications in the ground state. The analysis of this change is possible if we compare the non-trivial case with the field in the flat-space time. For instance, we can calculate the difference of energy in both cases. The result is measurable, at least for the electromagnetic field, and is called the *Casimir effect*. We develop this analysis starting with the energy-momentum tensor for the electromagnetic field considering the field in the topology Γ^d_D.

For the electromagnetic field, the energy-momentum tensor operator is

$$T^{\mu\lambda}(x) = -F^{\mu\alpha}(x)F^{\lambda}{}_{\alpha}(x) + \frac{1}{4}g^{\mu\lambda}F_{\beta\alpha}(x)F^{\alpha\beta}(x).$$

In order to get physical quantities, we have to calculate the expectation value of the operator $T^{\mu\lambda}$ in the vacuum state. This is not possible due to the product of field operators at the same point on the space-time. However, it is accomplished by relating the vacuum average of $T^{\mu\lambda}(x)$ to the Green function. For that we split the operator $T^{\mu\lambda}$ as

$$\begin{aligned} T^{\mu\lambda}(x) &= \lim_{x\to x'} T\left[-F^{\mu\nu}(x)F^{\lambda}{}_{\nu}(x') + \frac{1}{4}g^{\mu\lambda}F^{\nu\rho}(x)F_{\nu\rho}(x')\right] \\ &= \lim_{x\to x'}\left[-\mathcal{F}^{\mu\nu,\lambda}{}_{\nu}(x,x') + \frac{1}{4}g^{\mu\lambda}\mathcal{F}^{\nu\rho,}{}_{\nu\rho}(x,x')\right], \end{aligned} \tag{16.4}$$

where T is the time order operator and

$$\begin{aligned} \mathcal{F}^{\mu\nu,\lambda\rho}(x,x') &= T[F^{\mu\nu}(x)F^{\lambda\rho}(x')] \\ &= F^{\mu\nu}(x)F^{\lambda\rho}(x')\theta(x_0 - x'_0) + F^{\lambda\rho}(x')F^{\mu\nu}(x)\theta(x'_0 - x_0). \end{aligned}$$

Consider

$$\partial^{\mu}\theta(x_0 - x'_0) = n_0^{\mu}\delta(x_0 - x'_0),$$

where n_0^{μ} is the μ-component of the time-like vector $n_0 = (1,0,0,0)$, and the commutation relation, Eq. (16.1), to calculate $\mathcal{F}^{\mu\nu,\lambda\rho}(x,x')$. The result is

$$\begin{aligned} \mathcal{F}^{\mu\nu,\lambda\rho}(x,x') = \Gamma^{\mu\nu,\lambda\rho,\alpha\beta}(x,x')T[A_{\alpha}(x),A_{\beta}(x')] \\ -n_0^{\mu}\delta(x_0 - x'_0)I^{\nu,\lambda\rho}(x,x') \\ +n_0^{\nu}\delta(x_0 - x'_0)I^{\mu,\lambda\rho}(x,x'), \end{aligned}$$

where

$$\Gamma^{\mu\nu,\lambda\rho,\alpha\beta}(x,x') = (g^{\nu\alpha}\partial^{\mu} - g^{\mu\alpha}\partial^{\nu})(g^{\rho\beta}\partial'^{\lambda} - g^{\lambda\beta}\partial'^{\rho})$$

and

$$\begin{aligned} I^{\mu,\lambda\nu}(x,x') &= [A^{\mu}(x), F^{\lambda\nu}(x')] \\ &= [A^{\mu}(x), \partial'^{\lambda}A^{\nu}(x')] - [A^{\mu}(x), \partial'^{\nu}A^{\lambda}(x')] \\ &= in_0^{\nu}(g^{\mu\lambda} + \nabla^{-2}\partial^{\mu}\partial^{\lambda})\delta(\mathbf{x} - \mathbf{x}') \\ &\quad -in_0^{\lambda}(g^{\mu\nu} + \nabla^{-2}\partial^{\mu}\partial^{\nu})\delta(\mathbf{x} - \mathbf{x}'). \end{aligned}$$

Using Eq. (16.4), we obtain

$$T^{\mu\lambda}(x) = -\lim_{x\to x'}\{\Delta^{\mu\nu,\alpha\beta}(x,x')T[A_\alpha(x),A_\beta(x')] + 2i(n_0^\mu n_0^\lambda - \frac{1}{4}g^{\mu\nu})\delta(x-x'), \tag{16.5}$$

where

$$\Delta^{\mu\nu,\alpha\beta} = \Gamma^{\mu\nu,\lambda}{}_{\nu}{}^{,\alpha\beta} - \frac{1}{4}g^{\mu\lambda}\Gamma^{\nu\rho,}{}_{\nu\rho}{}^{,\alpha\beta}.$$

The vacuum expectation value of $T^{\mu\lambda}(x)$ is

$$\langle T^{\mu\nu}(x)\rangle = \langle 0|T^{\mu\nu}(x)|0\rangle = -i\lim_{x\to x'}\{\Gamma^{\mu\nu}(x,x')G_0(x-x') + 2(\eta^\mu\eta^\nu - \frac{1}{4}g^{\mu\nu})\delta(x-x')\},$$

where

$$\Gamma^{\mu\nu}(x,x') = \Gamma^{\mu\nu,}{}_{\rho\lambda}{}^{,\rho\lambda} = 2(\partial^\mu\partial'^\nu - \frac{1}{4}g^{\mu\nu}\partial^\rho\partial'_\rho).$$

We have used

$$iD_{\alpha\beta}(x-x') = \langle 0|T[A_\alpha(x)A_\beta(x)]|0\rangle = g_{\alpha\beta}G_0(x-x'),$$

with

$$G_0(x-x') = \frac{1}{4\pi^2 i}\frac{1}{(x-x')^2 - i\varepsilon}.$$

The interaction of the electromagnetic field with matter is described in some cases by imposing boundary conditions on the fields. For example, in the case of matter being a perfect conducting wall, the boundary conditions over the fields are

$$n^\nu F^*_{\mu\nu} = 0\,, \tag{16.6}$$

where $F^*_{\mu\nu} = \epsilon_{\mu\nu\alpha\beta}F^{\alpha\beta}$ is the dual of $F_{\mu\nu}$ and n^ν is a space-like vector orthogonal to the plane of the wall. This is equivalent to stating that $\mathbf{n}\cdot\mathbf{B} = 0$ and $\mathbf{n}\times\mathbf{E} = 0$, where $\mathbf{B}$ and $\mathbf{E}$ are the magnetic and electric fields, respectively. Otherwise, for permeable walls, the boundary conditions are

$$n^\nu F_{\mu\nu} = 0; \tag{16.7}$$

which, in terms of the electric and the magnetic fields, read $\mathbf{n}\cdot\mathbf{E} = 0$ and $\mathbf{n}\times\mathbf{B} = 0$.

We now turn our attention to calculate the energy-momentum tensor for α-dependent fields. Following the tilde conjugation rules, the doubled operator describing the energy-momentum tensor of the electromagnetic field is [275]

$$T^{\mu\lambda(ab)}(x) = -F^{\mu\alpha(ab)}(x)F^{\lambda(ab)}_{\alpha}(x) + \frac{1}{4}g^{\mu\lambda}F^{(ab)}_{\beta\alpha}(x)F^{\alpha\beta(ab)}(x), \tag{16.8}$$

where the indices $a, b = 1, 2$ are defined according to the doubled notation, and

$$F^{(ab)}_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^b_\mu.$$

The doubled free photon propagator is given by

$$\begin{aligned} iD^{(ab)}_{\alpha\beta}(x-x') &= \langle 0,\widetilde{0}|T[A^a_\alpha(x)A^b_\beta(x)]|0,\widetilde{0}\rangle \\ &= g_{\alpha\beta}G^{(ab)}_0(x-x'), \end{aligned} \tag{16.9}$$

where the non-zero components of $G^{(ab)}_0(x-x')$ are

$$G^{(ab)}_0(x-x') = \frac{1}{(2\pi)^4}\int d^4k\, e^{ik(x-x')}G^{(ab)}_0(k),$$

with

$$\left(G^{(ab)}_0(k)\right) = \begin{pmatrix} G_0(k) & 0 \\ 0 & -G^*_0(k) \end{pmatrix} = \begin{pmatrix} \frac{-1}{k^2+i\epsilon} & 0 \\ 0 & \frac{1}{k^2-i\epsilon} \end{pmatrix}.$$

In the configuration space, we have

$$\left(G^{(ab)}_0(x-x')\right) = \begin{pmatrix} G_0(x-x') & 0 \\ 0 & -G^*_0(x-x') \end{pmatrix}.$$

The vacuum average of the energy-momentum tensor

$$\langle T^{\mu\nu(ab)}\rangle = \langle 0,\widetilde{0}|T^{\mu\nu(ab)}|0,\widetilde{0}\rangle$$

reads

$$\begin{aligned} \langle T^{\mu\nu(ab)}\rangle = -i\lim_{x\to x'}\{&\Gamma^{\mu\nu}(x,x')G^{(ab)}_0(x-x') \\ &+2(n^\mu_0 n^\nu_0 - \frac{1}{4}g^{\mu\nu})\delta(x-x')\delta^{ab}\}. \end{aligned}$$

In terms of the α-dependent fields, we introduce the tensor

$$\begin{aligned} \langle T^{\mu\lambda(ab)}(x;\alpha)\rangle &= \langle 0,\widetilde{0}|T^{\mu\lambda(ab)}(x;\alpha)|0,\widetilde{0}\rangle \\ &= \langle 0(\alpha)|T^{\mu\lambda(ab)}(x)|0(\alpha)\rangle, \end{aligned}$$

which is given by

$$\begin{aligned} \langle T^{\mu\lambda(ab)}(x;\alpha)\rangle = -i\lim_{x\to x'}\{&\Gamma^{\mu\lambda}(x,x')G^{(ab)}(x-x';\alpha) \\ &+2(n^\mu_0 n^\lambda_0 - \frac{1}{4}g^{\mu\lambda})\delta(x-x')\delta^{ab}\}. \end{aligned}$$

In order to estimate the effect of the topology, characterized by the set of parameters α, we denote, with some regularization procedure, a finite energy-momentum tensor

$$\mathcal{T}^{\mu\lambda(ab)}(x;\alpha) = \langle T^{\mu\lambda(ab)}(x;\alpha)\rangle - \langle T^{\mu\lambda(ab)}(x)\rangle. \tag{16.10}$$

This is the central definition here and describes a renormalization procedure to obtain a finite expression describing measurable physical quantities. Explicitly we have

$$\mathcal{T}^{\mu\lambda(ab)}(x;\alpha) = -i\lim_{x\to x'}\{\Gamma^{\mu\lambda}(x,x')\overline{G}^{(ab)}(x-x';\alpha)\}, \tag{16.11}$$

where

$$\overline{G}^{(ab)}(x-x';\alpha) = G^{(ab)}(x-x';\alpha) - G^{(ab)}_0(x-x').$$

In the Fourier representation we get

$$G^{(ab)}(x-x';\alpha) = \frac{1}{(2\pi)^4}\int d^4k\, e^{ik(x-x')}G^{(ab)}(k;\alpha),$$

where

$$G^{(ab)}(k;\alpha) = B_k^{-1(ac)}(\alpha)G_0^{(cd)}(k)B_k^{(db)}(\alpha);$$

the components of $G_0^{(ab)}(k;\alpha)$ are

$$\overline{G}^{(11)}(k;\alpha) = \overline{G}^{(22)}(k;\alpha) = v_k^2(\alpha)[G_0(k) - G_0^*(k)],$$
$$\overline{G}^{(12)}(k;\alpha) = G^{(21)}(k;\alpha) = v_B(k,\alpha)[1+v_B^2(k,\alpha)]^{1/2}[G_0^*(k) - G_0(k)].$$

The generalized Bogoliubov transformation is

$$v^2(k_\alpha;\alpha) = \sum_{s=1}^{N+1} 2^{s-1}\sum_{\{\sigma_s\}}\left(\prod_{n=1}^{s} f(\alpha_{\sigma_n})\right) \times \sum_{l_{\sigma_1},\ldots,l_{\sigma_s}=1}^{\infty} \exp\{-\sum_{j=1}^{s}\alpha_{\sigma_j}l_{\sigma_j}k_{\sigma_j}\}, \tag{16.12}$$

where $\alpha = (\alpha_0,\alpha_1,\alpha_2,...,\alpha_N)$. We denote, without risk of confusion, $v_k^2(\alpha) = v^2(k_\alpha;\alpha)$. This leads to the general case of $(N+1)$-dimensions, considering $v_k^2(\alpha)$, we obtain

$$\overline{G}_0^{11}(x-x';\alpha) = \lim_{x'\to x}\sum_{s=1}^{N+1} 2^{s-1}\sum_{\{\sigma_s\}}\left(\prod_{n=1}^{s} f(\alpha_{\sigma_n})\right)\sum_{l_{\sigma_1},\ldots,l_{\sigma_s}=1}^{\infty} \times\Bigg[G_0^*(x'-x-i\sum_{j=1}^{s}\eta_{\sigma_j}\alpha_{\sigma_j}l_{\sigma_j}n_{\sigma_j}) - G_0(x-x'-i\sum_{j=1}^{s}\eta_{\sigma_j}\alpha_{\sigma_j}l_{\sigma_j}n_{\sigma_j})\Bigg], \tag{16.13}$$

where $\eta_{\sigma_j} = +1$, if $\sigma_j = 0$, and $\eta_{\sigma_j} = -1$ for $\sigma_j = 1,2,...,N$. To get the physical case of finite temperature and spatial confinement, α_0 has to be taken as a positive real number while α_n, for $n = 1,2,...,N$, must be pure imaginary of the form iL_n; in these cases, one finds that $\alpha_j^{*2} = \alpha_j^2$.

As a basic application, let us calculate the Stefan-Boltzmann radiation formula, by taking the (3+1)-Minkowski space, and one compactified dimension. The thermal effects appears by taking $\alpha = (\beta,0,0,0)$, such that

$$v_k^2(\beta) = \sum_{l=1}^{\infty} e^{-\beta k_0 l}\,. \tag{16.14}$$

As $\overline{G}^{11}(x-x';\beta) = G_0^{11}(x-x';\beta) - G_0(x-x')$, we have

$$\begin{aligned}\overline{G}^{(11)}(x-x';\beta) &= \frac{1}{(2\pi)^4}\int d^4k\, e^{ik(x-x')}G^{(11)}(k;\beta)\\ &= \frac{1}{(2\pi)^4}\int d^4k\, e^{ik(x-x')}\sum_{j=1}^{\infty} e^{\beta j k_0}[G_0(k)-G_0^*(k)]\\ &= 2\sum_{j=1}^{\infty} G_0(x-x'-i\beta j n_0).\end{aligned}$$

The average of the energy-momentum tensor operator at finite temperature in the vacuum is

$$\begin{aligned}\langle T^{\mu\nu(ab)}(x;\beta)\rangle &= \langle 0,\tilde{0}|T^{\mu\nu(ab)}(x;\beta)|0,\tilde{0}\rangle\\ &= -i\lim_{x\to x'}\{\Gamma^{\mu\nu}(x,x')G^{(ab)}(x-x';\beta)\\ &\quad +2(n_0^\mu n_0^\nu - \frac{1}{4}g^{\mu\nu})\delta(x-x')\delta^{ab}\}.\end{aligned}$$

This leads to

$$\begin{aligned}\mathcal{T}^{\mu\nu(11)}(\beta) &= -i\left\{\Gamma^{\mu\nu}(x,x')\overline{G}^{11}(x-x';\beta)\right\}\Big|_{x\to x'}\\ &= -\frac{2}{\pi^2}\sum_{l=1}^{\infty}\frac{g^{\mu\nu}-4n_0^\mu n_0^\nu}{(\beta l)^4} = \frac{-\pi^2}{45\beta^4}(g^{\mu\nu}-4n_0^\mu n_0^\nu)\,, \qquad (16.15)\end{aligned}$$

where we have used the Riemann zeta function $\zeta(4) = \sum_{l=1}^{\infty} l^{-4} = \pi^4/90$. As expected,

$$E(T) = \mathcal{T}^{00(11)}(\beta) = \frac{1}{15}\pi^2 T^4,$$

which gives the correct energy-density of the photon gas at temperature T, the Stefan-Boltzmann law.

In the more general situation of 4-dimensional space-time (corresponding to $N=3$), using the explicit form of $\overline{G}_0^{11}(x-x';\alpha)$, we obtain the renormalized α-dependent energy-momentum tensor

$$\begin{aligned}\mathcal{T}^{\mu\nu(11)}(\alpha) &= -i\lim_{x\to x'}\left\{\Gamma^{\mu\nu}(x,x')\overline{G}_0^{11}(x-x';\alpha)\right\}\\ &= -\frac{2}{\pi^2}\sum_{s=1}^{4}2^{s-1}\sum_{\{\sigma_s\}}\left(\prod_{n=1}^{s}f(\alpha_{\sigma_n})\right)\\ &\quad\times\sum_{l_{\sigma_1},\ldots,l_{\sigma_s}=1}^{\infty}\left[\frac{g^{\mu\nu}}{[\sum_{j=1}^{s}\eta_{\sigma_j}(\alpha_{\sigma_j}l_{\sigma_j})^2]^2}\right.\\ &\quad\left.-\frac{2\sum_{j,r=1}^{s}(1+\eta_{\sigma_j}\eta_{\sigma_r})(\alpha_{\sigma_j}l_{\sigma_j})(\alpha_{\sigma_r}l_{\sigma_r})n_{\sigma_j}^\mu n_{\sigma_r}^\nu}{[\sum_{j=1}^{s}\eta_{\sigma_j}(\alpha_{\sigma_j}l_{\sigma_j})^2]^3}\right]. \qquad (16.16)\end{aligned}$$

In the following we analyze the space and the time compactifications.

16.2 The Casimir effect

In this section we derive the Casimir effect at zero and non-zero temperature. We proceed with the same prescription for the energy-momentum tensor but with a proper definition of the parameter α for different options.

16.2.1 *Casimir effect at zero temperature*

Taking $\alpha = (0, 0, 0, iL)$, corresponding to confinement along the z-axis, we have

$$v_k^2(L) = \sum_{l=1}^{\infty} e^{-iLk_3 l} \,. \tag{16.17}$$

Using this v_k^2, and $\overline{G}_0^{11}(x - x'; L) = G_0^{11}(x - x'; L) - G_0(x - x')$, we get

$$\overline{G}_0^{11}(x - x'; L) = \sum_{l=1}^{\infty} [G_0^*(x' - x - Lln_3) - G_0(x - x' - Lln_3)] \tag{16.18}$$

where $n_3 = (n_3^\mu) = (0, 0, 0, 1)$. For this case, we obtain

$$\mathcal{T}^{\mu\nu(11)}(L) = -\frac{2}{\pi^2} \sum_{l=1}^{\infty} \frac{g^{\mu\nu} + 4n_3^\mu n_3^\nu}{(Ll)^4} = -\frac{\pi^2}{45L^4}(g^{\mu\nu} + 4n_3^\mu n_3^\nu), \tag{16.19}$$

The Casimir energy and pressure for the electromagnetic field under periodic boundary conditions are, respectively,

$$E(L) = \mathcal{T}^{00(11)}(L) = -\frac{\pi^2}{45L^4} \,,$$
$$P(L) = \mathcal{T}^{33(11)}(L) = -\frac{\pi^2}{15L^4} \,.$$

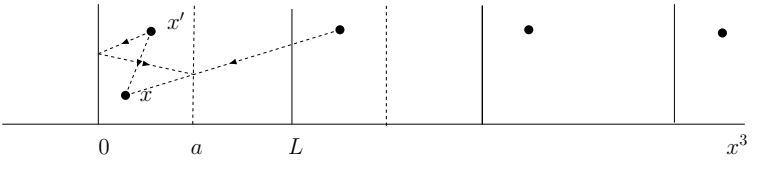


Fig. 16.1 Periodicity in x^3, with period L, and images for the electromagnetic field between two plates separated by a distance $a = L/2$. The images correspond to an even number of reflections on the walls.

These expressions correspond to the Casimir effect for the electromagnetic field in the topology $\Gamma_4^1 = \mathbb{S}^1 \times \mathbb{R}^3$ where $\mathbb{S}^1$ correspond to the compactification of x^3-axis in a circumference of length L. However, if we take $L = 2a$ in the Green functions that we have used, this corresponds to the contribution of even images used by Brown and Maclay to calculate the Casimir effect [273]. The even images are defined by the even number of reflections of the electromagnetic field in a region limited

by two conducting plates separated by a distance a; that is, the field propagates from x' to x reflecting on the walls an even number of times. These even images correspond also to a periodic function with period $L = 2a$, as it is shown in Fig. 16.1 Brown and Maclay proved that the odd images, i.e. the images generated by an odd number of reflections, do not contribute to the energy-momentum tensor. Notice that, with L we have an equivalent Stefan-Boltzmann law in the direction x^3, i.e. we have a symmetry by the change $L = 2a \leftrightarrow \beta$, basically as a result of the topology $\mathbb{S}^1$, where the theory is written for each case. This symmetry has been analyzed in different ways [260–263]. The basic observation is that when we consider symmetric boundary conditions on the two plates, these imply periodicity in the direction x^3, normal to the plates, with period $L = 2a$. The fields move unconstrained in the two transverse directions, obeying the symmetry $L = 2a \leftrightarrow \beta$. Using then $L = 2a$, the Casimir energy and pressure for the electromagnetic field between two parallel conducting plates, separated by a distance a, is

$$E(a) = \mathcal{T}^{00(11)}(a) = -\frac{\pi^2}{720a^4}\ ,$$
$$P(a) = \mathcal{T}^{33(11)}(a) = -\frac{\pi^2}{240a^4}\ .$$

The negative sign shows that the Casimir force between the plates is attractive.

16.2.2 *Casimir effect at non-zero temperature*

Assume that the electromagnetic field satisfies Dirichlet boundary conditions on parallel planes, corresponding to conducting plates, normal to the x^3-direction, at finite temperature. This case corresponds to the choice $\alpha = (\beta, 0, 0, i2a)$, resulting in

$$\mathcal{T}^{\mu\nu(11)}(\beta, a) = -\frac{2}{\pi^2}\left\{\sum_{l_0=1}^{\infty}\frac{g^{\mu\nu} - 4n_0^\mu n_0^\nu}{(\beta l_0)^4} + \sum_{l_3=1}^{\infty}\frac{g^{\mu\nu} + 4n_3^\mu n_3^\nu}{(2al_3)^4}\right.$$
$$\left. + 4\sum_{l_0,l_3=1}^{\infty}\frac{(\beta l_0)^2[g^{\mu\nu} - 4n_0^\mu n_0^\nu] + (2Ll_3)^2[g^{\mu\nu} + 4n_3^\mu n_3^\nu]}{[(\beta l_0)^2 + (2al_3)^2]^3}\right\}.$$

The Casimir energy ($\mathcal{T}^{00(11)}$) and pressure ($\mathcal{T}^{33(11)}$) are given respectively by

$$E(\beta, a) = \frac{\pi^2}{15\beta^4} - \frac{\pi^2}{720a^4} + \frac{8}{\pi^2}\sum_{l_0,l_3=1}^{\infty}\frac{3(\beta l_0)^2 - (2al_3)^2}{[(\beta l_0)^2 + (2al_3)^2]^3}, \tag{16.20}$$

$$P(\beta, a) = \frac{\pi^2}{45\beta^4} - \frac{\pi^2}{240a^4} + \frac{8}{\pi^2}\sum_{l_0,l_3=1}^{\infty}\frac{(\beta l_0)^2 - 3(2al_3)^2}{[(\beta l_0)^2 + (2al_3)^2]^3}. \tag{16.21}$$

The first two terms of these expressions reproduce the black-body radiation and the Casimir contributions for the energy and the pressure, separately. The last term represents the interplay between the two effects [241, 273].

Notice that the positive black-body contributions for E and P dominate in the high-temperature limit, while the energy and the pressure are negative for low T. The critical curve $\beta_c = \chi_0 a$, for the transition from negative to positive values of P, is determined by searching for the value of the ratio $\chi = \beta/a$ for which the pressure vanishes; this value, χ_0, is the solution of the transcendental equation

$$\frac{\pi^2}{45}\frac{1}{\chi^4} - \frac{\pi^2}{240} + \frac{8}{\pi^2}\sum_{l,n=1}^{\infty}\frac{(\chi l)^2 - 3(2n)^2}{[(\chi l)^2 + (2n)^2]^3} = 0,$$

given, numerically, by $\chi_0 \simeq 1.15$.

Define functions $f(\xi)$ and $g(\xi)$, with $\xi = \chi^{-1} = a/\beta$ [273],

$$f(\xi) = -\frac{1}{4\pi^2}\sum_{j,l=1}^{\infty}\frac{(2\xi)^4}{[(2l\xi)^2 + (j)^2]^2},$$

and

$$\begin{aligned} s(\xi) &= -\frac{d}{d\xi}f(\xi) \\ &= \frac{2^4}{\pi^2}\sum_{j,l=1}^{\infty}\frac{\xi^3 j^2}{[(2l\xi)^2 + (j)^2]^3}. \end{aligned}$$

The renormalized energy-momentum tensor reads

$$\mathcal{T}^{\mu\nu(11)}(\beta, a) = \frac{1}{a^4}f(\xi)(g^{\mu\nu} + 4n_3^\mu n_3^\nu) + \frac{1}{\beta a^3}(n^\mu n^\nu + n_3^\mu n_3^\nu)s(\xi).$$

The energy density, $E(\beta, a) = \mathcal{T}^{00(11)}(\beta, a)$, is then written as

$$E(\beta, a) = \frac{1}{a^4}[f(\xi) + \xi s(\xi)].$$

As this is a thermodynamical expression, the function $f(\xi)$ describes the free energy density for photons and $s(\xi)$ is the entropy density.

For the case of a cubic box of edge a at finite temperature, using Eq. (16.16) with $\alpha = (\beta, i2a, i2a, i2a)$, we have for the pressure

$$P(\beta, a) = T^{33(11)}(\beta, a) = \ g(\chi)\,\frac{1}{a^4}, \tag{16.22}$$

where $\chi = \frac{\beta}{a}$ and the function $g(\chi)$ is given by

$$\begin{aligned} g(\chi) = \frac{1}{\pi^2}\Bigg\{ & \mathcal{C}_e + \frac{\pi^4}{45}\frac{1}{\chi^4} + 8\sum_{l,n=1}^{\infty}\frac{1}{[\chi^2 l^2 + 4n^2]^2} + 4\sum_{l,n=1}^{\infty}\frac{\chi^2 l^2 - 12n^2}{[\chi^2 l^2 + 4n^2]^3} \\ & + 8\sum_{l,n,r=1}^{\infty}\frac{1}{[\chi^2 l^2 + 4(n^2 + r^2)]^2} + 16\sum_{l,n,r=1}^{\infty}\frac{\chi^2 l^2 + 4(n^2 - 3r^2)}{[\chi^2 l^2 + 4(n^2 + r^2)]^3} \\ & + 16\sum_{l,n,r,q=1}^{\infty}\frac{\chi^2 l^2 + 4(n^2 + r^2 - 3q^2)}{[\chi^2 l^2 + 4(n^2 + r^2 + q^2)]^3}\Bigg\}, \end{aligned}$$

with

$$\mathcal{C}_e = \frac{1}{4}\sum_{l,n=1}^{\infty}\frac{1}{[l^2+n^2]^2} + \frac{1}{6}\sum_{l,n,r=1}^{\infty}\frac{1}{[l^2+n^2+r^2]^2} - \frac{\pi^4}{720} \approx 0.00737\,. \qquad (16.23)$$

The pressure is always positive: for $T \to 0$,

$$T^{33(11)}(a) = \frac{\mathcal{C}_e}{\pi^2}\frac{1}{a^4}$$

For $T \to \infty$, the pressure in Eq. (16.22) is dominated by the term $\simeq T^{-4}$. A plot of the Casimir pressure as a function of T and a is presented in Fig. 16.2.

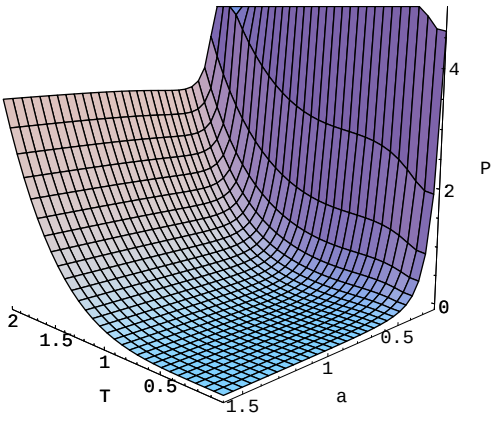


Fig. 16.2 Casimir pressure for the electromagnetic field in a cubic box under Dirichlet boundary conditions.

16.3 Casimir-Boyer model

Next we consider the Casimir-Boyer model [276, 277], corresponding to a mixed case of plates: one conducting plate at $x_3 = 0$ and the other one, a permeable plate, at $x_3 = d$. This is equivalent to taking a twisted boundary condition for the electromagnetic field [275]; corresponding to an anti-periodic boundary condition on the electromagnetic field in the topology $\mathbb{S}^1$. In order to have a Green function satisfying these conditions, we consider $\alpha = (\beta, 0, 0, i2a)$, $(n_0^\mu) = (1, 0, 0, 0)$ and $(n_3^\mu) = (0, 0, 0, 1)$. Then we have

$$v^2(k_0, k_1; \beta, a) = \sum_{l_0=1}^{\infty} e^{-\beta k_0 l_0} + \sum_{l_3=1}^{\infty}(-1)^{l_3} e^{-i2ak^3 l_3} + 2\sum_{l_0,l_3=1}^{\infty}(-1)^{l_3} e^{-\beta p_0 l_0 - i2ak^3 l_3}\,, \qquad (16.24)$$

and we find

$$\begin{aligned}\overline{G}^{(11)}(x-x';\beta,a) &= \frac{1}{(2\pi)^4}\int d^4k\, e^{ik(x-x')}\overline{G}^{(11)}(k;\beta,a)\\ &= \frac{1}{(2\pi)^4}\int d^4k\, e^{ik(x-x')}\\ &\quad\times v^2(k_0,k_1;\beta,a)\left[G_0(k)+\widetilde{G}_0(k)\right].\end{aligned}$$

Using this result in Eq. (16.11) we find the energy-momentum tensor

$$\begin{aligned}\mathcal{T}^{\mu\nu(11)}(\beta,a) = -\frac{2}{\pi^2}\Bigg\{&\sum_{l_0=1}^{\infty}\frac{g^{\mu\nu}-4n_0^\mu n_0^\nu}{(\beta l_0)^4}+\sum_{l_3=1}^{\infty}(-1)^{l_3}\frac{g^{\mu\nu}+4n_3^\mu n_3^\nu}{(2al_3)^4}\\ &+2\sum_{l_0,l_3=1}^{\infty}(-1)^{l_3}\frac{(\beta l_0)^2[g^{\mu\nu}-4n_0^\mu n_0^\nu]+(2Ll_3)^2[g^{\mu\nu}+4n_3^\mu n_3^\nu]}{[(\beta l_0)^2+(2al_3)^2]^3}\Bigg\}.\end{aligned}$$

Observe that for the term $a\to\infty$, the component $\mathcal{T}^{00(11)}(\beta)$ is the black-body radiation term, and for $\beta\to\infty$ $(T\to 0)$, we have the energy $E(a)=\mathcal{T}^{00(11)}(a)$,

$$E(a)=\frac{7}{8}\frac{\pi^2}{720a^4},$$

which is the Casimir energy for the Casimir-Boyer model [276, 275]. This expression is $-7/8$ of the Casimir energy for plates of the same material. The force, in this case, is repulsive.

Using $\xi=a/\beta$, we introduce

$$\bar{f}(\xi)=-\frac{1}{4\pi^2}\sum_{l_0,l_3=0'}^{\infty}(-1)^{l_3}\frac{(2\xi)^4}{[(2l_3\xi)^2+(l_0)^2]^2},$$

and

$$\begin{aligned}\bar{s}(\xi) &= -\frac{d}{d\xi}f(\xi)\\ &= \frac{2^4}{\pi^2}\sum_{l_0,l_3=0'}^{\infty}(-1)^{l_3}\frac{\xi^3 j^2}{[(2l_3\xi)^2+(l_0)^2]^3},\end{aligned}$$

where the notation $0'$ is to indicate that the term $l_0=l_3=0$ is excluded from the sum. We obtain

$$\mathcal{T}^{\mu\nu(11)}(\beta,a)=\frac{1}{a^4}\bar{f}(\xi)(g^{\mu\nu}+4n_3^\mu n_3^\nu)+\frac{1}{\beta a^3}(n_0^\mu n_0^\nu+n_3^\mu n_3^\nu)\bar{s}(\xi).$$

The energy density $E(\beta,a)=\mathcal{T}^{00(11)}(\beta,a)$ is written as

$$E(\beta,a)=\frac{1}{a^4}[\bar{f}(\xi)+\xi\bar{s}(\xi)].$$

The function $\bar{f}(\xi)$ is the free energy density for photons and $\bar{s}(\xi)$ is the entropy density.

From these applications, we observe that, the method based on the Bogoliubov transformation for compactified space-time regions provides an effective way to study the Casimir effect in different topologies. From a physical point of view, in addition, the Casimir effect is interpreted as a process of condensation of the electromagnetic field. The quasi-particles are described (for an arbitrary mode) by

$$a(\alpha) = u(\alpha)a - v(\alpha)\tilde{a}^{\dagger}$$
$$\tilde{a}^{\dagger}(\alpha) = u(\alpha)\tilde{a}^{\dagger} - v(\alpha)a,$$

with $a^{\dagger}(\alpha), \tilde{a}^{\dagger}(\alpha)$, $a(\alpha)$ and $\tilde{a}(\alpha)$ fulfilling the canonical algebra of the creation and destruction operators, that is $[a(\alpha), a^{\dagger}(\alpha)] = [\tilde{a}(\alpha), \tilde{a}^{\dagger}(\alpha)] = 1$. From these operators a vacuum state $|0(\alpha)\rangle$ is defined, such that $a(\alpha)|0(\alpha)\rangle = 0$. Therefore, regarding the operators a and $a^{\dagger}$, the state $|0(\alpha)\rangle$ describes a condensate, as is the case for the temperature. The result is that, in the vacuum state we have

$$\langle 0(\alpha)|a^{\dagger}a|0(\alpha)\rangle = \langle 0, \tilde{0}|a^{\dagger}(\alpha)a(\alpha)|0, \tilde{0}\rangle \neq 0.$$

This represents a modification of the energy spectrum in the vacuum, resulting in the Casimir effect. To derive a finite and measurable result, a renormalization procedure has to be introduced. Here we take the difference of the energy-momentum tensor in the topology Γ_D^d and the energy-momentum tensor written in the empty space-time. The result is the physical tensor $\mathcal{T}^{\mu\nu}(\alpha)$.

With these calculations, we observe the following facts. Since the energy for the empty space is not part of the Casimir energy, such a term is not included in the present calculations. Therefore, problems of renormalization, that plagues other methods, are not a part of the consideration here. Only the Casimir energy is calculated directly. The basic ingredient for this behavior is that the generalized Bogoliubov transformation separates the Green function into two parts. One is associated with the empty space-time; the other describes properties of the compactification. This fact represents a natural ease in the calculation of $\mathcal{T}^{\mu\nu}(\alpha)$, the renormalized energy, and hence the Casimir effect. As a final observation, in order to study the Casimir force in real media, we have to use $\epsilon(\mathbf{x}, \beta)$ (not $\epsilon_0 = 1$), the dielectric permittivity in the Drude model, for example [251].

Chapter 17

Casimir Effect for Fermions

The Casimir effect for a fermion field is of interest in considering, for instance, the structure of proton in particle physics. In particular, in the phenomenological MIT bag model [279], quarks are assumed to be confined in a small space region, of the order of 1.0 fm, in such a way that there is no fermionic current outside that region. The fermion field fulfills the bag model boundary conditions. The Casimir effect in such a small region is important to define the process of deconfinement. This may appear in heavy ion collisions at Relativistic Heavy Ion Collider (RHIC) or at Large Hadron Collider (LHC), giving rise to the quark-gluon plasma. For the quark field, the problem of the Casimir effect has been quite often addressed by considering the case of two parallel plates [259–263, 280, 281], although there are some calculations involving spherical geometries [241].

As first demonstrated by Johnson [282], for plates, the fermionic Casimir force is attractive as in the case of the electromagnetic field. On the other hand, depending on the geometry of confinement, the nature of the Casimir force can change. This is the case, for instance, for a spherical cavity and for the Casimir-Boyer model, using mixed boundary conditions for the electromagnetic field, such that the force is repulsive. [98, 264–266, 275–277]. Therefore, the analysis considering fermions in a topology of type Γ_D^d is of interest. We analyze the energy-momentum tensor for the Casimir effect of a fermion field in a d-dimensional box at finite temperature. As a particular case the Casimir energy and pressure for the field confined in a 3-dimensional parallelepiped box are calculated. It is found that the attractive or repulsive nature of the Casimir pressure on opposite faces changes depending on the relative magnitude of the edges. We also determine the temperature at which the Casimir pressure in a cubic box changes sign and estimate its value when the edge of the cube is of the order of the confining length for baryons. At the end we use these results to perform calculations for estimating the Casimir energy for a non-interacting massless QCD model.

17.1 Casimir effect in Γ_4^1

In order to treat the case of fermions, we follow in general the same prescription, developed for the electromagnetic field, to derive the physical (renormalized) energy-momentum tensor. The energy-momentum tensor for a massless fermionic field is

$$\begin{aligned} T^{\mu\nu}(x) &= \lim_{x'\to x} \langle 0|i\overline{\psi}(x')\gamma^\mu\partial^\nu\psi(x)|0\rangle \\ &= \lim_{x'\to x} \gamma^\mu\partial^\nu S(x-x') \\ &= -4i \lim_{x'\to x} \partial^\mu\partial^\nu G_0(x-x'), \end{aligned} \tag{17.1}$$

where

$$S(x-x') = -i\langle 0|T[\psi(x)\overline{\psi}(x')]|0\rangle$$

and $G_0(x-x')$ is the propagator of the free massless bosonic field. With $T^{\mu\nu}(x)$, we introduce the confined α-dependent energy-momentum tensor $\mathcal{T}^{\mu\nu(ab)}(x;\alpha)$ defined by

$$\mathcal{T}^{\mu\nu(ab)}(x;\alpha) = \langle T^{\mu\nu(ab)}(x;\alpha)\rangle - \langle T^{\mu\nu(ab)}(x)\rangle, \tag{17.2}$$

where $T^{\mu\nu(ab)}(x;\alpha)$ is a function of the field operators $\psi(x;\alpha)$, $\widetilde{\psi}(x;\alpha)$.

Using

$$S^{(ab)}(x-x') = \begin{pmatrix} S(x-x') & 0 \\ 0 & \widetilde{S}(x-x') \end{pmatrix},$$

with $\widetilde{S}(x-x') = -S^*(x'-x)$, we have

$$\mathcal{T}^{\mu\nu(ab)}(x;\alpha) = -4i \lim_{x'\to x} \partial^\mu\partial^\nu[G_{0f}^{(ab)}(x-x';\alpha) - G_{0f}^{(ab)}(x-x')], \tag{17.3}$$

corresponding to changing in Eq. (17.1), $S^{(ab)}(x-x')$ by $S(x-x')$. The 2×2 Green functions $G_{0f}^{(ab)}(x-x';\alpha)$ and $G_{0f}^{(ab)}(x-x')$ are

$$G_{0f}^{(ab)}(x-x') = \frac{1}{(2\pi)^4}\int d^4k\; G_{0f}^{(ab)}(k)\; e^{-ik\cdot(x-x')},$$

where

$$G_{0f}^{(ab)}(k) = \begin{pmatrix} G_0(k) & 0 \\ 0 & G_0^*(k) \end{pmatrix}.$$

Observe that, $G_{0f}^{(ab)}(k)$ is different from $G_0^{(ab)}(k)$ for bosons by a sign in the component $G_0^{(22)}(k)$. The α-counterpart is

$$G_{0f}^{(ab)}(x-x';\alpha) = \frac{1}{(2\pi)^4}\int d^4k\; G_{0f}^{(ab)}(k;\alpha)\; e^{-ik\cdot(x-x')}, \tag{17.4}$$

with

$$G_{0f}^{(ab)}(k;\alpha) = B^{-1(ac)}(k;\alpha)G_{0f}^{(cd)}(k)B^{(db)}(k;\alpha),$$

where $B_k^{(ab)}(\alpha)$ is the Bogoliubov transformation for fermions

$$\left(B^{(ab)}(k;\alpha)\right) = \begin{pmatrix} u_k(\alpha) & -v_k(\alpha) \\ v_k(\alpha) & u_k(\alpha) \end{pmatrix}.$$

Explicitly, the components of $G_0^{(ab)}(k;\alpha)$ are given by

$$\begin{aligned} G_{0f}^{11}(k;\alpha) &= G_0(k) + v_k^2(\alpha)[G_0^*(k) - G_0(k)], \\ G_{0f}^{12}(k;\alpha) &= G_0^{21}(k;\alpha) = v_k(\alpha)[1 - v_k^2(\alpha)]^{1/2}[G_0^*(k) - G_0(k)], \\ G_{0f}^{22}(k;\alpha) &= G_0^*(k) + v_k^2(\alpha)[G_0(k) - G_0^*(k)]. \end{aligned}$$

The physical quantities are derived from the component $G_{0f}^{11}(k;\alpha)$. Therefore, the physical α-tensor is given by the component $\mathcal{T}^{\mu\nu(11)}(x;\alpha)$.

Let us consider $\alpha = (\beta, 0, 0, 0)$. In this case $v_k(\beta)$ is defined through the fermion number distribution function,

$$v_k(\beta) = \frac{e^{-\beta k_0/2}}{[1 + e^{-\beta k_0}]^{1/2}}.$$

We write it as

$$v_k^2(\beta) = \sum_{l=1}^{\infty} (-1)^{l+1} e^{-\beta k_0 l}; \tag{17.5}$$

leading to the thermal Green function,

$$G_{0f}^{11}(k;\beta) = G_0(k) + \sum_{l=1}^{\infty} (-1)^{l+1} e^{-\beta k_0 l}[G_0^*(k) - G_0(k)].$$

Using this result in Eq. (17.4), we have

$$\begin{aligned} G_{0f}^{11}(x - x';\beta) = G_0(x - x') + \sum_{l=1}^{\infty} (-1)^{l+1} \\ \times [G_0^*(x' - x + i\beta l n_0) - G_0(x - x' - i\beta l n_0)], \end{aligned}$$

where $(n_0^\mu) = n_0 = (1, 0, 0, 0)$. Therefore, the renormalized tensor, given by Eq. (17.2), is

$$\begin{aligned} \mathcal{T}^{\mu\nu(11)}(\beta) = -4i \lim_{x' \to x} \sum_{l=1}^{\infty} (-1)^{l+1} \partial^\mu \partial^\nu \\ \times [G_0^*(x' - x + i\beta l \widehat{n}_0) - G_0(x - x' - i\beta l \widehat{n}_0)]. \end{aligned}$$

Performing the covariant derivatives, this expression reads

$$\mathcal{T}^{\mu\nu(11)}(\beta) = \frac{4}{\pi^2} \sum_{l=1}^{\infty} (-1)^l \left[\frac{g^{\mu\nu} - 4 n_0^\mu n_0^v}{(\beta l)^4} \right]. \tag{17.6}$$

Well known results for thermal fermionic fields can be derived from this tensor. For instance, the internal energy is given by $E(T) = \mathcal{T}^{00(11)}(\beta)$, that is,

$$E(T) = \frac{7\pi^2}{60} T^4, \tag{17.7}$$

where we have used the Riemann alternating zeta function

$$\varsigma(4) = \sum_{l=1}^{\infty}(-1)^{l+1}\,\frac{1}{l^4} = \frac{7\pi^4}{720}. \tag{17.8}$$

As another application, we derive the Casimir effect at zero temperature. For parallel plates perpendicular to the x^3-direction and separated by a distance a, instead of Eq. (17.5), we take $\alpha = i2a$, we write

$$v_k^2(a) = \sum_{l=1}^{\infty}(-1)^{l+1}e^{-i2ak_3l} \tag{17.9}$$

and use $n_3 = (n_3^\mu) = (0,0,0,1)$, a space-like vector. As a consequence, we derive

$$\mathcal{T}^{\mu\nu(11)}(a) = \frac{4}{\pi^2}\sum_{l=1}^{\infty}(-1)^l\left[\frac{g^{\mu\nu}+4n_3^\mu n_3^\nu}{(2al)^4}\right], \tag{17.10}$$

resulting in the Casimir energy and pressure given, respectively, by

$$E(a) = \mathcal{T}^{00(11)}(a) = -\frac{7\pi^2}{2880}\,\frac{1}{a^4}, \tag{17.11}$$

$$P(a) = \mathcal{T}^{33(11)}(a) = -\frac{7\pi^2}{960}\,\frac{1}{a^4}. \tag{17.12}$$

It is to be noticed that the choice of α as a pure imaginary number is required in order to obtain the spatial confinement, while the factor 2 is needed to ensure antiperiodic boundary conditions on the propagator and the bag model boundary conditions. In the next section we extend this procedure to the case where multiple compactifications of (imaginary) time and spatial coordinates are implemented simultaneously .

17.2 Compactification in higher dimensions

We calculate the Casimir effect for massless fermions in a topology Γ^d_{N+1}; i.e. within a d-dimensional box at finite temperature. We consider the $(1+N)$-dimensional Minkowski space with $v(\alpha)$ given by

$$\begin{aligned} v_k^2(\alpha) = &\sum_{j=0}^{N}\sum_{l_j=1}^{\infty}(-1)^{1+l_j}\,f(\alpha_j)\,\exp\{i\alpha_j l_j k_j\} \\ &+\sum_{j<r=0}^{N}2\,f(\alpha_j)f(\alpha_r)\sum_{l_j,l_r=1}^{\infty}(-1)^{2+l_j+l_r}\,\exp\{i\alpha_j l_j k_j + i\alpha_r l_r k_r\}+\cdots \\ &+2^N\,f(\alpha_0)f(\alpha_1)\cdots f(\alpha_N)\sum_{l_0,l_1,\ldots,l_N=1}^{\infty}(-1)^{N+1\sum_{r=1}^{N}l_r}\,\exp\{i\sum_{i=0}^{N}\alpha_i l_i k_i\}, \end{aligned} \tag{17.13}$$

where $\alpha = (\alpha_0, \alpha_1, \alpha_2, ..., \alpha_N)$, $f(\alpha_j) = 0$ for $\alpha_j = 0$ and $f(\alpha_j) = 1$ otherwise. This expression leads to the simultaneous compactification of any d $(1 \leq d \leq N+1)$ dimensions corresponding to the non-null parameters α_j , with α_0 corresponding to the time coordinate and α_n ($n = 1, ..., N$) referring to the spatial ones.

A more compact expression for $v_k^2(\alpha)$ is

$$v_k^2(\alpha) = \sum_{s=1}^{N+1} 2^{s-1} \sum_{\{\sigma_s\}} \left(\prod_{n=1}^{s} f(\alpha_{\sigma_n}) \right) \times \sum_{l_{\sigma_1},...,l_{\sigma_s}=1}^{\infty} (-1)^{s+\sum_{r=1}^{s} l_{\sigma_r}} \exp\{-\sum_{j=1}^{s} \alpha_{\sigma_j} l_{\sigma_j} k_{\sigma_j}\}. \tag{17.14}$$

where $\{\sigma_s\}$ denotes the set of all combinations with s elements, $\{\sigma_1, \sigma_2, ...\sigma_s\}$, of the first $N+1$ natural numbers $\{0, 1, 2, ..., N\}$, that is all subsets containing s elements, which we choose to write in an ordered form with $\sigma_1 < \sigma_2 < \cdots < \sigma_s$. Using this $v_k^2(\alpha)$ the (1,1)-component of the α-dependent Green function in the momentum space becomes

$$G_0^{11}(k;\alpha) = G_0(k) + \sum_{s=1}^{N+1} 2^{s-1} \sum_{\{\sigma_s\}} \left(\prod_{n=1}^{s} f(\alpha_{\sigma_n}) \right) \times \sum_{l_{\sigma_1},...,l_{\sigma_s}=1}^{\infty} (-1)^{s+\sum_{r=1}^{s} l_{\sigma_r}} \exp\{i \sum_{j=1}^{s} \alpha_{\sigma_j} l_{\sigma_j} k_{\sigma_j}\} [G_0^*(k) - G_0(k)].$$

Taking the inverse Fourier transform of this expression and defining the vectors $n_0 = (1, 0, 0, 0, ...)$, $n_1 = (0, 1, 0, 0, ...), ...,$ $n_N = (0, 0, 0, ..., 1)$, in the $(1+N)$-dimensional Minkowski space, written in the the contravariant coordinates, the energy-momentum tensor is

$$\mathcal{T}^{\mu\nu(11)}(\alpha) = -4i \sum_{s=1}^{N+1} 2^{s-1} \sum_{\{\sigma_s\}} \left(\prod_{n=1}^{s} f(\alpha_{\sigma_n}) \right) \sum_{l_{\sigma_1},...,l_{\sigma_s}=1}^{\infty} (-1)^{s+\sum_{r=1}^{s} l_{\sigma_r}} \times \partial^\mu \partial^\nu \lim_{x' \to x} \left[G_0^*(x' - x + \sum_{j=1}^{s} \xi_{\sigma_j} \alpha_{\sigma_j} l_{\sigma_j} n_{\sigma_j}) - G_0(x - x' - \sum_{j=1}^{s} \xi_{\sigma_j} \alpha_{\sigma_j} l_{\sigma_j} n_{\sigma_j}) \right], \tag{17.15}$$

where $\xi_{\sigma_j} = +1$, if $\sigma_j = 0$, and $\xi_{\sigma_j} = -1$ for $\sigma_j = 1, 2, ..., N$.

In order to get the physical conditions of finite temperature and spatial confinement, α_0 has to be taken as a positive real number while α_n, for $n = 1, 2, ..., N$, must be pure imaginary of the form $i2a_n$; in these cases, one finds that $\alpha_j^{*2} = \alpha_j^2$. Considering such choices for the parameters α_j and using the explicit form of $G_0(x)$

for the 4-dimensional space-time (corresponding to $N = 3$), we obtain

$$\mathcal{T}^{\mu\nu(11)}(\alpha) = -\frac{4}{\pi^2}\sum_{s=1}^{4} 2^{s-1} \sum_{\{\sigma_s\}} \left(\prod_{n=1}^{s} f(\alpha_{\sigma_n})\right) \times \sum_{l_{\sigma_1},\ldots,l_{\sigma_s}=1}^{\infty} (-1)^{s+\sum_{r=1}^{s} l_{\sigma_r}} \frac{1}{[\sum_{j=1}^{s} \xi_{\sigma_j}(\alpha_{\sigma_j} l_{\sigma_j})^2]^2} \times \left[g^{\mu\nu} - \frac{2\sum_{j,r=1}^{s}(1+\xi_{\sigma_j}\xi_{\sigma_r})(\alpha_{\sigma_j} l_{\sigma_j})(\alpha_{\sigma_r} l_{\sigma_r}) n^{\mu}_{\sigma_j} n^{\nu}_{\sigma_r}}{\sum_{j=1}^{s} \xi_{\sigma_j}(\alpha_{\sigma_j} l_{\sigma_j})^2}\right]. \tag{17.16}$$

It is important to observe that the results given by Eqs. (17.6) and (17.10) are particular cases of the energy-momentum tensor given by Eq. (17.16), corresponding to $\alpha = (\beta, 0, 0, 0)$ and $\alpha = (0, 0, 0, i2a)$ respectively. Another important aspect is that $\mathcal{T}^{\mu\nu(11)}(\alpha)$ is traceless, as it should be. To obtain the physical meaning of $\mathcal{T}^{\mu\nu(11)}(\alpha)$, we have to analyze particular cases. Thus we rederive, first, some known results considering $N = 3$. Let us emphasize that Eq. (17.14) is the generalization of the Bogoliubov transformation, compatible with the generalizations of the Matsubara formalism, for the case of fermions.

17.3 Casimir effect for two plates

The particular case of two parallel plates at zero temperature has already been analyzed. For this case, taking $\alpha = (0, 0, 0, i2a)$, Eq. (17.16) reduces to Eq. (17.10) and the standard Casimir effect is recovered. Let us then consider two parallel plates at finite temperature. Then both time and space compactification need to be considered; this is carried out by taking $\alpha = (\beta, 0, 0, i2a)$ in Eq. (17.16), where $\beta^{-1} = T$ is the temperature and a is the distance between plates perpendicular to the x^3-axis. Therefore we find,

$$\mathcal{T}^{\mu\nu(11)}(\beta, a) = \frac{4}{\pi^2}\left\{\sum_{l_0=1}^{\infty}(-1)^{l_0}\frac{[g^{\mu\nu} - 4n_0^{\mu}n_0^{\nu}]}{(\beta l_0)^4} + \sum_{l_3=1}^{\infty}(-1)^{l_3}\frac{[g^{\mu\nu} + 4n_3^{\mu}n_3^{\nu}]}{(2al_3)^4} - 2\sum_{l_0,l_3=1}^{\infty}(-1)^{l_0+l_3}\left[\frac{(\beta l_0)^2[g^{\mu\nu} - 4n_0^{\mu}n_0^{\nu}]}{[(\beta l_0)^2 + (2al_3)^2]^3} + \frac{(2al_3)^2[g^{\mu\nu} + 4n_3^{\mu}n_3^{\nu}]}{[(\beta l_0)^2 + (2al_3)^2]^3}\right]\right\}.$$

Using the summation in Eq. (17.8), the Casimir energy $E(\beta, a) = \mathcal{T}^{00(11)}(\beta, a)$ is given by

$$E(\beta, a) = \frac{7\pi^2}{60}\frac{1}{\beta^4} - \frac{7\pi^2}{2880}\frac{1}{a^4} - \frac{8}{\pi^2}\sum_{l_0,l_3=1}^{\infty}(-1)^{l_0+l_3}\frac{3(\beta l_0)^2 - (2al_3)^2}{[(\beta l_0)^2 + (2al_3)^2]^3}.$$

Taking the limit $a \to \infty$, this energy reduces to the Stefan-Boltzmann term given in Eq. (17.7), while making $\beta \to \infty$ one regains the Casimir effect for two plates at zero temperature presented in Eq. (17.11). The third term, which stands for the correction due to temperature and spatial compactification, remains finite as $\beta \to 0$ and, as expected, the high temperature limit is dominated by the positive contribution of the Stefan-Boltzmann term.

The Casimir pressure, $P(\beta, a) = \mathcal{T}^{33(11)}(\beta, a)$, is similarly obtained as

$$P(\beta,a) = \frac{7\pi^2}{180}\frac{1}{\beta^4} - \frac{7\pi^2}{960}\frac{1}{a^4} + \frac{8}{\pi^2}\sum_{l_0,l_3=1}^{\infty}(-1)^{l_0+l_3}\frac{(\beta l_0)^2 - 3(2al_3)^2}{[(\beta l_0)^2 + (2al_3)^2]^3}. \qquad (17.17)$$

It is to be noted that for low temperatures (large β) the pressure is negative but, as the temperature increases, a transition to positive values happens. It is possible to determine the critical curve of this transition, $\beta_c = \chi_0 a$, by searching for a value of the ratio $\chi = \beta/a$ for which the pressure vanishes; this value, χ_0, is the solution of the transcendental equation

$$\frac{7\pi^2}{180}\frac{1}{\chi^4} - \frac{7\pi^2}{960} + \frac{8}{\pi^2}\sum_{l,n=1}^{\infty}(-1)^{l+n}\frac{(\chi l)^2 - 3(2n)^2}{[(\chi l)^2 + (2n)^2]^3} = 0,$$

given, numerically, by $\chi_0 \simeq 1.38177$.

In the following sections we shall discuss situations in which the field is compactified in more than one space directions. We start by describing the Casimir effect for the massless fermion field in a rectangular waveguide, that is, considering compactification of two space directions, then we include temperature.

17.4 Casimir effect for a waveguide

The situation of a rectangular waveguide is defined here by considering the confinement along the x^2- and the x^3-axis. Then the Casimir effect at zero temperature is obtained from Eq. (17.16) by taking $\alpha = (0, 0, i2a_2, i2a_3)$, that is

$$\begin{aligned}\mathcal{T}^{\mu\nu(11)}(a_2,a_3) = \frac{1}{4\pi^2}\Bigg\{&\sum_{l_2=1}^{\infty}(-1)^{l_2}\frac{[g^{\mu\nu}+4n_2^\mu n_2^\nu]}{(a_2l_2)^4} + \sum_{l_3=1}^{\infty}(-1)^{l_3}\frac{[g^{\mu\nu}+4n_3^\mu n_3^\nu]}{(L_3l_3)^4}\\ &- 2\sum_{l_2,l_3=1}^{\infty}(-1)^{l_2+l_3}\Bigg[\frac{(a_2l_2)^2[g^{\mu\nu}+4n_2^\mu n_2^\nu] + (a_3l_3)^2[g^{\mu\nu}+4n_3^\mu n_3^\nu]}{[(a_2l_2)^2+(a_3l_3)^2]^3}\\ &+ \frac{4(a_2l_2)(a_3l_3)[n_2^\mu n_3^\nu + n_3^\mu n_2^\nu]}{[(a_2l_2)^2+(a_3l_3)^2]^3}\Bigg]\Bigg\}. \qquad (17.18)\end{aligned}$$

Making use of Eq. (17.8), the Casimir energy, $E(a_2, a_3) = \mathcal{T}^{00(11)}(a_2, a_3)$, is given by

$$E(a_2,a_3) = -\frac{7\pi^2}{2880}\left(\frac{1}{a_2^4}+\frac{1}{a_3^4}\right) - \frac{1}{2\pi^2}\sum_{l_2,l_3=1}^{\infty}\frac{(-1)^{l_2+l_3}}{[(a_2l_2)^2+(a_3l_3)^2]^2}, \qquad (17.19)$$

while the Casimir pressure , $P_c(L_2, L_3) = \mathcal{T}^{33(11)}(L_2, L_3)$, reads

$$P(a_2, a_3) = -\frac{7\pi^2}{2880}\left(\frac{3}{a_3^4} - \frac{1}{a_2^4}\right) + \frac{1}{2\pi^2}\sum_{l_2,l_3=1}^{\infty}(-1)^{l_2+l_3}\frac{(a_2 l_2)^2 - 3(a_3 l_3)^2}{[(a_2 l_2)^2 + (a_3 l_3)^2]^3}. \quad (17.20)$$

For a square waveguide, $a_2 = a_3 = a$, the Casimir energy and the Casimir pressure (in this case, $\mathcal{T}^{33(11)} = \mathcal{T}^{22(11)}$) reduce, respectively, to

$$E(a) = -\left(\frac{7\pi^2}{1440} + \frac{\mathcal{C}_2}{2\pi^2}\right)\frac{1}{a^4}, \quad (17.21)$$

$$P(a) = -\left(\frac{7\pi^2}{1440} + \frac{\mathcal{C}_2}{2\pi^2}\right)\frac{1}{a^4}, \quad (17.22)$$

where the constant $\mathcal{C}_2$ is given by

$$\mathcal{C}_2 = \sum_{l,n=1}^{\infty}\frac{(-1)^{l+n}}{(l^2+n^2)^2} \simeq 0.19368.$$

We find that E and P for a square waveguide behave, as functions of a , in the same way as in the case of two parallel plates, both being negative, but with the energy decreasing (increasing in absolute value) and the pressure increasing (smaller absolute value) in the waveguide case as compared with the case of two plates.

On the other hand, if the case $a_2 \neq a_3$ is considered, although E remains negative whatever the ratio $\xi = a_3/a_2$ is, it is clear from Eq. (17.20) that the sign of the Casimir pressure depends heavily on the relative magnitude of a_2 and a_3. In fact, a transition from negative to positive pressure is observed as ξ is increased; this feature is presented in Fig. 17.1 where we plot $P = \mathcal{T}^{33(11)}$ for some rectangular waveguides (characterized by different values of ξ) as a function of a $(= a_2)$. These plots indicate the existence of a specific value of the ratio ξ, ξ_0, for which the Casimir pressure vanishes identically. This value is the solution of the transcendental equation

$$-\frac{7\pi^2}{2880}\left(\frac{3}{\xi^4} - 1\right) + \frac{1}{2\pi^2}\sum_{l,n=1}^{\infty}(-1)^{l+n}\frac{l^2 - 3(\xi n)^2}{[l^2 + (\xi n)^2]^3} = 0,$$

which is given, numerically, by $\xi_0 \simeq 1.44742$; all rectangular waveguides with the ratio between a_3 and a_2 equal to ξ_0 have null Casimir pressure $P = \mathcal{T}^{33(11)}$.

It is important to note that a similar reasoning applies to $\mathcal{T}^{22(11)}(a_2, a_3)$, which is obtained from $\mathcal{T}^{33(11)}$ by exchanging $a_2 \leftrightarrow a_3$. So the force on the faces of the wage-guide perpendicular to the x^2-direction will also change from attractive to repulsive if the ratio $a_2/a_3 = \xi^{-1}$ increases, passing by the value ξ_0. It is clear that $\mathcal{T}^{33(11)}$ and $\mathcal{T}^{22(11)}$ will never be simultaneously positive; in fact, both are negative for $\xi_0^{-1} < \xi < \xi_0$ but they have opposite signs whenever $\xi > \xi_0$ or $\xi < \xi_0^{-1}$. It is also worth mentioning that, in a sense, this transition is similar to the transition from negative to positive pressures for two plates as the temperature is increased;

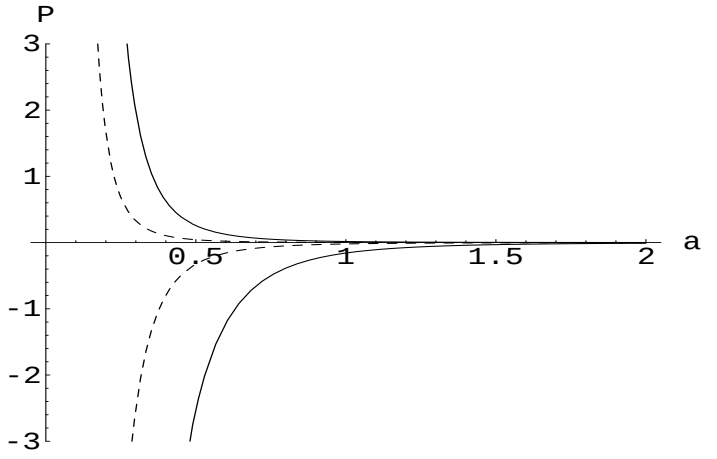


Fig. 17.1 The Casimir pressure, $P = \mathcal{T}^{33(11)}$, for some rectangular waveguides, as a function of a $(= a_2)$: the full and the dashed lines below the horizontal axis correspond to $\xi = 0.8$ and $\xi = 1.2$, respectively; the dashed and the full lines above the horizontal axis refer to $\xi = 1.5$ and $\xi = 2.0$, respectively.

the effect in both cases arises from the compactification of a second space-time coordinate.

In order to incorporate the effect of temperature in the waveguide, we consider Eq. (17.16) with $\alpha = (\beta, 0, i2a_2, i2a_3)$. Then the Casimir energy becomes

$$\begin{aligned} E(\beta, a_2, a_3) = {} & \frac{7\pi^2}{60}\frac{1}{\beta^4} - \frac{7\pi^2}{2880}\left(\frac{1}{a_2^4} + \frac{1}{a_3^4}\right) \\ & + \frac{8}{\pi^2}\sum_{l_0,l_2=1}^{\infty}(-1)^{l_0+l_2}\frac{3(\beta l_0)^2 - (2a_2 l_2)^2}{[(\beta l_0)^2 + (2a_2 l_2)^2]^3} \\ & + \frac{8}{\pi^2}\sum_{l_0,l_3=1}^{\infty}(-1)^{l_0+l_3}\frac{3(\beta l_0)^2 - (2a_3 l_3)^2}{[(\beta l_0)^2 + (2a_3 l_3)^2]^3} \\ & - \frac{1}{2\pi^2}\sum_{l_2,l_3=1}^{\infty}\frac{(-1)^{l_2+l_3}}{[(a_2 l_2)^2 + (a_3 l_3)^2]^2} \\ & - \frac{16}{\pi^2}\sum_{l_0,l_2,l_3=1}^{\infty}(-1)^{l_0+l_2+l_3}\frac{3(\beta l_0)^2 - (2a_2 l_2)^2 - (2a_3 l_3)^2}{[(\beta l_0)^2 + (2a_2 l_2)^2 + (2a_3 l_3)^2]^3}, \end{aligned} \tag{17.23}$$

while the Casimir pressure, $P = \mathcal{T}^{33(11)}$, is given by

$$\begin{aligned} P(\beta, a_2, a_3) = & \frac{7\pi^2}{180}\frac{1}{\beta^4} - \frac{7\pi^2}{2880}\left(\frac{3}{a_3^4} - \frac{1}{a_2^4}\right) \\ & + \frac{8}{\pi^2}\sum_{l_0,l_3=1}^{\infty}(-1)^{l_0+l_3}\frac{(\beta l_0)^2 - 3(2a_3 l_3)^2}{[(\beta l_0)^2 + (2a_3 l_3)^2]^3} \\ & + \frac{8}{\pi^2}\sum_{l_0,l_2=1}^{\infty}\frac{(-1)^{l_0+l_2}}{[(\beta l_0)^2 + (2a_2 l_2)^2]^2} \\ & + \frac{1}{2\pi^2}\sum_{l_2,l_3=1}^{\infty}(-1)^{l_2+l_3}\frac{(a_2 l_2)^2 - 3(a_3 l_3)^2}{[(a_2 l_2)^2 + (a_3 l_3)^2]^3} \\ & - \frac{16}{\pi^2}\sum_{l_0,l_2,l_3=1}^{\infty}(-1)^{l_0+l_2+l_3}\frac{(\beta l_0)^2 + (2a_2 l_2)^2 - 3(2a_3 l_3)^2}{[(\beta l_0)^2 + (2a_2 l_2)^2 + (2a_3 l_3)^2]^3}. \end{aligned} \tag{17.24}$$

For simplicity, we concentrate on the problem of a square waveguide at finite temperature. As in the two-plate case, the Casimir energy changes sign from negative to positive values with increasing temperature, as expected since the Stefan-Boltzmann term dominates all others as $\beta \to 0$. Let us then look at the Casimir pressure $P = \mathcal{T}^{33(11)}$ $(= \mathcal{T}^{22(11)})$. Taking $a_2 = a_3 = a$ and defining $\chi = \beta/a$, Eq. (17.24) is written as

$$P(\chi, L) = g(\chi)\,\frac{1}{a^4}, \tag{17.25}$$

where

$$\begin{aligned} g(\chi) = & \frac{7\pi^2}{180}\frac{1}{\chi^4} - \frac{7\pi^2}{1440} - \frac{\mathcal{C}_2}{2\pi^2} \\ & + \frac{8}{\pi^2}\sum_{l,n=1}^{\infty}(-1)^{l+n}\frac{(\chi l)^2 - 3(2n)^2}{[(\chi l)^2 + (2n)^2]^3} \\ & + \frac{8}{\pi^2}\sum_{l,n=1}^{\infty}\frac{(-1)^{l+n}}{[(\chi l)^2 + (2n)^2]^2} \\ & - \frac{16}{\pi^2}\sum_{l,n,r=1}^{\infty}(-1)^{l+n+r}\frac{(\chi l)^2 + (2n)^2 - 3(2r)^2}{[(\chi l)^2 + (2n)^2 + (2r)^2]^3}. \end{aligned} \tag{17.26}$$

As for two plates, in a square waveguide the Casimir pressure changes sign from negative to positive values as the temperature increases, the transition point given by the value of χ, χ_0, such that $g(\chi_0) = 0$. Numerically it is found that $\chi_0 \simeq 1.50448$, and so the critical curve is given by $\beta_c = \chi_0\, a$. In the general case, $a_2 \neq a_3$, increasing the temperature tends to make all diagonal components of $\mathcal{T}^{\mu\nu(11)}$ positive.

17.5 Casimir effect for a box

The fermion field is confined in a 3-dimensional closed box having the form of a rectangular parallelepiped with faces a_1, a_2 and a_3. At zero temperature, the physical energy-momentum tensor is obtained from Eq. (17.16) by taking $\alpha = (0, i2a_1, i2a_2, i2a_3)$. The Casimir energy is then given by

$$\begin{aligned} E(a_1,a_2,a_3) = &-\frac{7\pi^2}{2880}\left(\frac{1}{a_1^4}+\frac{1}{a_2^4}+\frac{1}{a_3^4}\right) \\ &-\frac{1}{2\pi^2}\sum_{l_1,l_2=1}^{\infty}\frac{(-1)^{l_1+l_2}}{[(a_1l_1)^2+(a_2l_2)^2]^2} \\ &-\frac{1}{2\pi^2}\sum_{l_1,l_3=1}^{\infty}\frac{(-1)^{l_1+l_3}}{[(a_1l_1)^2+(a_3l_3)^2]^2} \\ &-\frac{1}{2\pi^2}\sum_{l_2,l_3=1}^{\infty}\frac{(-1)^{l_2+l_3}}{[(a_2l_2)^2+(a_3l_3)^2]^2} \\ &+\frac{1}{\pi^2}\sum_{l_1,l_2,l_3=1}^{\infty}\frac{(-1)^{l_1+l_2+l_3}}{[(a_1l_1)^2+(a_2l_2)^2+(a_3l_3)^2]^2}, \end{aligned} \tag{17.27}$$

and the Casimir pressure, $P = \mathcal{T}^{33(11)}$, reads

$$\begin{aligned} P(a_1,a_2,a_3) = &-\frac{7\pi^2}{2880}\left(\frac{3}{a_3^4}-\frac{1}{a_1^4}-\frac{1}{a_2^4}\right) \\ &+\frac{1}{2\pi^2}\sum_{l_1,l_3=1}^{\infty}(-1)^{l_1+l_3}\frac{(a_1l_1)^2-3(a_3l_3)^2}{[(a_1l_1)^2+(a_3l_3)^2]^3} \\ &+\frac{1}{2\pi^2}\sum_{l_1,l_2=1}^{\infty}\frac{(-1)^{l_1+l_2}}{[(a_1l_1)^2+(a_2l_2)^2]^2} \\ &+\frac{1}{2\pi^2}\sum_{l_2,l_3=1}^{\infty}(-1)^{l_2+l_3}\frac{(a_2l_2)^2-3(a_3l_3)^2}{[(a_2l_2)^2+(a_3l_3)^2]^3} \\ &-\frac{1}{\pi^2}\sum_{l_1,l_2,l_3=1}^{\infty}(-1)^{l_1+l_2+l_3}\frac{(a_1l_1)^2+(a_2l_2)^2-3(a_3l_3)^2}{[(a_1l_1)^2+(a_2l_2)^2+(a_3l_3)^2]^3}. \end{aligned} \tag{17.28}$$

For a cubic box ($a_1 = a_2 = a_3 = a$), the Casimir energy and pressure, respectively, become

$$E(a) = -\left(\frac{7\pi^2}{960}+\frac{3\mathcal{C}_2-\mathcal{C}_3}{2\pi^2}\right)\frac{1}{a^4},$$

$$P(a) = -\left(\frac{7\pi^2}{2880}+\frac{3\mathcal{C}_2-\mathcal{C}_3}{6\pi^2}\right)\frac{1}{a^4},$$

where the constant $\mathcal{C}_3$ is given by

$$\mathcal{C}_3 = \sum_{l,n,r=1}^{\infty} \frac{(-1)^{l+n+r}}{(l^2+n^2+r^2)^2} \simeq -0.06314,$$

and the constant $\mathcal{C}_2 = 0.1937$ was given earlier. In this case one has $\mathcal{T}^{33(11)} = \mathcal{T}^{22(11)} = \mathcal{T}^{11(11)}$. It is clear that both energy and pressure in cubic boxes behave similarly to the cases of two parallel plates and of square waveguides. In Fig. 17.2 the Casimir pressure for all these symmetrical cases is plotted, for comparison. It is curious that, in the natural units, the Casimir pressure is three times the energy for parallel plates, they are equal in a square waveguide, while in a cubic box, $P(a) = E(a)/3$.

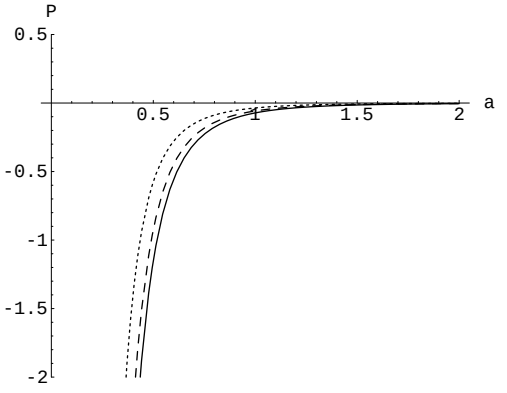


Fig. 17.2 The Casimir pressure, P, for two parallel plates separated by a distance L (full line); for a square waveguide with transversal section of edge L (dashed line); and for a cubic box of edge L (dotted line).

Changing the relative magnitude of the edges of the parallelepiped box leads to similar effects as in the case of the rectangular waveguide. For example, taking $a_1 = a_2 = a$ and defining $\xi = a_3/a$, one can show that $P(a,\xi) = \mathcal{T}^{33(11)}(a,\xi)$ vanishes for $\xi = \xi_0 \simeq 1.68433$, being negative for $\xi < \xi_0$ and positive for $\xi > \xi_0$. However, as in the case of the waveguide, $\mathcal{T}^{22(11)}$ ($= \mathcal{T}^{11(11)}$ in the present situation) will be negative whenever $\mathcal{T}^{33(11)} > 0$.

To treat the effect of temperature in the case of a box, all four coordinates in the Minkowski space have to be compactified by considering $\alpha = (\beta, i2a_1, 12a_2, i2a_3)$ in Eq. (17.16). This amounts to the addition to Eqs. (17.27) and (17.28) terms involving β and the distances a_j like those appearing in Eqs. (17.23) and (17.24). In the simpler case of a cubic box at finite temperature, the expressions for the

Casimir energy and pressure are

$$E(\beta,a) = \frac{7\pi^2}{60}\frac{1}{\beta^4} - \left(\frac{7\pi^2}{960}+\frac{\mathcal{C}}{2\pi^2}\right)\frac{1}{a^4} + \frac{24}{\pi^2}\sum_{l,n=1}^{\infty}(-1)^{l+n}\frac{3\beta^2l^2-4a^2n^2}{[\beta^2l^2+4a^2n^2]^3}$$
$$-\frac{48}{\pi^2}\sum_{l,n,r=1}^{\infty}(-1)^{l+n+r}\frac{3\beta^2l^2-4a^2(n^2+r^2)}{[\beta^2l^2+4a^2(n^2+r^2)]^3}$$
$$+\frac{32}{\pi^2}\sum_{l,n,r,q=1}^{\infty}(-1)^{l+n+r+q}\frac{3\beta^2l^2-4a^2(n^2+r^2+q^2)}{[\beta^2l^2+4a^2(n^2+r^2+q^2)]^3}, \qquad (17.29)$$

$$P(\chi,a) = \frac{1}{a^4}\left\{\frac{7\pi^2}{180}\frac{1}{\chi^4} - \left(\frac{7\pi^2}{2880}+\frac{\mathcal{C}}{6\pi^2}\right) + \frac{16}{\pi^2}\sum_{l,n=1}^{\infty}\frac{(-1)^{l+n}}{[\chi^2l^2+4n^2]^2}\right.$$
$$+\frac{8}{\pi^2}\sum_{l,n=1}^{\infty}(-1)^{l+n}\frac{\chi^2l^2-12n^2}{[\chi^2l^2+4n^2]^3} - \frac{16}{\pi^2}\sum_{l,n,r=1}^{\infty}\frac{(-1)^{l+n+r}}{[\chi^2l^2+4(n^2+r^2)]^2}$$
$$-\frac{32}{\pi^2}\sum_{l,n,r=1}^{\infty}(-1)^{l+n+r}\frac{\chi^2l^2+4(n^2-3r^2)}{[\chi^2l^2+4(n^2+r^2)]^3}$$
$$\left.+\frac{32}{\pi^2}\sum_{l,n,r,q=1}^{\infty}(-1)^{l+n+r+q}\frac{\chi^2l^2+4(n^2+r^2-3q^2)}{[\chi^2l^2+4(n^2+r^2+q^2)]^3}\right\}, \qquad (17.30)$$

where $\chi = \beta/L$ and the constant $\mathcal{C}$ is defined by

$$\mathcal{C} = 3\,\mathcal{C}_2 - 2\,\mathcal{C}_3$$
$$= 3\sum_{l,n=1}^{\infty}\frac{(-1)^{l+n}}{(l^2+n^2)^2} - 2\sum_{l,n,r=1}^{\infty}\frac{(-1)^{l+n+r}}{(l^2+n^2+r^2)^2} \simeq 0.707\,. \qquad (17.31)$$

The plot of P, as a function of the temperature ($T = \beta^{-1}$) and of the size of the cube edge (L), is shown in Fig. 17.3. The Casimir pressure changes sign from negative to positive values when the ratio $\chi = \beta/a$ passes through the value $\chi_0 \simeq 2.00$. The critical curves,

$$T_c = \frac{1}{\chi_0\, a}\,, \qquad (17.32)$$

for all symmetrical cases analyzed here (parallel plates, square waveguide and cubic box) appears in Fig. 17.4. It is important to note that the behavior of $T_c \times a$, in all three cases, is very similar, with T_c scaling with the inverse of the length a.

Let us present an estimate about of the critical temperature $T_c = (\chi_0 a)^{-1}$. Taking $a = 1$ we have $T_c = (\chi_0)^{-1} \approx 0.5$. However, $a = 1$ means, $a \approx 1$fm, a length of the order of hadron radius; corresponding to $T_c = (\chi_0 a)^{-1} \approx 100\,\mathrm{MeV}$. This temperature is of the same order of magnitude as the temperature for the deconfinement transition for hadrons. Let us analyze this fact in more detail, for a more realistic model of QCD with massless quarks and gluons.

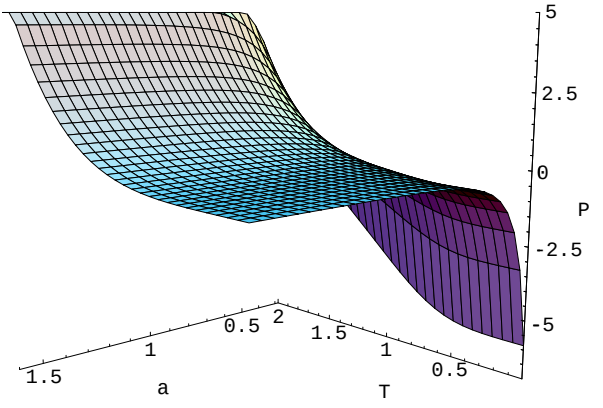


Fig. 17.3 Casimir pressure for free fermionic field in a box at finite temperature.

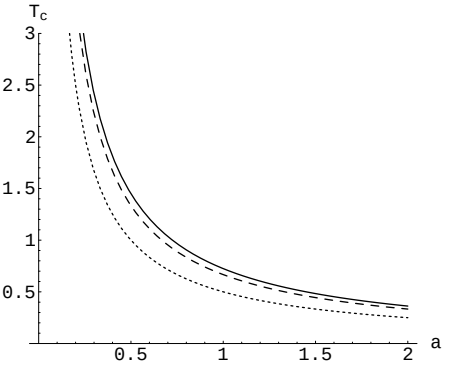


Fig. 17.4 Critical curves for the transitions from negative to positive Casimir pressure, induced by the temperature, for: (i) two parallel plates separated by a distance L (full line); (ii) square waveguide of transversal section of edge L (dashed line); (iii) cubic box of edge L (dotted line). In all cases, the points below the curves correspond to $P_c < 0$, while above them one has $P_c > 0$.

17.6 Casimir effect for a non-interacting massless QCD

The QCD Lagrangian is given by

$$\mathcal{L} = \overline{\psi}(x)[iD_\mu\gamma^\mu - m]\psi(x) - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{1}{2\alpha'}(\partial^\mu A^r_\mu(x))^2 + A^r_\mu(x)t^r J^\mu(x)\,.$$

where

$$F^r_{\mu\nu} = \partial_\mu A^r_\nu(x) - \partial_\nu A^r_\mu(x) + gc^{rsl}A^s_\mu(x)A^l_\nu(x),$$

$F_{\mu\nu} = \sum_r F^r_{\mu\nu} t^r$, is the field tensor describing the gluons; t^r and c^{rsl} are, respectively, the generators and the structure constants of the gauge group $SU(3)$; $D_\mu = \partial_\mu + igA^r_\mu(x)t^r$ is the covariant derivative; $\psi(x)$ is the quark field, carrying flavor and color quantum numbers. The term $\frac{1}{2\alpha'}(\partial^\mu A^r_\mu(x))^2$ is the Gauge fixing term. We consider an approximation for $\mathcal{L}$ describing a baryon-free massless quark-gluon plasma, confined in a space-time with topology Γ^4_4, where the circumferences are specified by the set of parameters α. For high temperatures, to zero-order approximation, the interactions and the quark mass can be discarded. In order to calculate the Casimir energy and pressure, the results for bosonic and fermionic fields have to be combined.

The free energy-momentum tensor for the quark field is given by

$$\begin{aligned} T^{\mu\nu}_q(x) &= in_c \lim_{x'\to x} \sum_f \overline{\psi}(x)\gamma^\mu \partial'^\nu \psi(x'), \\ &= in_c n_f \lim_{x'\to x} \{\overline{\psi}(x)\gamma^\mu \partial'^\nu \psi(x')\}, \end{aligned}$$

where n_c and n_f are the number of colors and flavors, respectively, in the $SU(3)$ non-abelian gauge theory. From $T^{\mu\nu}_q(x)$, we introduce the renormalized tensor $\mathcal{T}^{\mu\nu(ab)}_q(x;\alpha)$ by

$$\mathcal{T}^{\mu\nu(ab)}_q(x;\alpha) = \langle T^{\mu\lambda(ab)}_q(x;\alpha)\rangle - \langle T^{\mu\lambda(ab)}_q(x)\rangle, \tag{17.33}$$

where

$$\langle T^{\mu\lambda(ab)}_q(x)\rangle = -i4n_c n_f \lim_{x'\to x} \partial'^\nu \partial^\mu G^{(ab)}_{0f}(x-x'), \tag{17.34}$$

$$\langle T^{\mu\lambda(ab)}_q(x;\alpha)\rangle = -i4n_c n_f \lim_{x'\to x} \partial'^\nu \partial^\mu G^{(ab)}_{0f}(x-x';\alpha). \tag{17.35}$$

Neglecting self-interaction of gluons, the energy-momentum tensor for the gluon field is similar as for the electromagnetic field, up to the color number, n_g. Then we have

$$\begin{aligned} \mathcal{T}^{\mu\nu(11)}_g(\alpha) &= -in_g \lim_{x'\to x} \left\{\Gamma^{\mu\nu}(x,x')\bar{G}^{11}_0(x-x';\alpha)\right\} \\ &= -\frac{2n_g}{\pi^2} \sum_{s=1}^{4} 2^{s-1} \sum_{\{\sigma_s\}} \left(\prod_{n=1}^{s} f(\alpha_{\sigma_n})\right) \\ &\quad \times \sum_{l_{\sigma_1},\ldots,l_{\sigma_s}=1}^{\infty} \left[\frac{g^{\mu\nu}}{[\sum_{j=1}^{s} \eta_{\sigma_j}(\alpha_{\sigma_j} l_{\sigma_j})^2]^2}\right. \\ &\quad \left. - \frac{2\sum_{j,r=1}^{s}(1+\eta_{\sigma_j}\eta_{\sigma_r})(\alpha_{\sigma_j} l_{\sigma_j})(\alpha_{\sigma_r} l_{\sigma_r}) n^\mu_{\sigma_j} n^\nu_{\sigma_r}}{[\sum_{j=1}^{s} \eta_{\sigma_j}(\alpha_{\sigma_j} l_{\sigma_j})^2]^3}\right]; \end{aligned} \tag{17.36}$$

and for the quark field

$$\begin{aligned}\mathcal{T}_q^{\mu\nu(11)}(\alpha) &= -i4n_c n_f \partial^\mu \partial^\nu [\bar{G}_0^{11}(x-x';\alpha)]_{x'\to x} \\ &= -\frac{4n_c n_f}{\pi^2} \sum_{s=1}^{4} \sum_{\{\sigma_s\}} \left(\prod_{n=1}^{s} f(\alpha_{\sigma_n}) \right) \sum_{l_{\sigma_1},\ldots,l_{\sigma_s}=1}^{\infty} (-1)^{s+\sum_{r=1}^{s} l_{\sigma_r}} \\ &\quad \times 2^{s-1} \left[\frac{g^{\mu\nu}}{[\sum_{j=1}^{s} \eta_{\sigma_j} (\alpha_{\sigma_j} l_{\sigma_j})^2]^2} \right. \\ &\quad \left. - \frac{2\sum_{j,r=1}^{s} (1+\eta_{\sigma_j}\eta_{\sigma_r})(\alpha_{\sigma_j} l_{\sigma_j})(\alpha_{\sigma_r} l_{\sigma_r}) n_{\sigma_j}^{\mu} n_{\sigma_r}^{\nu}}{[\sum_{j=1}^{s} \eta_{\sigma_j} (\alpha_{\sigma_j} l_{\sigma_j})^2]^3} \right]. \end{aligned} \tag{17.37}$$

The energy-momentum tensor for the quark-gluon system, in our approximation, is

$$\mathcal{T}_{qg}^{\mu\nu(11)}(\alpha) = \mathcal{T}_q^{\mu\nu(11)}(\alpha) + \mathcal{T}_g^{\mu\nu(11)}(\alpha).$$

Considering the case of a cubic box of edge L at finite temperature, we have $\alpha = (\beta, iL, iL, iL)$ and the gluon contribution for the Casimir pressure is

$$P_g(\beta, L) = T_g^{33(11)}(\beta, L) = n_g \, g(\chi) \, \frac{1}{L^4}$$

where

$$\begin{aligned} g(\chi) = \frac{2}{\pi^2} \Bigg\{ & \mathcal{C}_g + \frac{\pi^4}{90} \frac{1}{\chi^4} + 4 \sum_{l,n=1}^{\infty} \frac{1}{[\chi^2 l^2 + n^2]^2} + 2 \sum_{l,n=1}^{\infty} \frac{\chi^2 l^2 - 3n^2}{[\chi^2 l^2 + n^2]^3} \\ & + 4 \sum_{l,n,r=1}^{\infty} \frac{1}{[\chi^2 l^2 + n^2 + r^2]^2} + 8 \sum_{l,n,r=1}^{\infty} \frac{\chi^2 l^2 + n^2 - 3r^2}{[\chi^2 l^2 + n^2 + r^2]^3} \\ & + 8 \sum_{l,n,r,q=1}^{\infty} \frac{\chi^2 l^2 + n^2 + r^2 - 3q^2}{[\chi^2 l^2 + n^2 + r^2 + q^2]^3} \Bigg\}, \end{aligned}$$

with $\chi = \frac{\beta}{L}$ and

$$\mathcal{C}_g = 2 \sum_{l,n=1}^{\infty} \frac{1}{[l^2 + n^2]^2} + \frac{4}{3} \sum_{l,n,r=1}^{\infty} \frac{1}{[l^2 + n^2 + r^2]^2} - \frac{\pi^4}{90} \approx 0.582 \, .$$

The pressure of the gluon field is always positive: for $T \to 0$,

$$T_g^{33(11)}(L) = n_g \, \frac{2\mathcal{C}_g}{\pi^2} \, \frac{1}{L^4};$$

for $T \to \infty$, the pressure is dominated by the term $n_g \pi^2 T^4/45$.

For the quark field we have

$$P_q(\beta, L) = T_q^{33(11)}(\beta, L) = n_c n_f \, f(\chi) \, \frac{1}{L^4}$$

where

$$f(\chi) = \frac{1}{\pi^2}\left\{\mathcal{C}_f + \frac{7\pi^4}{180}\frac{1}{\chi^4} + 16\sum_{l,n=1}^{\infty}\frac{(-1)^{l+n}}{[\chi^2 l^2 + n^2]^2}\right.$$
$$+8\sum_{l,n=1}^{\infty}(-1)^{l+n}\frac{\chi^2 l^2 - 3n^2}{[\chi^2 l^2 + n^2]^3}$$
$$-16\sum_{l,n,r=1}^{\infty}\frac{(-1)^{l+n+r}}{[\chi^2 l^2 + n^2 + r^2]^2}$$
$$-32\sum_{l,n,r=1}^{\infty}(-1)^{l+n+r}\frac{\chi^2 l^2 + n^2 - 3r^2}{[\chi^2 l^2 + n^2 + r^2]^3}$$
$$\left.+32\sum_{l,n,r,q=1}^{\infty}(-1)^{l+n+r+q}\frac{\chi^2 l^2 + n^2 + r^2 - 3q^2}{[\chi^2 l^2 + n^2 + r^2 + q^2]^3}\right\}$$

with $\chi = \frac{\beta}{L}$ and

$$\mathcal{C}_f = -8\sum_{l,n=1}^{\infty}\frac{(-1)^{l+n}}{[l^2+n^2]^2} + \frac{16}{3}\sum_{l,n,r=1}^{\infty}\frac{(-1)^{l+n+r}}{[l^2+n^2+r^2]^2} - \frac{7\pi^4}{180} \approx -5.67$$

For the quark field the pressure changes sign from negative to positive as the temperature is increased: for $T \to 0$,

$$P_q(\beta, L) = n_c n_f \frac{\mathcal{C}_f}{\pi^2}\frac{1}{L^4} < 0;$$

for $T \to \infty$, the pressure is dominated by the term $\sim T^4$, which is positive.

The total Casimir pressure for the system of free, massless, quarks and gluons is given by

$$P_{qg}(\beta, L) = [n_c n_f\, f(\chi) + n_g\, g(\chi)]\;\frac{1}{L^4}\,. \tag{17.38}$$

For high temperatures both parcels give positive contributions to the Casimir pressure, but for low T, there exists a competition between quark and gluon contributions to determine the nature of the pressure, since they have opposite signs. Considering a hadron specified by two flavors, u and d, each with 3 colors and an octet of gluons, we have $n_g = 8$, $n_c = 3$ and $n_f = 2$; in this case, the low-T pressure is negative and a transition to positive pressure appears by raising the temperature. The value of $\chi = \beta/L$ at which the pressure vanishes, in the case of a cubic box, is the root of the equation $n_c n_f f(\chi) + n_g g(\chi) = 0$ which is obtained, numerically, as $\chi_c \approx 2.66$; this leads to the critical curve

$$T_c = \chi_c^{-1}\,\frac{1}{L}\,.$$

If we take $L \approx 1$fm, a length of the order of a hadron radius, one finds $T_c \approx 75\,\mathrm{MeV}$. Such an estimative provides a rough idea of the importance of Casimir effect in the

deconfinement transition for hadrons; this is to be compared with the estimated temperature, 175 MeV, for the deconfinement of quarks and gluons in lattice QCD. This points to the fact that we have to analyze the Casimir effect in QCD in more detail. The Casimir energy may change the deconfining temperature, estimated by using lattice gauge theory, in production of the quark-gluon plasma RHIC.

We have also to emphasize that, as for the case of the electromagnetic field, for fermions and non-abelian gauge fields the Casimir effect is also described as an effect of condensation of the vacuum, due to the use of the Bogoliubov transformation. These examples show that this method provides an important tool for studies of this nature, in particular for QCD. However, the case of a topology like S^3 has to be considered to get a better understanding of the role of the Casimir effect in the process of confinement and deconfinement of quarks and gluons.

Chapter 18

Compactified $\lambda\varphi^4$ Theory

This chapter is devoted to the compactified $\lambda\varphi^4$ theory, considering its N-component version. We work in the Euclidian space-time and treat compactified space and time coordinates with the generalized Matsubara formalism presented in Chapter 15. At $T = 0$ and with only one spatial dimension compactified, we compare the boundary-dependent renormalized coupling constant for the model with and without Wick ordering and discuss the breaking of the $O(N)$ symmetry induced by varying the compactification length. Taking the compactified model at finite temperature, the spontaneous symmetry breaking is considered and the equation for the critical curve in the $\beta \times L$ plane is derived.

18.1 Compactification of a d-dimensional subspace

Let us consider the N-component, massive, $\lambda\varphi^4$ theory described by the Lagrangian density,

$$\mathcal{L} = \frac{1}{2}\partial_\mu\varphi_a\partial^\mu\varphi_a + \frac{1}{2}m^2\varphi_a\varphi_a + \frac{u}{4!}(\varphi_a\varphi_a)^2, \tag{18.1}$$

in D-dimensional Euclidian space-time, where u is the coupling constant, m is the mass and summation over repeated flavor index a is assumed. To simplify the notation, in the following, we drop the flavor index, summation over them being understood in field products. We consider the system in thermal equilibrium with a reservoir at temperature β^{-1} and confined to a $(d-1)$-dimensional spatial parallelepiped box of sides L_j, $j = 2, 3, ..., d$. We use Cartesian coordinates $\mathbf{r} = (x_1, ..., x_d, \mathbf{z})$, where $\mathbf{z}$ is a $(D-d)$-dimensional vector, with corresponding momentum $\mathbf{k} = (k_1, ..., k_d, \mathbf{q})$, $\mathbf{q}$ being a $(D-d)$-dimensional vector in momentum space. Then we use a generalized Matsubara prescription, performing the following multiple replacements,

$$\int \frac{dk_i}{2\pi} \to \frac{1}{L_i}\sum_{n_i=-\infty}^{+\infty} ; \qquad k_i \to \frac{2n_i\pi}{L_i} , \quad i = 1, 2..., d. \tag{18.2}$$

This generalizes the standard procedure used in finite temperature field theory, as for instance in [283] We consider the large N limit, in which $N \to \infty$, $u \to 0$, with

$Nu = \lambda$ fixed.

We start from the well-known expression for the one-loop contribution for the effective potential for the non-compactified theory, as discussed in Chapter 4,

$$U_1(\varphi_0) = \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s} \left[\frac{\lambda\varphi_0^2}{2}\right]^s \int \frac{d^D k}{(2\pi)^D} \frac{1}{(k^2+m^2)^s}, \tag{18.3}$$

where m is the physical mass. For the *Wick-ordered* model, since in this case the tadpoles are suppressed, it is unnecessary to perform a mass renormalization to order $\frac{1}{N}$ in the one-loop approximation, the parameter m in Eq. (18.1) playing in this case the role of the physical mass.

We introduce dimensionless parameters $c^2 = m^2/4\pi^2\mu^2$, $(L_i\mu)^2 = a_i^{-1}$, $g = (u/8\pi^2)$, $(\varphi_0/\mu) = \phi_0$, where φ_0 is the normalized vacuum expectation value of the field (the classical field) and μ is a mass scale. In terms of these parameters and performing the Matsubara replacements Eq. (18.2), the one-loop contribution to the effective potential is written as,

$$\begin{aligned} U_1(\phi_0, a_1, ..., a_d) = \mu^D \sqrt{a_1 \cdots a_d} \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s} g^s \phi_0^{2s} \sum_{n_1,...,n_d=-\infty}^{+\infty} \\ \times \int \frac{d^{D-d}q}{(a_1 n_1^2 + \cdots + a_d n_d^2 + c^2 + \mathbf{q}^2)^s}. \end{aligned} \tag{18.4}$$

Using formula Eq. (10.12) to perform the integration over the $(D-d)$ non-compactified momentum variables, we obtain

$$U_1(\phi_0, a_1, ..., a_d) = \mu^D \sqrt{a_1 \cdots a_d} \sum_{s=1}^{\infty} f(D,d,s) g^s \phi_0^{2s} A_d^{c^2}(s - \frac{D-d}{2}; a_1, ..., a_d), \tag{18.5}$$

where

$$f(D,d,s) = \pi^{(D-d)/2} \frac{(-1)^{s+1}}{2s\Gamma(s)} \Gamma(s - \frac{D-d}{2}) \tag{18.6}$$

and $A_d^{c^2}$ is the Epstein-Hurwitz multivariable zeta function defined by,

$$\begin{aligned} A_d^{c^2}(\nu; a_1, ..., a_d) = \sum_{n_1,...,n_d=-\infty}^{+\infty} (a_1 n_1^2 + \cdots + a_d n_d^2 + c^2)^{-\nu} = \frac{1}{c^{2\nu}} \\ + 2 \sum_{i=1}^{d} \sum_{n_i=1}^{\infty} (a_i n_i^2 + c^2)^{-\nu} \\ + 2^2 \sum_{i<j=1}^{d} \sum_{n_i,n_j=1}^{\infty} (a_i n_i^2 + a_j n_j^2 + c^2)^{-\nu} + \cdots \\ + 2^d \sum_{n_1,...,n_d=1}^{\infty} (a_1 n_1^2 + \cdots + a_d n_d^2 + c^2)^{-\nu}. \end{aligned} \tag{18.7}$$

We proceed by generalizing to several variables the mode-sum regularization procedure described in [284, 285]. Using the identity,

$$\frac{1}{\Delta^\nu} = \frac{1}{\Gamma(\nu)} \int_0^\infty dt\; t^{\nu-1} e^{-\Delta t}, \tag{18.8}$$

we get

$$A_d^{c^2}(\nu; a_1, ..., a_d) = \frac{1}{\Gamma(\nu)} \int_0^\infty dt\; t^{\nu-1} e^{-c^2 t} \left[1 + 2 \sum_{i=1}^{d} T_1(t, a_i) + \right.$$
$$\left. + 2^2 \sum_{i,j=1}^{d} T_2(t, a_i, a_j) + \cdots + 2^d T_d(t, a_1, ..., a_d) \right], \tag{18.9}$$

where

$$T_1(t, a_i) = \sum_{n_i=1}^{\infty} e^{-a_i n_i^2 t}\,, \tag{18.10}$$

$$T_j(t, a_1, ..., a_j) = T_{j-1}(t, a_1, ..., a_{j-1}) T_1(t, a_j), \quad j = 2, ..., d. \tag{18.11}$$

Considering the property of the function T_1,

$$T_1(t, a_i) = -\frac{1}{2} + \sqrt{\frac{\pi}{a_i t}} \left[\frac{1}{2} + S(\frac{\pi^2}{a_i t}) \right], \tag{18.12}$$

where

$$S(x) = \sum_{n=1}^{\infty} e^{-n^2 x}, \tag{18.13}$$

we find that the surviving terms in Eq. (18.9) are proportional to $(a_1 \cdots a_d)^{-(1/2)}$. Therefore,

$$A_d^{c^2}(\nu; a_1, ..., a_d) = \frac{\pi^{\frac{d}{2}}}{\sqrt{a_1 \cdots a_d}} \frac{1}{\Gamma(\nu)} \int_0^\infty dt\; t^{(\nu - \frac{d}{2}) - 1} e^{-c^2 t}$$
$$\times \left[1 + 2 \sum_{i=1}^{d} S(\frac{\pi^2}{a_i t}) + 2^2 \sum_{i<j=1}^{d} S(\frac{\pi^2}{a_i t}) S(\frac{\pi^2}{a_j t}) \right.$$
$$\left. + \cdots + 2^d \prod_{i=1}^{d} S(\frac{\pi^2}{a_i t}) \right]. \tag{18.14}$$

Using the explicit form of the function $S(x)$ and the representation for Bessel functions of the third kind, K_ν,

$$2(a/b)^{\frac{\nu}{2}} K_\nu(2\sqrt{ab}) = \int_0^\infty dx\; x^{\nu-1} e^{-(a/x) - bx}, \tag{18.15}$$

we obtain

$$A_d^{c^2}(\nu;a_1,...,a_d) = \frac{2^{\nu-\frac{d}{2}+1}\pi^{2\nu-\frac{d}{2}}}{\sqrt{a_1\cdots a_d}\,\Gamma(\nu)}\left[2^{\nu-\frac{d}{2}-1}\Gamma(\nu-\frac{d}{2})(\frac{m}{\mu})^{d-2\nu}\right.$$
$$+2\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}(\frac{m}{\mu^2 L_i n_i})^{\frac{d}{2}-\nu}K_{\nu-\frac{d}{2}}(mL_i n_i)+\cdots$$
$$+2^d\sum_{n_1,\ldots,n_d=1}^{\infty}(\frac{m}{\mu^2\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}})^{\frac{d}{2}-\nu}$$
$$\left.K_{\nu-\frac{d}{2}}(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2})\right]. \tag{18.16}$$

Taking $\nu = s-(D-d)/2$ in Eq. (18.16), the one-loop correction to the effective potential in D dimensions with a compactified d-dimensional subspace is

$$U_1(\phi_0,a_1,...,a_d) = \sum_{s=1}^{\infty}u^s\varphi_0^{2s}h(D,s)\left[2^{s-\frac{D}{2}-2}\Gamma(s-\frac{D}{2})m^{D-2s}\right.$$
$$+\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}(\frac{m}{L_i n_i})^{\frac{D}{2}-s}K_{\frac{D}{2}-s}(mL_i n_i)$$
$$+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}})^{\frac{D}{2}-s}$$
$$\times K_{\frac{D}{2}-s}(m\sqrt{L_i^2n_i^2+L_j^2n_j^2})+\cdots$$
$$+2^{d-1}\sum_{n_1,\cdots n_d=1}^{\infty}(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}})^{\frac{D}{2}-s}$$
$$\left.\times K_{\frac{D}{2}-s}(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2})\right], \tag{18.17}$$

with

$$h(D,s) = \frac{1}{2^{D/2-s-1}\pi^{D/2-2s}}\frac{(-1)^{s+1}}{s\Gamma(s)}, \tag{18.18}$$

where we have recovered the original parameters and eliminated the auxiliary mass scale μ.

18.2 Subtraction scheme

We consider in the following the zero external momentum four-point function, which will be used to define the coupling constant. The four-point function to leading order

in $1/N$ is given by the sum of all diagrams of the type depicted in Fig. 18.1. This gives

$$\Gamma_D^{(4)}(0,\{L_i\}) = \frac{u}{1+Nu\Sigma(D,\{L_i\})}, \tag{18.19}$$

where $\Sigma(D,\{L_i\})$ corresponds to the one-loop (bubble) subdiagram in Fig. 18.1. To obtain an expression for $\Sigma(D,\{L_i\})$, we use concurrently dimensional and zeta function analytic regularizations, to evaluate formally the integral over the continuous momenta and the summation over the Matsubara frequencies. These results contain terms proportional to Γ-functions which are singular for even dimensions. We subtract them to get finite quantities. To have an uniform procedure in any dimension, these subtractions are also performed for odd dimension D, where no poles of Γ-functions are present. In what follows this subtraction procedure is called *renormalization*, although it is not a perturbative renormalization, and the quantities obtained are denoted *renormalized* quantities.

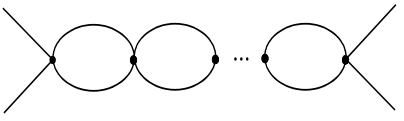


Fig. 18.1 Typical diagram contributing to the four-point function at leading order in $\frac{1}{N}$. To each vertex there is a factor $\frac{\lambda}{N}$ and for each single bubble a color circulation factor of N.

To proceed, we use the normalization conditions,

$$\frac{\partial^2}{\partial\varphi^2}U(D,\{L_i\})\bigg|_{\varphi_0=0} = m^2 \tag{18.20}$$

and

$$\frac{\partial^4}{\partial\varphi^4}U(D,\{L_i\})\bigg|_{\varphi_0=0} = \lambda. \tag{18.21}$$

We deduce that formally the single bubble function, $\Sigma(D,\{L_i\})$, is obtained from the coefficient of the fourth power of the field ($s=2$) in Eq. (18.17). Such a coefficient is divergent for even dimensions and a renormalization procedure is needed. Then using Eqs. (18.21) and (18.17) we can write $\Sigma(D,\{L_i\})$ in the form,

$$\Sigma(D,\beta,L) = \Sigma_1(D) + \Sigma_2(D,\{L_i\}), \tag{18.22}$$

where the L_i-dependent contribution $\Sigma_2(D,\{L_i\})$, coming from the second term

between brackets in Eq. (18.17), is given by

$$\Sigma_2(D,\{L_i\}) = \frac{3}{2}\frac{1}{(2\pi)^{D/2}}\left[\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_i n_i}\right)^{\frac{D}{2}-2} K_{\frac{D}{2}-2}(mL_i n_i) + \right.$$
$$+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}}\right)^{\frac{D}{2}-2}$$
$$\times K_{\frac{D}{2}-2}\left(m\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}\right) + \cdots +$$
$$+ 2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}}\right)^{\frac{D}{2}-2}$$
$$\left.\times K_{\frac{D}{2}-2}\left(m\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}\right)\right] \tag{18.23}$$

The first term between brackets in Eq. (18.17) gives

$$\Sigma_1(D) \propto \Gamma(2-\frac{D}{2})m^{D-4}. \tag{18.24}$$

We find that, for even dimensions $D \geq 4$, $\Sigma_1(D)$ is divergent, due to the pole of the Γ-function. Accordingly this term must be subtracted to give the renormalized single bubble function $\Sigma_R(D,\{L_i\})$,

$$\Sigma_R(D,\{L_i\}) = \Sigma_2(D,\{L_i\}). \tag{18.25}$$

It is important to note that $\Sigma_1(D)$ does not depend on $\{L_i\}$. As mentioned before, the term $\Sigma_1(D)$ is also subtracted for odd dimension D also which corresponds to a finite renormalization. Using properties of Bessel functions, we find from Eq. (18.23) that, for any dimension D, $\Sigma_R(D,\beta,L)$ satisfies the conditions

$$\lim_{L_i\to\infty}\Sigma_R(D,\{L_i\}) = 0\,, \qquad \lim_{L_i\to 0}\Sigma_R(D,\{L_i\}) \to \infty, \tag{18.26}$$

and $\Sigma_R(D,\{L_i\}) > 0$ for any values of D, and L_i.

The L_i-dependent renormalized coupling constant $\lambda_R(D,\{L_i\})$ to the leading order in $1/N$ is defined by,

$$N\Gamma_D^{(4)}(0,\{L_i\}) \equiv \lambda_R(D,\{L_i\}) = \frac{\lambda}{1+\lambda\Sigma_R(D,\{L_i\})}. \tag{18.27}$$

The renormalized coupling constant in the absence of boundaries is,

$$\lambda_R(D) = N\lim_{L_i\to\infty}\Gamma_{D,R}^{(4)}(0,\{L_i\}) = \lambda, \tag{18.28}$$

where we have used Eq. (18.26). Thus we conclude that we have made a choice of the renormalization scheme such that the constant $\lambda = Nu$ introduced in the Lagrangian corresponds to the physical large N coupling constant in the unbounded space. Then the L_i-dependent renormalized coupling constant is,

$$\lambda_R(D,\{L_i\}) = \frac{\lambda}{1+\lambda\Sigma_R(D,\{L_i\})}. \tag{18.29}$$

18.3 The zero-temperature compactified model

We study in this section the boundary behavior of the mass and the coupling constant when only one spatial dimension is compactified. We consider the cases with Wick-ordering and without Wick-ordering.

18.3.1 *Wick-ordered model*

As we mentioned earlier, no mass renormalization is needed if we take the Wick-ordered model. In the case of only one compactified spatial dimension, particularizing Eq. (18.17) for $d = 1$, $L_1 = L$ for $d = 1$, we obtain from Eqs. (18.21) and (18.25),

$$\Sigma_R(D, L) = \frac{3}{2}\frac{1}{(2\pi)^{D/2}}\sum_{n=1}^{\infty}\left[\frac{m}{nL}\right]^{D/2-2} K_{\frac{D}{2}-2}(mnL), \tag{18.30}$$

which gives the L -dependent renormalized coupling constant,

$$\lambda_R(D, L) = \frac{\lambda}{1 + \lambda\Sigma_R(D, L)}. \tag{18.31}$$

An exact result is obtained in dimension $D = 3$. Using [286],

$$K_{n+\frac{1}{2}}(z) = K_{-n-\frac{1}{2}}(z), \qquad K_{\frac{1}{2}}(z) = \sqrt{\frac{\pi}{2z}}e^{-z}, \tag{18.32}$$

we obtain the coupling constant in the large N limit,

$$\lambda_R^W(D = 3, L) = \frac{8\pi m\lambda(e^{mL} - 1)}{8m\pi(e^{mL} - 1) + 3\lambda}, \tag{18.33}$$

where the superscript W is used to indicate explicitly Wick-ordering. A plot of $\lambda_R^W(D = 3, L)$ is given in Fig. 18.2.

18.3.2 *The model without Wick-ordering*

The effect of suppression of Wick-ordering is that the renormalized mass cannot be taken as the coefficient m of the term $\varphi_a\varphi_a$ in the Lagrangian. We must take an L-corrected physical mass which is obtained from Eq. (18.20). We get,

$$m_R^2(L) = m^2 + \frac{4\lambda(N + 2)}{N(2\pi)^{D/2}}\sum_{n=1}^{\infty}\left[\frac{m_R(L)}{Ln}\right]^{D/2-1} K_{\frac{D}{2}-1}(m_R(L)nL). \tag{18.34}$$

To obtain the L-dependent coupling constant the constant mass parameter m should be replaced in Eq. (18.31) and Eq. (18.30) by the L-corrected mass $m_R(L)$ and the resulting system of equations should be solved with respect to $m_R(L)$. Exact closed expressions are not possible, since it would be equivalent to solving the Dyson-Schwinger equations exactly.

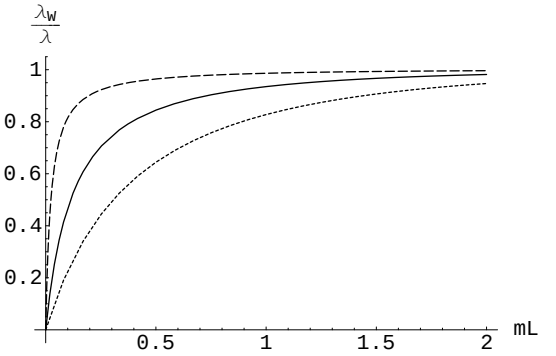


Fig. 18.2 Renormalized coupling constant (in units of $\frac{1}{N}$) for the Wick-ordered model as a function of the separation between the planes in dimension $D = 3$. The dashed, full and dotted lines correspond, respectively, to $\lambda/m = 0.2, 1.0$ and 3.0.

Nevertheless, results can be obtained, both analytic and numerical, for $D = 4$. We take an integral representation for the Bessel function [286],

$$K_\nu(z) = \frac{\sqrt{\pi}}{\Gamma(\nu + \frac{1}{2})}(\frac{z}{2})^\nu \int_1^\infty e^{-zt}(t^2-1)^{\nu-\frac{1}{2}}dt, \tag{18.35}$$

valid for $Re(\nu) > -\frac{1}{2}$ and $|arg(z)| < \frac{\pi}{2}$. Using this representation, the L-dependent renormalized mass is

$$m_R^2(L) = m^2 + \frac{4\lambda(N+2)}{N}F(D)m_R^{D-2}(L) \times \int_{m_R(L)L}^\infty \frac{d\tau}{m_R(L)L}\left[\left(\frac{\tau}{m_R(L)L}\right)^2 - 1\right]^{\frac{D-3}{2}} \frac{1}{e^\tau - 1}, \tag{18.36}$$

where

$$F(D) = \frac{1}{2^D}\frac{1}{\pi^{\frac{D-1}{2}}}\frac{1}{\Gamma(\frac{D-1}{2})}.$$

When D is odd, the power $(D-3)/2$ is an integer and Newton binomial theorem gives an algebraic equation for $m_R^2(L)$. When D is even the expansion of

$$\left[\left(\frac{\tau}{m_R(L)L}\right)^2 - 1\right]^{\frac{D-3}{2}}$$

yields an infinite power series leading to

$$m_R^2(L) = m^2 + \frac{4\lambda(N+2)}{NL^{D-2}}\sum_{k=0}^\infty g(D,k)(m_R(L)L)^{2k}\int_{m_R(L)L}^\infty d\tau \frac{\tau^{D-3-2k}}{e^\tau - 1} \tag{18.37}$$

where

$$g(D,k) = F(D)(-1)^k C^k_{\frac{D-3}{2}}$$

and the C's are the generalized binomial coefficients,

$$C_n^k = \frac{n!}{k!(n-k)!}.$$

For $k = 0$, the Debye integral is

$$I(x,n) = \int_x^\infty d\tau \frac{\tau^n}{e^\tau - 1} = \sum_{q=1}^\infty e^{-qx}\, x^n \left(\frac{1}{q} + \frac{n}{q^2} + \cdots + \frac{n!}{q^{n+1}}\right), \tag{18.38}$$

which is valid for $x > 0$ and $n \geq 1$. For $k > D-3)/2$, the exponent of τ in Eq. (18.37) becomes negative and the integral is undefined. Then for small values of L, a generalization to negative odd powers of the argument of the integrand in the Debye integral can be carried out [245] and the integral has the expansion

$$J(u,n) = \int_u^\infty d\tau \frac{\tau^{-n}}{e^\tau - 1} = -\sum_{q=0, q\neq n}^\infty \frac{B_q}{q!}\frac{u^{q-n}}{q-n} - \frac{1}{n!}B_n \ln u + \alpha_n \tag{18.39}$$

where B_k are the Bernoulli numbers and α_n is a constant. Now using this result in Eq. (18.37) we have, in the small L regime, the following expression

$$m_R^2(L) = m^2 + \frac{4\lambda(N+2)}{NL^{D-2}}\left[A(L,D) + B(L,D)\right], \tag{18.40}$$

where,

$$A(L,D) = \sum_{k=0}^{k\leq \frac{D-3}{2}} g(D,k)(m_R(L)L)^{2k} I(m_R(L)L, D-3-2k) \tag{18.41}$$

and

$$B(L,D) = \sum_{k>\frac{D-3}{2}}^{k=\infty} g(D,k) m_R(L)L)^{2k} J(m_R(L)L, D-3-2k). \tag{18.42}$$

This provides a non-perturbative expression for the L-corrected renormalized mass in the small L regime, for even dimensional Euclidean space. In arbitrary even dimensions, for L sufficiently small, the series in Eq. (18.42) can be truncated, giving an approximate algebraic equation for the L-corrected mass. Use this expression in Eq. (18.31) gives the L-corrected coupling constant in the small L regime. We will not perform these manipulations here. Instead, we get some exact results for $D = 3$.

In dimension $D = 3$, using Eqs. (18.32) the sum over n in Eq. (18.34) can be performed exactly. We obtain a closed transcendental equation for the L-corrected renormalized mass,

$$m_R^2(L) = m^2 - \frac{\lambda(N+2)}{N\pi L}\log(1 - e^{-m_R(L)L}), \tag{18.43}$$

or, in the large N limit,

$$m_R^2(L) = m^2 - \frac{\lambda}{\pi L}\log(1 - e^{-m_R(L)L}). \tag{18.44}$$

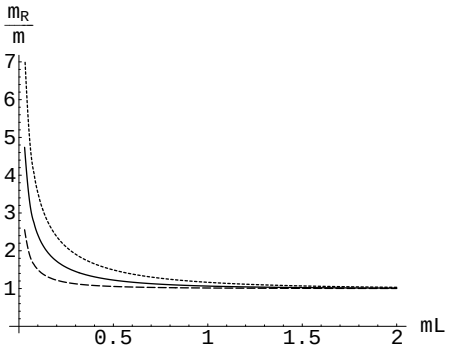


Fig. 18.3 Renormalized mass for the non-Wick-ordered model as a function of the spacing L between the planes in dimension $D = 3$. The dashed, full and dotted lines correspond, respectively, to $\lambda/m = 0.2, 1.0$ and 3.0.

The large N renormalized mass is plotted as a function of L in Fig. 18.3.

An exact expression for the coupling constant in the large N limit as a function of the renormalized L-dependent mass is

$$\lambda_R(D=3,L) = \frac{8\pi m_R(L)\lambda(e^{m_R(L)L}-1)}{8\pi m_R(L)(e^{m_R(L)L}-1)+3\lambda}. \tag{18.45}$$

In Fig. 18.4 the L-corrected coupling constant for the non-Wick-ordered model in dimension $D = 3$, in the same scale used in Fig. 18.2 is presented. Comparison of the coupling constant for Wick-ordered and without Wick-ordering shows quite different behaviors. The coupling constant without Wick-ordering slightly decreases for decreasing values of L until some minimum value and then starts to increase. In the Wick-ordered model the coupling constant tends monotonically to zero as L goes to zero. In the non-Wick ordered model it has a non-vanishing value even for very small values of L. In fact, numerical analysis of the solution of Eq. (18.45) shows that $m_R(L)L \to 0$ and $m_R^2(L)L \to \infty$ as $L \to 0$ and, therefore, the L-corrected non-Wick-ordered coupling constant has a non-vanishing value at $L = 0$. This value is equal to the free space value λ. As a general conclusion it can be said that for the non-Wick-ordered model the L-dependent renormalized coupling constant departs slightly to lower values, from the free space coupling constant. Furthermore this departure is smaller for smaller values of λ.

For space dimension $D > 2$ the correction in L to the squared mass is positive and the L-dependent squared mass is a monotonically increasing function of $\frac{1}{L}$. If we start in the disordered phase with a negative squared mass m^2, the model exhibits spontaneous symmetry breaking of the $O(N)$ symmetry to $O(N-1)$, but for a sufficiently small critical value of L the symmetry is restored. The critical value of L, L_c is defined as the value of L for which the inverse squared correlation

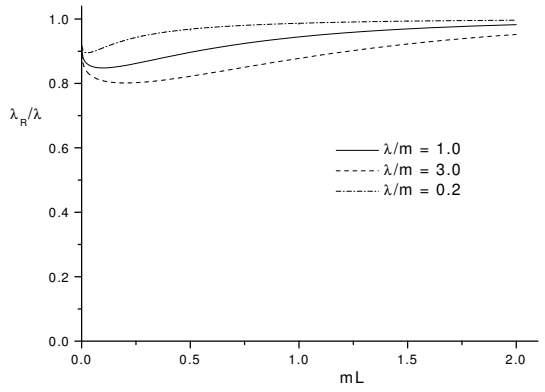


Fig. 18.4 Renormalized coupling constant (in units of $\frac{1}{N}$) for the non-Wick ordered model as a function of the distance between the planes in dimension $D = 3$.

length, $\xi^{-2}(L, \varphi_0)$, vanishes in the gap equation,

$$\xi^{-2}(L,\varphi_0) = m^2 + 2\lambda\varphi_0^2 + \frac{2\lambda(N+2)}{NL}\sum_{n=-\infty}^{+\infty}\int\frac{d^{D-1}k}{(2\pi)^{D-1}}\,\frac{1}{\mathbf{k}^2+\omega_n^2+\xi^{-2}(L,\varphi_0)}, \tag{18.46}$$

where φ_0 is different from zero in the ordered phase. In the neighborhood of the critical point φ_0 vanishes and the gap equation reduces to Eq. (18.34). In the small L regime, we may use an asymptotic formula for small values of the argument of Bessel functions,

$$K_\nu(z) \approx \frac{1}{2}\Gamma(\nu)\left(\frac{z}{2}\right)^{-\nu} \quad (z \sim 0\,; \quad Re(\nu) > 0) \tag{18.47}$$

in Eq. (18.34). Then taking $m_R(L) = 0$ in the resulting equation, it is not difficult to obtain the large N critical value of L in the Euclidian space dimension D ($D > 2$),

$$(L_c)^{D-2} = -\frac{4\lambda g(D)}{m^2}, \tag{18.48}$$

where

$$g(D) = \frac{1}{4\pi^{\frac{D}{2}}}\Gamma(\frac{D}{2}-1)\zeta(D-2), \tag{18.49}$$

$\zeta(D-2)$ being the Riemann zeta function. For $D = 3$ the zeta function in $g(D)$ has a pole and a subtraction procedure is needed: we use the Laurent expansion of $\zeta(z)$,

$$\zeta(z) = \frac{1}{z-1} + \gamma_0 - \gamma_1\,(z-1) + \cdots\,, \tag{18.50}$$

where $\gamma_0 \simeq 0.577$ and $\gamma_1 \simeq 0.0728$ (the Euler-Mascheroni and the first Stieltjes constants, respectively). We get the critical value of L in dimension $D = 3$,

$$(L_c) = -\frac{\lambda\gamma_0}{16m^2}\pi^{-\frac{5}{2}}, \tag{18.51}$$

The result above extends to a phase transition driven by a spatial boundary, estimates and numerical simulations for temperature-driven transitions [287, 288].

Taking the Wick-ordering, which eliminates all contributions from the tadpoles, we decouple in some sense the boundary behavior of the coupling constant from boundary behavior of the mass. Wick-ordering is a useful and simplifying procedure in applications of the field theory to particle physics, but the same is not necessarily true in applications of field theory to investigate critical phenomena, where the contribution from tadpoles are physically significant. As a consequence of the suppression of Wick-ordering the boundary behavior of the coupling constant is sensibly modified with respect to the monotonic behavior in the Wick-ordered case (see comments following Eq. (18.45)).

18.4 The compactified model at finite temperature: spontaneous symmetry breaking

We consider in this section the non-Wick-ordered model; we get the β- and L-corrected effective potential to one-loop approximation from Eq. (18.17), taking $d = 2$, with $L_1 = \beta$ and $L_2 = L$. Then the renormalized physical mass is obtained from Eqs. (18.20) and (18.17),

$$\begin{aligned} m^2(\beta, L) = m^2 + \frac{4\mu^{4-D}\lambda}{(2\pi)^{D/2}} \\ \times \left[\sum_{n=1}^{\infty} (\frac{m}{n\beta})^{\frac{D}{2}-1} K_{\frac{D}{2}-1}(n\beta m) + \sum_{n=1}^{\infty} (\frac{m}{nL})^{\frac{D}{2}-1} K_{\frac{D}{2}-1}(nLm) \right. \\ \left. + 2 \sum_{n_1,n_2=1}^{\infty} (\frac{m}{\sqrt{\beta^2 n_1^2 + L^2 n_2^2}})^{\frac{D}{2}-1} K_{\frac{D}{2}-1}(m\sqrt{\beta^2 n_1^2 + L^2 n_2^2}) \right] \end{aligned} \tag{18.52}$$

Using Eq. (18.32), we obtain for the physical mass and the renormalized one-loop diagram, the following expressions

$$\begin{aligned} \Sigma_R(D, \beta, L)(\beta, L) = \frac{3\mu}{8\pi m} \left[(e^{m\beta} - 1)^{-1} + (e^{mL} - 1)^{-1} \right. \\ \left. + 2 \sum_{n_1,n_2=1}^{\infty} e^{-m\sqrt{\beta^2 n_1^2 + L^2 n_2^2}} \right], \end{aligned} \tag{18.53}$$

and

$$\begin{aligned} m^2(\beta, L) = m^2 + \frac{\mu\lambda}{\pi} \left[-\frac{\log(1 - e^{-m\beta})}{\beta} - \frac{\log(1 - e^{-mL})}{L} \right. \\ \left. + 2 \sum_{n_1,n_2=1}^{\infty} \frac{e^{-m\sqrt{\beta^2 n_1^2 + L^2 n_2^2}}}{\sqrt{\beta^2 n_1^2 + L^2 n_2^2}} \right]. \end{aligned} \tag{18.54}$$

18.4.1 *Mass behavior and critical curve*

The critical curve is a curve in the $\beta \times L$ plane and is defined by the vanishing of, $\xi^{-2}(\beta, L, \varphi_0)$, the inverse squared correlation length, in the gap equation,

$$\begin{aligned}\xi^{-2}(\beta, L, \varphi_0) = m^2 + \lambda\varphi_0^2 \\ + \frac{\lambda(N+2)}{2N\beta L} \sum_{n_1,n_2=-\infty}^{\infty} \\ \times \int \frac{d^{D-2}q}{(2\pi)^{D-2}} \frac{1}{\mathbf{q}^2 + (\frac{2\pi n_1}{\beta})^2 + (\frac{2\pi n_2}{L})^2 + \xi^{-2}(\beta, L, \varphi_0)},\end{aligned} \tag{18.55}$$

where φ_0 is different from zero in the ordered phase.

Close to the critical curve, φ_0 vanishes and the gap equation at one-loop order reduces, in the large N limit, to Eq. (18.52). In the neighborhood of criticality, $m^2 \approx 0$, the asymptotic formula for small values of the argument of Bessel functions, Eq. (18.47) may be used and Eq. (18.52) becomes,

$$\begin{aligned}m^2(\beta, L) \approx m^2 + \frac{4\lambda\mu^{4-D}}{(\pi)^{D/2}}\Gamma\left(\frac{D}{2} - 1\right) \\ \times \left[(\beta^{2-D} + L^{2-D})\zeta(D-2) + 2E_2\left(\frac{D-2}{2}; \beta, L\right)\right],\end{aligned} \tag{18.56}$$

where $\zeta(D-2)$ is the Riemann zeta function,

$$\zeta(D-2) = \sum_{n=1}^{\infty} \frac{1}{n^{D-2}}, \tag{18.57}$$

and $E_2((D-2)/2; \beta, L)$ is the two-variable Epstein zeta function,

$$E_2\left(\frac{D-2}{2}; \beta, L\right) = \sum_{n_1,n_2=1}^{\infty} \frac{1}{(\beta^2 n_1^2 + L^2 n_2^2)^{\frac{D-2}{2}}}\,. \tag{18.58}$$

$\zeta(D-2)$ has an analytical extension to the whole complex D-plane, having an unique simple pole of residue 1 at $D = 3$.

We can also obtain an analytic continuation of the two-variable Epstein zeta function, writing it in terms of the one-variable Riemann zeta functions plus an analytic part, if we use the analytic extension of the one-variable Epstein-Hurwitz zeta function [284, 289],

$$\begin{aligned}\sum_{n=1}^{\infty} \frac{1}{(n^2 + p^2)^{\nu}} = -\frac{1}{2}\frac{1}{p^{2\nu}} + \frac{\sqrt{\pi}}{2p^{2\nu-1}\Gamma(\nu)} \\ \times \left[\Gamma\left(\nu - \frac{1}{2}\right) + 4\sum_{n=1}^{\infty}(\pi p n)^{\nu-\frac{1}{2}} K_{\nu-\frac{1}{2}}(2\pi p n)\right].\end{aligned} \tag{18.59}$$

Using this expression to perform first the summation over n_2 in Eq. (18.58), we get

$$E_2\left(\frac{D-2}{2};\beta,L\right) = \frac{1}{L^{D-2}}\sum_{n_1=1}^{\infty}\left(\sum_{n_2=1}^{\infty}\frac{1}{(n_2^2+L^{-2}\beta^2 n_1^2)^{\frac{D-2}{2}}}\right)$$
$$= -\frac{1}{2}\frac{1}{\beta^{D-2}}\,\zeta(D-2) + \frac{\sqrt{\pi}}{2}\frac{\Gamma\left(\frac{D-3}{2}\right)}{\Gamma\left(\frac{D-2}{2}\right)}\frac{1}{L\beta^{D-3}}\,\zeta(D-3)$$
$$+\frac{\sqrt{2\pi}}{\Gamma\left(\frac{D-2}{2}\right)}\frac{1}{L}\sum_{n_1,n_2=1}^{\infty}\left(\frac{\pi}{L\beta}\frac{n_1}{n_2}\right)^{\frac{D-3}{2}}K_{\frac{D-3}{2}}\left(2\pi\frac{\beta}{L}n_1n_2\right).$$

However, under the interchange $\beta \leftrightarrow L$ this expression is not symmetrical, a symmetry that is expected from the definition of the two-variable Epstein zeta function. In order to preserve the $\beta \leftrightarrow L$ symmetry of Eq. (18.58), we adopt a symmetrized summation and define

$$E_2\left(\frac{D-2}{2};\beta,L\right) = \frac{1}{2}\left[\sum_{n_1=1}^{\infty}\left(\sum_{n_2=1}^{\infty}\frac{1}{(\beta^2n_1^2+L^2n_2^2)^{\frac{D-2}{2}}}\right)\right.$$
$$\left.+\sum_{n_2=1}^{\infty}\left(\sum_{n_1=1}^{\infty}\frac{1}{(\beta^2n_1^2+L^2n_2^2)^{\frac{D-2}{2}}}\right)\right], \qquad (18.60)$$

where the parentheses indicate that the sums must be performed in this order.

The symmetric analytical extension of the two-variables Epstein function [285] is then given by

$$E_2\left(\frac{D-2}{2};\beta,L\right) = -\frac{1}{4}\left(\frac{1}{\beta^{D-2}}+\frac{1}{L^{D-2}}\right)\zeta(D-2)$$
$$+\frac{\sqrt{\pi}\,\Gamma\left(\frac{D-3}{2}\right)}{4\,\Gamma\left(\frac{D-2}{2}\right)}\left(\frac{1}{L\beta^{D-3}}+\frac{1}{\beta L^{D-3}}\right)\zeta(D-3)$$
$$+\frac{\sqrt{\pi}}{\Gamma\left(\frac{D-2}{2}\right)}W_2\left(\frac{D-3}{2};\beta,L\right), \qquad (18.61)$$

where the analytic part W_2 is

$$W_2\left(\frac{D-3}{2};\beta,L\right) = \frac{1}{L}\sum_{n_1,n_2=1}^{\infty}\left(\frac{\pi}{L\beta}\frac{n_1}{n_2}\right)^{\frac{D-3}{2}}K_{\frac{D-3}{2}}\left(2\pi\frac{\beta}{L}n_1n_2\right)$$
$$+\frac{1}{\beta}\sum_{n_1,n_2=1}^{\infty}\left(\frac{\pi}{\beta L}\frac{n_1}{n_2}\right)^{\frac{D-3}{2}}K_{\frac{D-3}{2}}\left(2\pi\frac{L}{\beta}n_1n_2\right). \qquad (18.62)$$

This procedure will be generalized for multivariable Epstein zeta functions in Chapter 21.

Then we find that the function $E_2((D-2)/2;\beta,L)$ has two simple poles at $D=4$ and $D=3$. The solution of Eq. (18.56) for $m_R(\beta,L)=0$ and $m^2<0$ defines the critical curve in dimension D, with $D\neq 4$ and $D\neq 3$, as

$$m^2+\frac{4\lambda\mu^{4-D}}{(\pi)^{D/2}}\Gamma\left(\frac{D}{2}-1\right)\left[(\beta_c^{2-D}+L_c^{2-D})\zeta(D-2)+2E_2\left(\frac{D-2}{2};\beta_c,L_c\right)\right]=0. \qquad (18.63)$$

For $D = 4$ the generalized zeta function E_2 has a pole and for $D = 3$ both the Riemann zeta function and E_2 have poles. We cannot obtain a critical curve in dimensions $D = 4$ and $D = 3$ by a limiting procedure from Eq. (18.63). For $D = 4$, which corresponds to the physically interesting case of the system at $T \neq 0$ confined between two parallel planes embedded in a 3-dimensional Euclidean space, Eqs. (18.56) and (18.63) are meaningless. To obtain a critical curve in $D = 4$, a regularization procedure is carried out using Eq. (18.50). Then from Eq. (18.61), we redefine the mass as,

$$\lim_{D\to 4^-}\left[m^2 + \frac{1}{D-4}\frac{4\lambda}{\pi^2\beta L}\right] = m^2 \,, \tag{18.64}$$

in terms of which we obtain the critical curve in dimension $D = 4$,

$$m^2 + \frac{\lambda}{3}\left(\frac{1}{\beta_c^2} + \frac{1}{L_c^2}\right) + \frac{\pi\gamma_0}{\beta_c L_c} + 4\sqrt{\pi}W_2(2;\beta_c, L_c) = 0 \,, \tag{18.65}$$

where we have used $\zeta(2) = \pi^2/6$ and $\Gamma(1/2) = \sqrt{\pi}$.

We have presented a formalism that accounts for compactification of the $\lambda\varphi^4$ theory in a d-dimensional subspace. This includes both cases of only spatial coordinates and simultaneous compactification of time and spatial coordinates. In both cases, equations for the L- and β and L-dependent mass and coupling constant are derived. A critical value for L in the case $d = 1$ is obtained and an equation for the critical curve in the $\beta \times L$ plane is derived.

The case of simultaneous compactification of time and spatial coordinates leads to the study of spontaneous symmetry breaking in a spatially compactified theory. In fact, consider the system initially at a high enough temperature such that, for a small enough, but *fixed*, value of L, $m_R^2(\beta, L) > 0$. In this case, the potential

$$V(\varphi) = \frac{1}{2}m_R^2(\beta, L)\varphi^2 + \lambda(\beta, L)\varphi^4 \tag{18.66}$$

has only one minimum at $\varphi = 0$. As the temperature is lowered, eventually, $m_R^2(\beta, L)$ vanishes. As the temperature is lowered further, $m_R^2(\beta, L)$ becomes negative. When this situation is attained the potential has two minima, the original symmetry is spontaneously broken.

Chapter 19

Phase Transitions in Confined Systems: Application to Superconducting Films

The idea of describing thermodynamical phases through classical (in general complex) fields, the order parameters, was first introduced by Landau [290]. The free energy of a system is written as a functional of the order parameter, $\phi(\mathbf{r})$, and the equilibrium state is obtained by a variational principle. First- and second-order phase transitions can be described by choosing an appropriated expansion of the free energy functional around the critical point.

19.1 Overview

For a second-order phase transition, the free energy [291] is written (in natural units, $\hbar = c = k_B = 1$) as

$$F[\phi(\mathbf{r})] = \int d\mathbf{r}\, \mathcal{F}(\phi(\mathbf{r}), \nabla\phi(\mathbf{r}))\,, \tag{19.1}$$

with the free energy density given by

$$\mathcal{F}(\phi(\mathbf{r}), \nabla\phi(\mathbf{r})) = |\nabla\phi(\mathbf{r})|^2 + a(T)\,|\phi(\mathbf{r})|^2 + \frac{b}{2}\,|\phi(\mathbf{r})|^4\,, \tag{19.2}$$

where $a(T) = \alpha(T - T_0)$, T_0 being the critical temperature, and $b > 0$ is independent of the temperature T. The truncated expansion Eq. (19.2), is assumed to be correct near the transition point, where the order parameter is close to zero. In equilibrium, the order parameter satisfies the equation

$$\nabla^2\phi(\mathbf{r}) - a(T)\phi(\mathbf{r}) - b|\phi(\mathbf{r})|^2\phi(\mathbf{r}) = 0. \tag{19.3}$$

Neglecting spatial variations of ϕ, the possible solutions are $\phi_0 = 0$ and $\phi_0^2 = -a(T)/b$; the null solution is stable when $T > T_0$, while the other one gives the true minimum of the free energy for $T < T_0$, corresponding to the ordered phase. The spatial changes of the order parameter $\phi(\mathbf{r})$ are characterized by the Ginzburg-Landau (GL) coherence length $\eta^2 = 1/|a(T)|$.

In this chapter, our aim is to address the question of second-order phase transitions for systems with compactified dimensions (that is, in films, wires and grains), using methods of the quantum theory of fields.

Under a field theoretical point of view, the Ginzburg-Landau free energy density in the absence of external fields, Eq. (19.2), can be considered as the Hamiltonian density for the Euclidean self-interacting scalar field theory, the $\lambda\phi^4$ model. Therefore, we take advantage of this similarity to explore the powerful methods of quantum field theory to treat fluctuations of the order parameter in the GL model.

A large amount of work has already been done on applications of the Ginzburg-Landau model to the study of the superconducting transition, both in the single component and in the N- component versions of the model, using the renormalization group approach [292–298]. Questions concerning stability and the existence of phase transitions may also be raised if one considers field theories in the presence of spatial boundaries. In particular, an analysis of the renormalization group in finite size geometries can be found in [133, 299]. These studies have been performed to take into account boundary effects on scaling laws. The existence of phase transitions would be in this case associated to some spatial parameters describing the breaking of translational invariance, for instance the distance L between planes confining the system. Also in other contexts, the influence of boundaries in the behavior of systems undergoing transitions have been investigated [300, 301].

Here, we shall take a distinct route, analyzing directly the effects of boundaries on the transition. Such confined systems will be modelled by compactifying spatial dimensions. Compactification will be engendered as a generalization of the Matsubara (imaginary-time) prescription to account for constraints on the spatial coordinates. In the original Matsubara formalism, the time is rotated to the imaginary axis, $t \to i\tau$ where τ (the Euclidean time) is limited to the interval $0 \leq \tau \leq \beta$, with $\beta = 1/T$ standing for the inverse temperature. The fields then fulfill periodic (bosons) or anti-periodic (fermions) boundary conditions and are compactified on the τ-axis in an S^1-topology, the circumference of length β. Such a formalism leads to the description of a system in thermal equilibrium at the temperature β^{-1}. Since in an Euclidean field theory space and time are treated on the same footing, one can envisage a generalization of the Matsubara approach to any set of spatial coordinates as well [231, 232, 302, 303] as presented in Chapter 15. In such a case, however, the interpretation of this prescription is quite different: it provides a general and practical way to account for systems confined in limited regions of space at finite temperature. Distinctly, here, we will be concerned with stationary field theories and shall employ the generalized Matsubara prescription to implement spatial compactification. No imaginary-time compactification will be done, the temperature will be introduced through the mass parameter in the Hamiltonian.

Let us consider a system described by an N-component bosonic field, $\varphi_a(\mathbf{r})$ with $a = 1, 2, ..., N$, in a D-dimensional Euclidean space, constrained to a d-dimensional ($d \leq D$) parallelepiped box with edges $L_1, L_2, \ldots, L_d$, satisfying periodic boundary conditions on its faces, that is, $\forall a$, $\varphi_a(x_i \leq 0, \mathbf{z}) = \varphi_a(x_i \geq L_i, \mathbf{z})$. The generating

functional for correlation functions is

$$\mathcal{Z}[\varphi_a] = \int \mathcal{D}\varphi_1 \cdots \mathcal{D}\varphi_N \times \exp\left[- \int_0^{L_1} dx_1 \cdots \int_0^{L_d} dx_d \int d^{D-d}\mathbf{z}\, \mathcal{H}(\varphi(\mathbf{r}), \nabla\varphi(\mathbf{r})) \right] , \quad (19.4)$$

where $\mathcal{H}(\varphi(\mathbf{r}), \nabla\varphi(\mathbf{r}))$ is the Hamiltonian density, $\mathbf{r} = (x_1, ..., x_d, \mathbf{z})$ with $\mathbf{z}$ being a $(D-d)$-dimensional vector; the corresponding momentum is $\mathbf{k} = (k_1, ..., k_d, \mathbf{q})$, $\mathbf{q}$ referring to a $(D-d)$-dimensional vector in momentum space. For the coordinates $x_1, \ldots, x_d$, the field is defined in the intervals $[0,\, L_1], \ldots, [0,\, L_d]$, it will have a mixed series-integral Fourier expansion of the form,

$$\varphi_a(\{x_i\}, \mathbf{z}) = \frac{1}{L_1 \cdots L_d} \sum_{n_1,\ldots,n_d=-\infty}^{\infty} \quad (19.5)$$

$$\times \int d^{D-d}\mathbf{q}\, e^{-i\omega_{n_1} x_1 - \cdots - i\omega_{n_d} x_d - i\mathbf{q}\cdot\mathbf{z}} \overline{\varphi}_a(\omega_{n_1}, \ldots, \omega_{n_d}, \mathbf{q}) , \quad (19.6)$$

where $\omega_{n_i} = 2\pi n_i / L_i$, $i = 1, \ldots, d$. The Feynman rules should be modified, as described in Chapters 15 and 18, according to the generalized Matsubara prescription,

$$\int \frac{dk_i}{2\pi} \to \frac{1}{L_i} \sum_{n_i=-\infty}^{+\infty} ; \qquad k_i \to \frac{2n_i\pi}{L_i} , \quad i = 1, 2..., d. \quad (19.7)$$

In this sense we will refer equivalently in this and following chapters to confinement in a segment of length L_i, or to compactification of the coordinate x_i with a compactification length L_i. General arguments based on topology have been given in Chapter 15. The development of these applications to first- and second order phase transitions is provided by the detailed consideration presented there.

Thus, for $D = 3$ and $d = 1, 2, 3$ we have respectively the system constrained to a slab of thickness L_1 (a film), to a wire of rectangular section $L_1 \times L_2$ and to a parallelepiped of volume $L_1 \times L_2 \times L_3$ (a grain). Studies using this approach have been performed [95, 285] with the spontaneous symmetry breaking in the $\lambda\phi^4$ theory. Also, if the Ginzburg-Landau model confined to limited regions of space is considered, the question of how the critical temperature depends on the relevant lengths of the system can be considered. This method will be applied to the Ginzburg-Landau model to both second- and first-order phase transitions. A physical application is found to the problem of superconducting transitions in films, wires and grains. For second-order phase transitions the critical temperature decreases with the inverse of the relevant linear dimension characterizing the confined system. This agrees generally with scaling arguments [133, 299].

19.2 Second-order phase transition in superconducting films

In this section we consider the N-component Ginzburg-Landau model in D-dimensions at leading order in $1/N$, the system being contained between two parallel

planes a distance L apart from one another (compactification of one spatial dimension). From a physical point of view, for $D = 3$, this corresponds to a film-like material undergoing a second-order phase transition. The large N limit allows us to incorporate in the model the L-dependent corrections to the coupling constant in a non-perturbative manner. It is interesting to investigate how the physically relevant quantities, such as the coupling constant, the mass, and in particular the critical temperature, depend on L. After a redefinition of the physical mass (mass renormalization), the equation relating the transition temperature and the film thickness is established. Finally it is important to find the effect of renormalising the coupling constant.

19.2.1 *The effective potential for the Ginzburg-Landau model with one compactified dimension*

We consider the N-component vector model described by the Ginzburg-Landau Hamiltonian density,

$$\mathcal{H} = \nabla\varphi_a \cdot \nabla\varphi_a + \bar{m}_0^2 \varphi_a \varphi_a + u\,(\varphi_a \varphi_a)^2\,, \tag{19.8}$$

in Euclidian D-dimensional space, where u is the coupling constant and $\bar{m}_0^2$ is an L-modified mass parameter such that

$$\lim_{L\to\infty} \bar{m}_0^2(L,T) = m_0^2(T) \equiv \alpha\,(T - T_0)\,, \tag{19.9}$$

$m_0^2(T)$ being the bulk mass parameter present in the usual free space Ginzburg-Landau model and T_0 the bulk transition temperature. Summation over repeated indices a is assumed. In the following we will consider the model described by the Hamiltonian (19.8) and take the large N limit with $Nu = \lambda$ fixed.

The system is confined between two parallel planes, normal to the x-axis separated by a distance L; we use Cartesian coordinates $\mathbf{r} = (x, \mathbf{z})$, where $\mathbf{z}$ is a $(D-1)$-dimensional vector, with corresponding momentum $\mathbf{k} = (k_x, \mathbf{q})$, $\mathbf{q}$ being a $(D-1)$-dimensional vector in momentum space.

The partition function is obtained from Eq. (19.4) with $d = 1$,

$$\mathcal{Z} = \int \mathcal{D}\varphi_1 \cdots \mathcal{D}\varphi_N \exp\left[-\int_0^L dx \int d^{D-1}\mathbf{z}\; \mathcal{H}(\varphi, \nabla\varphi) \right], \tag{19.10}$$

where the field $\varphi(x, \mathbf{z})$ satisfies periodic boundary conditions along the x-axis, $\varphi(x = 0, \mathbf{z}) = \varphi(x = L, \mathbf{z})$. Then the field has a mixed series integral Fourier expansion of the form,

$$\varphi(x, \mathbf{z}) = \sum_{n=-\infty}^{\infty} \int d^{D-1}\mathbf{q}\; e^{-i\omega_n x\, - i\mathbf{q}\cdot\mathbf{z}} \overline{\varphi}(\omega_n, \mathbf{q})\,, \tag{19.11}$$

where $\omega_n = 2\pi n/L$. Following Eq. (19.7), for the particular case of $d = 1$, the modified Feynman rules are,

$$\int \frac{dk_x}{2\pi} \to \frac{1}{L} \sum_{n=-\infty}^{+\infty}\,, \qquad k_x \to \frac{2n\pi}{L} \equiv \omega_n\,. \tag{19.12}$$

We start from the well known expression for the one-loop contribution to the effective potential in unbounded space presented in Chapter 4,

$$U_1(\varphi_0) = \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s} \left[12\lambda\varphi_0^2\right]^s \int \frac{d^D k}{(2\pi)^D} \frac{1}{(k^2+m^2)^s}, \tag{19.13}$$

where m is the physical mass and φ_0 is the normalized vacuum expectation value of the field, the classical field. We introduce dimensionless parameters

$$c = \frac{m}{2\pi\mu}, \;\; b = \frac{1}{L\mu}, \;\; g = \frac{\lambda}{4\pi^2\mu^{4-D}}, \;\; \phi_0^2 = \frac{\varphi_0^2}{\mu^{D-2}}, \tag{19.14}$$

where μ is a mass scale. In terms of these parameters the one-loop contribution to the effective potential is written as,

$$U_1(\phi_0, b) = \mu^D \, b \sum_{s=1}^{\infty} \frac{(-1)^s}{2s} \left[12g\phi_0^2\right]^s \sum_{n=-\infty}^{+\infty} \int \frac{d^{D-1}q'}{(b^2n^2 + c^2 + \mathbf{q}'^2)^s} \;, \tag{19.15}$$

where $\mathbf{q}' = \mathbf{q}/2\pi\mu$ is dimensionless.

Using the dimensional regularization formula, Eq. (10.12),

$$\int \frac{d^D p}{(2\pi)^D} \frac{1}{(p^2+M)^s} = \frac{\Gamma\left(s - \frac{D}{2}\right)}{(4\pi)^{\frac{D}{2}}\Gamma(s)} \frac{1}{M^{s-\frac{D}{2}}} \;, \tag{19.16}$$

Eq. (19.15) can be cast in the form

$$U_1(\phi_0, b) = \mu^D \, b \sum_{s=1}^{\infty} f(D,s) \left[12g\phi_0^2\right]^s A_1^{c^2}\left(s - \frac{D-1}{2}; b\right), \tag{19.17}$$

where

$$f(D,s) = \pi^{(D-1)/2} \frac{(-1)^{s+1}}{2s\Gamma(s)} \Gamma(s - \frac{D-1}{2}) \tag{19.18}$$

and $A_1^{c^2}\left(s - \frac{D-1}{2}; b\right)$ is one of the Epstein-Hurwitz zeta functions [284] defined by

$$A_K^{c^2}(\nu; b_1, ..., b_K) = \sum_{n_1,...,n_K=-\infty}^{+\infty} \left(b_1^2 n_1^2 + \cdots + b_K^2 n_K^2 + c^2\right)^{-\nu}, \tag{19.19}$$

which is regular for $\mathrm{Re}(\nu) > \mathrm{K}/2$ (in our case $\mathrm{Re(s)} > \mathrm{D}/2$).

The function $A_1^{c^2}(\nu; b)$ is analytically continued to the whole complex ν-plane [284] as follows (this is the simplest case of the developments in Sec. 18.1): using the identity [286]

$$\frac{1}{\Delta^\nu} = \frac{1}{\Gamma(\nu)} \int_0^\infty dt \; t^{\nu-1} e^{-\Delta t}, \tag{19.20}$$

we write

$$\begin{aligned} A_1^{c^2}(\nu; b) &= \sum_{n=-\infty}^{+\infty} \frac{1}{\left(b^2n^2 + c^2\right)^\nu} \;=\; \frac{1}{c^{2\nu}} + 2\sum_{n=1}^{\infty} \frac{1}{(b^2n^2+c^2)^\nu} \\ &= \frac{1}{\Gamma(\nu)} \int_0^\infty dt \; t^{\nu-1} e^{-c^2 t} \left[1 + 2\, T_1(t,b)\right] \;, \end{aligned} \tag{19.21}$$

where the function $T_1(t,b)$ is given by

$$T_1(t,b) = \sum_{n=1}^{\infty} e^{-b^2 n^2 t}\,. \tag{19.22}$$

The function $T_1(t,b)$ possesses the property

$$T_1(t,b) = -\frac{1}{2} + \sqrt{\frac{\pi}{b^2 t}}\left[\frac{1}{2} + S(\frac{\pi^2}{b^2 t})\right], \tag{19.23}$$

with $S(x)$ defined by

$$S(x) = \sum_{n=1}^{\infty} e^{-n^2 x}\,. \tag{19.24}$$

Next, considering the representation for Bessel functions of the third kind, $K_\nu(z)$ [286],

$$2(a/b)^{\frac{\nu}{2}} K_\nu(2\sqrt{ab}) = \int_0^\infty dx\; x^{\nu-1} e^{-(a/x)-bx}, \tag{19.25}$$

it is found that

$$A_1^{c^2}(\nu;b) = \frac{2^{\nu+\frac{1}{2}}\pi^{2\nu-\frac{1}{2}}}{b\,\Gamma(\nu)}\left[2^{\nu-\frac{3}{2}}\Gamma\left(\nu-\frac{1}{2}\right)(2\pi c)^{1-2\nu} + 2\sum_{n=1}^{\infty}\left(\frac{n}{2\pi cb}\right)^{\nu-\frac{1}{2}} K_{\nu-\frac{1}{2}}\left(\frac{2\pi cn}{b}\right)\right]. \tag{19.26}$$

Taking $\nu = s - (D-1)/2$ in Eq. (19.26) and inserting it in Eq. (19.17), we obtain the one-loop correction to the effective potential in D dimensions, with one compactified dimension. Recovering the dimensional parameters we find,

$$U_1(\varphi_0, L) = \sum_{s=1}^{\infty}\left[12\lambda\varphi_0^2\right]^s h(D,s)\left[2^{s-\frac{D}{2}-2}\Gamma(s-\frac{D}{2})m^{D-2s} + \sum_{n=1}^{\infty}\left(\frac{m}{Ln}\right)^{\frac{D}{2}-s} K_{\frac{D}{2}-s}(mLn)\right], \tag{19.27}$$

where

$$h(D,s) = \frac{1}{2^{D/2+s-1}\pi^{D/2}}\frac{(-1)^{s+1}}{s\Gamma(s)}\,. \tag{19.28}$$

As already mentioned in Chapter 18 in the general case, there are terms proportional to $\Gamma(s-D/2)$, $s=1,2,\ldots$, in Eq. (19.27). These terms lead to divergent contributions when D is even; finite quantities are obtained by subtraction of these divergent (polar) terms. In order to have an uniform renormalization scheme in any dimension, these subtractions should be done even in the case of odd dimensions, where no poles of Γ-functions are present. In these cases a finite renormalization is performed. It is important to note that the first term in the brackets subtracted to achieve renormalization is independent of L. This makes this subtraction consistent.

The physical mass and the coupling constant are obtained by using the conditions,

$$\left.\frac{\partial^2}{\partial\varphi_0^2}U(\varphi_0,L)\right|_{\varphi_0=0} = m^2\,, \tag{19.29}$$

$$\left.\frac{\partial^4}{\partial\varphi_0^4}U(\varphi_0,L)\right|_{\varphi_0=0} = \lambda\,, \tag{19.30}$$

where U is the sum of the tree-level and one-loop contributions to the effective potential.

19.3 Mass renormalization and transition temperature

Initially, we shall neglect corrections to the coupling constant, that is, we assume that λ corresponds to the renormalized coupling constant. Then, from Eqs. (19.27) and (19.29), subtracting the term proportional to $\Gamma(1-D/2)$, we get the L-dependent physical mass

$$m^2(L,T) = \bar{m}_0^2(L,T) + \frac{24\lambda}{(2\pi)^{D/2}}\sum_{n=1}^{\infty}\left(\frac{m}{nL}\right)^{\frac{D}{2}-1}K_{\frac{D}{2}-1}(nLm)\,. \tag{19.31}$$

The dependence of the critical temperature T_c on L can be determined. If we start in the ordered phase with a negative squared mass, the model exhibits spontaneous symmetry breaking, $O(N)$ symmetry to $O(N-1)$, but for sufficiently small values of T^{-1} and L the symmetry is restored and the squared physical mass in Eq. (19.31) vanishes. This equation is to be interpreted as an L-dependent Dyson-Schwinger equation, which cannot be solved in a closed form. Limiting ourselves to the neighborhood of criticality ($m^2 \approx 0$) and considering L finite and sufficiently small, we may use the asymptotic formula for small values of the argument of Bessel functions,

$$K_\nu(z) \approx \frac{1}{2}\Gamma(\nu)\left(\frac{z}{2}\right)^{-\nu} \quad (z\sim 0\,;\quad Re(\nu)>0)\,. \tag{19.32}$$

Then Eq. (19.31) reduces to

$$m^2(L,T) \approx \bar{m}_0^2(L,T) + \frac{6\lambda}{\pi^{D/2}L^{D-2}}\Gamma\left(\frac{D}{2}-1\right)\zeta(D-2) \tag{19.33}$$

where

$$\zeta(z) = \sum_{n=1}^{\infty}\frac{1}{n^z} \tag{19.34}$$

is the Riemann zeta function, which is a meromorphic function having only a simple pole at $z=1$.

For $D=3$, Eq. (19.33) is not well defined due to the pole of $\zeta(D-2)$. However, it can be made physically meaningful by the following regularization procedure: using the Laurent expansion of $\zeta(z)$,

$$\zeta(z) = \frac{1}{z-1} + \gamma_0 - \gamma_1\,(z-1) + \cdots\,, \tag{19.35}$$

where $\gamma_0 \simeq 0.577$ and $\gamma_1 \simeq 0.0728$ (the Euler-Mascheroni and the first Stieltjes constants, respectively), we define the L-dependent bare mass in such a way that the pole at $D = 3$ is suppressed, that is, we take

$$\bar{m}_0^2(L,T) \approx M - \frac{1}{(D-3)}\frac{6\lambda}{\pi L}\,, \tag{19.36}$$

where M is independent of D. To fix M, the simplest choice satisfying Eq (19.9) is

$$M = m_0^2(T) = \alpha\,(T - T_0)\;, \tag{19.37}$$

where T_0 is the bulk critical temperature. In this case, taking the limit as $D \to 3$, the L-dependent renormalized mass term in the vicinity of criticality becomes

$$m^2(L,T) \approx \alpha\,(T - T_c(L))\;, \tag{19.38}$$

where the modified, L-dependent, transition temperature is

$$T_c(L) = T_0 - C_1\frac{\lambda}{\alpha L}\;, \tag{19.39}$$

with the constant C_1 given by

$$C_1 = \frac{6\gamma_0}{\pi} \approx 1.1024\,. \tag{19.40}$$

From this equation, we find that for L smaller than

$$L_{\min} = C_1\frac{\lambda}{\alpha T_0}\;, \tag{19.41}$$

$T_c(L)$ becomes negative, meaning that the transition does not occur. In other words, superconductivity is suppressed in films with thickness smaller than $L_{\min}$.

19.3.1 *Effect of the coupling-constant correction on $T_c(L)$*

We now consider the effect of the L-correction to the coupling constant on the critical temperature for films. The renormalized coupling constant will be defined in terms of the four-point function at zero external momenta which, at leading order in $\frac{1}{N}$, is given by the sum of all chains of one-loop diagrams of the type shown in Fig. 18.1. This is a geometric series whose sum is given by

$$\Gamma_D^{(4)}(\mathbf{p}=0,m,L) = \frac{u}{1 + Nu\Pi(D,m,L)}\,, \tag{19.42}$$

where $\Pi(D,m,L) \equiv \Pi(\mathbf{p}=0,D,m,L)$ corresponds to the one-loop subdiagram,

$$\Pi(D,m,L) = \frac{1}{L}\sum_{n=-\infty}^{\infty}\int\frac{d^{D-1}q}{(2\pi)^{D-1}}\frac{1}{[\mathbf{q}^2 + \omega_n^2 + m^2]^2}\,. \tag{19.43}$$

This subdiagram can be calculated with the regularization technique used earlier. However, comparing Eq. (19.43) with Eq. (19.15), $\Pi(D,m,L)$ is obtained directly from the $s = 2$ term in Eq. (19.27) for the one-loop contribution to the

effective potential. Again, suppressing the term proportional to $\Gamma(2 - D/2)$, the renormalized one-loop subdiagram is,

$$\Pi_R(D, m, L) = \frac{1}{(2\pi)^{D/2}} \sum_{n=1}^{\infty} \left[\frac{m}{nL}\right]^{(D-4)/2} K_{\frac{D-4}{2}}(nLm)\,. \tag{19.44}$$

From the properties of Bessel functions, for any dimension D, $\Pi_R(D, m, L)$ is positive for all values of D and L. It satisfies the conditions

$$\lim_{L\to\infty} \Pi_R(D, m, L) = 0 \quad \text{and} \quad \lim_{\mathrm{L}\to 0} \Pi_{\mathrm{R}}(\mathrm{D}, \mathrm{m}, \mathrm{L}) \to \infty\,. \tag{19.45}$$

Let us define the L-dependent renormalized coupling constant $u_R(m, D, L)$, at the leading order in $1/N$, as

$$\Gamma^{(4)}_{D,R}(\mathbf{p} = 0, m, L) \equiv u_R(D, m, L) = \frac{u}{1 + Nu\Pi_R(D, m, L)} \tag{19.46}$$

and the renormalized coupling constant in the absence of boundaries as

$$u_R(D, m) = \lim_{L\to\infty} \Gamma^{(4)}_{D,R}(\mathbf{p} = 0, m, L)\,. \tag{19.47}$$

From Eq. (19.46) and Eq. (19.45) we get $u_R(D, m) = u$. In other words, we have made a choice of the renormalization scheme such that the constant u corresponds to the renormalized coupling constant in the absence of spatial constraints. From Eq. (19.46) we define the L-dependent large N renormalized coupling constant

$$\lambda_R(D, m, L) \equiv \lim_{u\to 0\,;\ N\to\infty} N u_R(D, m, L) = \frac{\lambda}{1 + \lambda\Pi_R(D, m, L)}\,, \tag{19.48}$$

with $\lambda = Nu$.

Considering the L-correction to the coupling constant, the Dyson-Schwinger equation for the mass Eq (19.31) becomes

$$\begin{aligned} m^2(L, T) = \bar{m}_0^2(L, T) + \frac{24\lambda_R(D, m, L)}{(2\pi)^{D/2}} \\ \times \sum_{n=1}^{\infty} \left[\frac{m}{nL}\right]^{\frac{D-2}{2}} K_{\frac{D-2}{2}}(nLm)\,. \end{aligned} \tag{19.49}$$

The set of coupled equations Eqs. (19.44), (19.48) and (19.49), form a complicated set since on their right hand sides $m = m(D, T, L)$. Nevertheless, limiting ourselves to the neighborhood of criticality, $m^2(D, T, L) \approx 0$, we may investigate the behavior of the system by using in Eqs. (19.44) and (19.49) the asymptotic formula Eq. (19.32) for small values of the argument of the Bessel function. Making such an approximation, Eq. (19.49) reduces to Eq. (19.33) with λ replaced by $\lambda_R(D, m, L)$. So it remains to calculate the renormalized coupling constant close to criticality.

Inserting Eq. (19.32) into Eq. (19.44), we obtain

$$\Pi_R(D, L) \approx \frac{1}{8\pi^{D/2}} L^{4-D} \Gamma\left(\frac{D-4}{2}\right) \zeta(D-4)\,, \tag{19.50}$$

which shows that the renormalized one-loop subdiagram is independent of the mass close to criticality. This result leads to the renormalized coupling constant, for $m^2 \approx 0$,

$$\lambda_R(D,L) \approx \frac{\lambda}{1+\lambda C(D) L^{4-D}\zeta(D-4)}\,, \tag{19.51}$$

where $C(D) = \frac{1}{8\pi^{D/2}}\Gamma(\frac{D-4}{2})$. With $\Gamma(-1/2) = -2\sqrt{\pi}$ and $\zeta(-1) = -1/12$, $\lambda_R(D,L)$ is finite and positive for $D = 3$.

The mass, close to criticality and for dimension D, thus becomes

$$m^2(L,T) \approx \bar{m}_0^2(L,T) + \frac{6\lambda_R(D,L)}{\pi^{D/2}L^{D-2}}\Gamma\left(\frac{D}{2}-1\right)\zeta(D-2)\,, \tag{19.52}$$

with $\lambda_R(D,L)$ given by Eq. (19.51). Although $\lambda_R(D,L)$ remains finite as $D \to 3^+$, the mass is singular, due to the pole of $\zeta(D-2)$ and a regularization procedure is needed. Following the same steps that led from Eq. (19.33) to Eq. (19.38), with λ replaced by $\lambda_R(3,L)$, we obtain the critical temperature as a function of L,

$$T_c(L) = T_0 - \frac{48\pi C_1\lambda}{48\pi\alpha L + \alpha\lambda L^2}\,. \tag{19.53}$$

This result may be compared with the critical temperature for a film deduced from the Ginzburg-Landau model in which the L-correction to the coupling constant is neglected, obtained from Eq. (19.52) by taking $\lambda_R = \lambda$. In this lowest level of approximation, the critical temperature is simply a linear decreasing function of $1/L$. In Fig. 19.1, both curves are plotted for comparison.

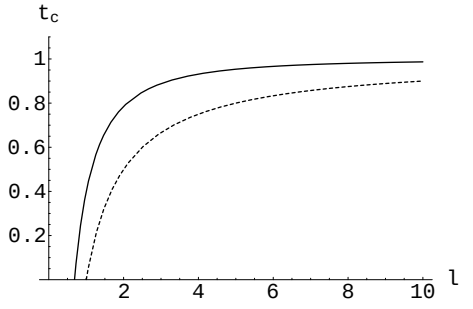


Fig. 19.1 Reduced transition temperature, $t_c = T_c/T_0$, for films as a function of the reduced thickness, $l = L/L_{\min}$ (with $L_{\min} = C_1\lambda/(\alpha T_0)$), fixing $\lambda L_{\min} = 100$ (solid line). The dashed line corresponds to $t_c(l) = 1 - l^{-1}$, obtained without considering L-corrections to the coupling constant in the Ginzburg-Landau model.

We find that the critical temperature, Eq. (19.53), decreases from T_0, as L diminishes reaching zero for a minimal thickness $L'_{\min}$, below which the transition is suppressed. This minimal thickness is given by

$$L'_{\min} = \frac{24\pi}{\lambda}\left[\sqrt{1+\frac{\lambda L_{\min}}{12\pi}}\ -1\right], \tag{19.54}$$

where $L_{\min} = C_1\lambda/(\alpha T_0)$ is the minimal thickness for the existence of the ordered phase in the approximation of neglecting L-corrections to the coupling constant, Eq. (19.41). This minimal thickness, not considering coupling constant corrections, coincides with the result for the standard, two-component, Ginzburg-Landau model [304], except for a simple symmetry factor. We also find that the predicted minimal film thickness, for the N-component model including the L-correction to the coupling constant ($L'_{\min}$), is lower than the value $L_{\min}$ but the general behavior of both curves $t_c(l)$ in Fig. 19.1, is very similar.

It is important to note that the results obtained here might be applicable to any physical system undergoing a second-order phase transition in a film described by the Ginzburg-Landau model. For example, the decrease of the transition temperature with the inverse of the film thickness was experimentally observed for superconductors [305]. In fact, the results presented in this section do not depend on particular physical systems, appearing only as a topological consequence of the compactification in one spatial dimension of the Ginzburg-Landau model. This is in contrast to other calculations that used modifications of the microscopic interactions in bulk superconductors, in order to explain the variations of the critical temperature with the thickness of the film.

19.4 Critical behavior of type-II superconducting films in a magnetic field

Until now, we have considered phase transitions in confined systems not taking into account the possible existence of an external magnetic field interacting with the order parameter of a type II superconducting film. In this respect, for the case of superconductors, we have neglected the minimal coupling with the vector potential when an external magnetic field is applied and, in its absence, the intrinsic gauge fluctuations. In this chapter, we investigate how the transition temperature for a film behaves as a function of its thickness and of the intensity of an applied magnetic field [306, 307].

19.4.1 *Coupling-constant correction in the presence of an external magnetic field*

We shall take the uniform external magnetic field, $\mathbf{H} = H\hat{e}_3$, normal to the film. To describe the critical curve of a type-II superconductor close to the upper critical field, we will neglect gauge fluctuations of the magnetic vector potential [293, 294], that is, we take $\nabla \times \mathbf{A} = \mathbf{H}$. Therefore, the Hamiltonian density is

$$\mathcal{H} = |(\nabla - ie\mathbf{A})\phi|^2 + \bar{m}_0^2\,|\phi|^2 + u\left(|\phi|^2\right)^2, \tag{19.55}$$

where, as before, ϕ is an N-component vector and $\bar{m}_0^2$ is the mass parameter which depends on L, H and T, in such way that

$$\lim_{L\to\infty}\lim_{H\to 0}\bar{m}_0^2(L,H,T) = m_0^2(T) \equiv \alpha\,(T - T_0)\,. \tag{19.56}$$

Let us initially consider the Hamiltonian density (19.55) referring to a bulk superconductor. We choose a gauge such that $\mathbf{A} = (0, xH, \mathbf{0})$. In this case, the part of the hamiltonian $H = \int d^D r\,\mathcal{H}$ quadratic in ϕ becomes, after an integration by parts, $-\int d^D r\,\phi\mathcal{D}\phi$ where the differential operator $\mathcal{D}$ is

$$\mathcal{D} = \nabla^2 - 2i\omega x\partial_y - \omega^2 x^2 - m_0^2, \tag{19.57}$$

with $\omega = eH$ being the cyclotron frequency. Thus the natural basis to expand the field operators is the set of the normalized eigenfunctions of the operator $\mathcal{D}$, the Landau basis,

$$\chi_{l,p_y,\mathbf{p}}(\mathbf{r}) = \frac{1}{\sqrt{2^l l!}}\left(\frac{\omega}{\pi}\right)^{\frac{1}{4}} e^{i\mathbf{p}\cdot\mathbf{z}} e^{ip_y y} e^{-\omega(x-p_y/\omega)^2/2} H_l\left[\sqrt{\omega}(x - \frac{p_y}{\omega})\right], \tag{19.58}$$

where H_l are the Hermite polynomials; the corresponding energy eigenvalues are

$$E_l(|\mathbf{p}|) = |\mathbf{p}|^2 + (2l+1)\omega + m_0^2 \tag{19.59}$$

where $\mathbf{p}$ and $\mathbf{z}$ are $(D-2)$-dimensional vectors.

The propagator can be written as [293, 294]

$$G(\mathbf{r},\mathbf{r}') = \int \frac{d^{D-2}p}{(2\pi)^{D-1}} \int dp_y \sum_{l=0}^{\infty} \frac{\chi_{l,p_y,\mathbf{p}}(\mathbf{r})\chi^{\star}_{l,p_y,\mathbf{p}}(\mathbf{r}')}{|\mathbf{p}|^2 + (2l+1)\omega + m_0^2}. \tag{19.60}$$

To calculate the coupling-constant correction, we have to find the appropriate expression for the single one-loop subdiagram in Fig. 18.1. This is a complicated expression that will be treated here within the approximation of neglecting all Landau levels except the lowest one. Such an approximation is valid when the magnetic field is high and, so, the Landau levels are well separated. Thus, the use of this approximation will lead to results that are applicable at low temperatures. Notice that, this observation is not restricted to the bulk case but it also applies to a film if the magnetic field is perpendicular to the film plane.

Now, taking into account the prescription given by Eq. (19.12), we obtain the expression of the single one-loop subdiagram in the form

$$\Pi(D,L,\omega) = \frac{1}{L}\sum_{n=-\infty}^{\infty} \frac{\omega}{2\pi} \int \frac{d^{D-3}k}{(2\pi)^{D-3}}\, \frac{1}{\left[\mathbf{k}^2 + \omega_n^2 + m^2 + \omega\right]^2}, \tag{19.61}$$

$\mathbf{k}$ being a $(D-3)$-dimensional vector and $\omega_n = 2\pi n/L$.

The sum over n and the integral over k can be treated using the formalism developed in the preceding sections. Again, using the dimensional regularization

formula Eq. (10.12) and the analytic extension for the Epstein-Hurwitz zeta function, Eq. (19.26), we obtain

$$\Pi(D,L,\omega) = \frac{\omega}{2(2\pi)^{D/2}}\left[\frac{1}{4}\Gamma\left(3-\frac{D}{2}\right)\left(\frac{m^2+\omega}{2}\right)^{\frac{D}{2}-3} + \sum_{n=1}^{\infty}\left(\frac{\sqrt{m^2+\omega}}{nL}\right)^{\frac{D}{2}-3} K_{\frac{D}{2}-3}(nL\sqrt{m^2+\omega})\right]. \quad (19.62)$$

As before, we suppress the term containing $\Gamma(3-\frac{D}{2})$ in the above equation, leading to the renormalized one-loop subdiagram

$$\Pi_R(D,L,\omega) = \frac{\omega}{2(2\pi)^{D/2}}\sum_{n=1}^{\infty}\left(\frac{\sqrt{m^2+\omega}}{nL}\right)^{\frac{D}{2}-3} K_{\frac{D}{2}-3}(nL\sqrt{m^2+\omega}). \quad (19.63)$$

The renormalized zero external momenta four-point function at leading order in $1/N$ is given by the sum of chains of single one-loop diagrams of the kind shown in Fig. 19.1. This sum gives for the L and ω-dependent four-point function, with the lowest Landau level approximation, the expression

$$\Gamma^{(4)}_{D,R}(0,L,\omega) \equiv u_R(D,L,\omega) = \frac{u}{1+Nu\,\Pi_R(D,L,\omega)}. \quad (19.64)$$

We define the renormalized coupling constant

$$\lambda_R(D,L,\omega) \equiv \lim_{N\to\infty\,,\,u\to 0} Nu_R(D,L,\omega)\lambda_R(D,L,\omega) = \frac{\lambda}{1+\lambda\,\Pi_R(D,L,\omega)}, \quad (19.65)$$

where $\lambda = Nu$ corresponds to the renormalized coupling constant in the absence of boundaries and of external field.

19.4.2 *The gap equation and the critical curve*

In order to study the critical behavior of a type-II film of thickness L, in an external magnetic field perpendicular to it, we have to consider the large N gap equation for the correlation length, properly adapted to the present situation. In the disordered phase, $\varphi_0 = 0$, and we have

$$\xi^{-2} = \bar{m}_0^2 + \omega + \frac{24\,\lambda_R}{L}\sum_{n=-\infty}^{\infty}\frac{\omega}{2\pi}\int\frac{d^{D-3}k}{(2\pi)^{D-3}}\,\frac{1}{\mathbf{k}^2+\omega_n^2+\xi^{-2}}. \quad (19.66)$$

It is important to observe that, in the presence of a magnetic field, the correlation length is related to the renormalized mass by $\xi^{-2} = m^2(L,\omega)+\omega$, since the pole of the propagator occurs at $m^2(L,\omega) = -\omega$ [293, 294]. Notice that $\lambda_R(D,L,\omega)$, the renormalized (L,ω)-dependent coupling constant, is itself a function of ξ^{-2}, via the mass $m(L,\omega)$ present in Π_R. Criticality, as usual, is reached by making $\xi^{-2}\to 0$.

Calculating the sum and the integral in the above expression, in a similar manner as that used to get Eq. (19.31), Eq. (19.66) becomes

$$\xi^{-2} = \bar{m}_0^2 + \omega + \frac{24\omega\,\lambda_R}{(2\pi)^{D/2}}\sum_{n=1}^{\infty}\left[\frac{\xi^{-1}}{nL}\right]^{\frac{D-4}{2}} K_{\frac{D-4}{2}}(nL\xi^{-1})\,. \quad (19.67)$$

Close to criticality, $\xi^{-2} \approx 0$, using (19.32), we obtain

$$\xi^{-2} \approx \bar{m}_0^2 + \omega_c + \frac{3\,\omega_c \lambda_R(D,L,\omega_c)}{\pi^{D/2}} \Gamma(\frac{D}{2} - 2) L^{4-D} \zeta(D-4), \tag{19.68}$$

where

$$\lambda_R(D,L,\omega_c) \approx \frac{\lambda}{1 + \lambda\,\omega_c\, A(D) L^{6-D} \zeta(D-6)}, \tag{19.69}$$

with $A(D) = \frac{1}{32\pi^{D/2}}\Gamma(\frac{D}{2} - 3)$. Notice that we have used the subscript c in the cyclotron frequency (actually, the external field) to indicate that we are in the region of criticality.

We find immediately that there are no divergences in Eq. (19.68) and (19.69) as $D \to 3$. Therefore, no renormalization procedure is needed and we are allowed to make the simplest choice for the mass parameter: $\bar{m}_0^2 = \alpha(T - T_0)$. In this way, making $D = 3$ and $\xi^{-2} = 0$ in Eqs. (19.68) and (19.69), we obtain the critical curve for a film in a perpendicular magnetic field as

$$\alpha(T_c - T_0) + \omega_c + \frac{1440\,\lambda\,\omega_c\, L}{2880\,\pi + \lambda\,\omega_c\, L^3} = 0\,, \tag{19.70}$$

where we have used that $\Gamma(-3/2) = 4\sqrt{\pi}/3$ and $\zeta(-3) = 1/120$. Notice that, as $L \to \infty$, the critical curve given by Eq. (19.70) reduces to $\alpha(T_c - T_0) + \omega_c = 0$, reproducing the known result for the upper critical field in bulk superconductors $H_{c2} = \eta^{-2}$.

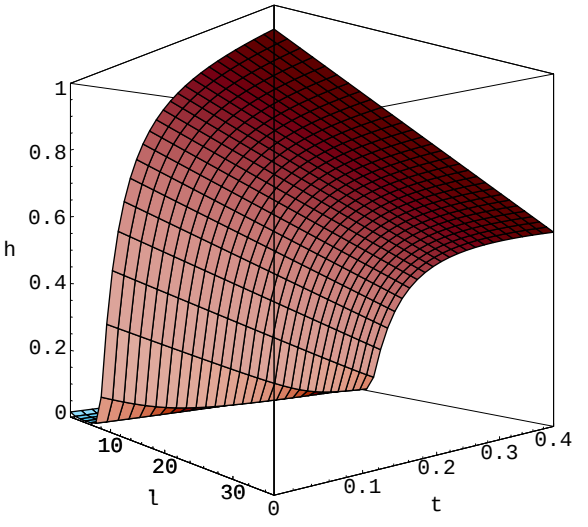


Fig. 19.2 Plot of the surface $h = h(l,t)$, fixing $\beta = 10^3$.

We can rewrite Eq. (19.70) in a way such that the upper critical field is expressed as a function of the critical temperature and the film thickness. Using the zero-temperature Ginzburg-Landau coherence length, $\eta_0 = (\alpha T_0)^{-1/2}$, we can introduce the following dimensionless quantities,

$$h = \omega_c \, \eta_0^2 \,, \qquad t = \frac{T_c}{T_0} \,, \qquad l = \frac{L}{\eta_0} \,, \tag{19.71}$$

corresponding respectively to reduced critical field, critical temperature and film thickness. With these parameters, Eq. (19.70) becomes

$$\begin{aligned} h(l,t) = \frac{1}{2\gamma l^3} \Big\{ & -1440\gamma l + \gamma l^3 (1-t) - 2880\pi \\ & + \left[(1440\gamma l - \gamma l^3 (1-t) + 2880\pi)^2 + 11520\pi\gamma l^3 (1-t) \right]^{1/2} \Big\} \,, \end{aligned} \tag{19.72}$$

where $\gamma = \lambda\eta_0$. The surface $h = h(l,t)$ is illustrated in Fig. 19.2. We recall that, since we have used the lowest Landau level approximation in our calculations, this surface is only meaningful for high values of the external field, that is for low temperatures and relatively thick films.

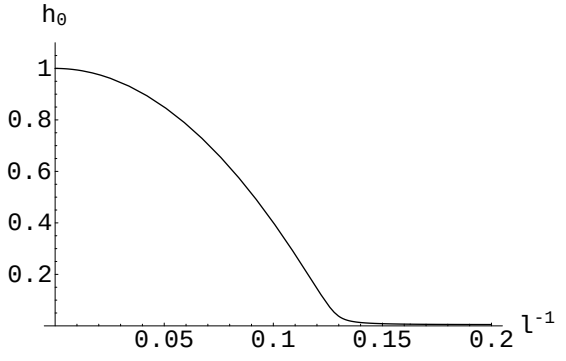


Fig. 19.3 Zero-temperature reduced critical field as a function of the inverse of the reduced film thickness, for $\gamma = 10^3$.

We can see from Fig. 19.2 that each value of l defines a critical line on the $h \times t$ plane, corresponding to a film of thickness L. This set of critical lines also suggests the existence of a minimal value for the thickness L below which superconductivity is suppressed. Indeed, this can be seen from the plot of the reduced critical field at zero temperature, h_0, as a function of the inverse of the reduced film thickness, shown in Fig. 19.3. As before, we emphasize that our results are obtained within the framework of field theory, emerging from the topological nature of the spatial compactification, and do not depend on specific characteristics of the material and of the sample.

Chapter 20

Second-Order Phase Transition in Wires and Grains

We now generalize the procedure presented earlier to account for second-order phase transitions in wires and grains. From a physical point of view superconducting transitions are considered. The compactification process has to be extended to more than one spatial dimension. General arguments based on topology to compactify an arbitrary number of dimensions have been given in Chapter 15. This allows us to introduce temperature as well as confined spatial dimensions along any direction. For the sake of generality, we consider initially the D-dimensional Ginzburg-Landau model with d ($\leq D$) compactified coordinates. Fixing $D = 3$, the cases $d = 2$ and $d = 3$ will correspond to wires and grains respectively.

20.1 Compactification of a d-dimensional subspace

For such a general situation, the partition function is given by Eq. (19.4), with the Hamiltonian density Eq. (19.8), and the generalized Matsubara prescription is taken as in Eq. (19.7). We consider λ to be the renormalized coupling constant, i.e., we will work initially in the approximation of neglecting boundary corrections to the coupling constant, and take $\overline{m}_0^2$ as the boundary-modified mass parameter depending on $\{L_i\}$ $i = 1, 2, ..., d$, in such a way that,

$$\lim_{\{L_i\}\to\infty} \overline{m}_0^2(L_1, ..., L_d, T) = m_0^2(T) \equiv \alpha\,(T - T_0)\,, \tag{20.1}$$

with $m_0^2(T)$ being the bulk mass parameter. In this case, the one-loop contribution to the effective potential, Eq. (19.13), becomes

$$U_1(\phi_0, b_1, ..., b_d) = \mu^D b_1 \cdots b_d \sum_{s=1}^{\infty} \frac{(-1)^s}{2s} [12 g \phi_0^2]^s \times \sum_{n_1,\ldots,n_d=-\infty}^{+\infty} \int \frac{d^{D-d}\mathbf{q}}{(b_1^2 n_1^2 + \cdots + b_d^2 n_d^2 + c^2 + \mathbf{q}^2)^s}, \tag{20.2}$$

where we have used the dimensionless quantities given in Eq. (19.14), now with $b_i = (L_i \mu)^{-1}$ for $i = 1, 2, \ldots, d$.

Using the dimensional regularization formula, Eq. (10.12) to perform the integration over the $D-d$ non-compactified momentum variables, the above expression becomes

$$U_1(\phi_0, b_1, ..., b_d) = \mu^D b_1 \cdots b_d \sum_{s=1}^{\infty} f(D,d,s) \times [12 g \phi_0^2]^s \, A_d^{c^2}\left(s - \frac{D-d}{2}; b_1, ..., b_d\right), \tag{20.3}$$

with

$$f(D,d,s) = \pi^{(D-d)/2} \frac{(-1)^{s+1}}{2s\Gamma(s)} \Gamma(s - \frac{D-d}{2}), \tag{20.4}$$

and $A_d^{c^2}$ is the multivariable Epstein-Hurwitz function defined in Eq. (19.19).

The analytical extension of the multivariable Epstein-Hurwitz function can be carried out by a generalization of the procedure shown in the preceding chapter. This has been presented in Sec. 18.1; we repeat it here with the present notation. Using Eq. (19.20), we get,

$$A_d^{c^2}(\nu; b_1, ..., b_d) = \frac{1}{\Gamma(\nu)} \int_0^{\infty} dt \; t^{\nu-1} e^{-c^2 t} \left[1 + 2 \sum_{i=1}^{d} T_1(t, b_i) + 4 \sum_{i<j=1}^{d} T_2(t, b_i, b_j) + \cdots + 2^d \, T_d(t, b_1, ..., b_d) \right], \tag{20.5}$$

where, the function T_1 is given by Eq. (19.22) and

$$T_j(t, b_1, ..., b_j) = \prod_{l=1}^{j} T_1(t, b_l) \;, \qquad j = 2, ..., d. \tag{20.6}$$

Considering the property of Eq. (19.23) for the function T_1, the surviving terms in Eq. (20.5) are those proportional to $(b_1 \cdots b_d)^{-1}$, and we find

$$A_d^{c^2}(\nu; b_1, ..., b_d) = \frac{\pi^{\frac{d}{2}}}{b_1 \cdots b_d} \frac{1}{\Gamma(\nu)} \int_0^{\infty} dt \; t^{(\nu - \frac{d}{2})-1} e^{-c^2 t} \left[1 + 2 \sum_{i=1}^{d} S(\frac{\pi^2}{b_i^2 t}) + 4 \sum_{i<j=1}^{d} S(\frac{\pi^2}{b_i^2 t}) S(\frac{\pi^2}{b_j^2 t}) + \cdots + 2^d \prod_{i=1}^{d} S(\frac{\pi^2}{b_i^2 t}) \right], \tag{20.7}$$

with $S(x)$ given by Eq. (19.24). Using again the representation of Eq. (19.25) for

the Bessel function K_ν, we find

$$A_d^{c^2}(\nu; b_1, ..., b_d) = \frac{2^{\nu-\frac{d}{2}+1}\pi^{2\nu-\frac{d}{2}}}{b_1 \cdots b_d\, \Gamma(\nu)} \left[2^{\nu-\frac{d}{2}-1}\Gamma\left(\nu - \frac{d}{2}\right)(2\pi c)^{d-2\nu} \right.$$
$$+ 2\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{n_i}{2\pi c b_i}\right)^{\nu-\frac{d}{2}} K_{\nu-\frac{d}{2}}\left(\frac{2\pi c n_i}{b_i}\right) + \cdots$$
$$+ 2^d \sum_{n_1,...,n_d=1}^{\infty}\left(\frac{1}{2\pi c}\sqrt{\frac{n_1^2}{b_1^2} + \cdots + \frac{n_d^2}{b_d^2}}\right)^{\nu-\frac{d}{2}}$$
$$\left. \times\, K_{\nu-\frac{d}{2}}\left(2\pi c\sqrt{\frac{n_1^2}{b_1^2} + \cdots + \frac{n_d^2}{b_d^2}}\right)\right]. \tag{20.8}$$

Taking $\nu = s - (D-d)/2$ in this equation and inserting it in Eq. (20.3), we obtain the one-loop correction to the effective potential in D dimensions with a compactified d-dimensional subspace. Recovering the dimensional parameters we get

$$U_1(\varphi_0, L_1, ..., L_d) = \sum_{s=1}^{\infty}\left[12g\varphi_0^2\right]^s h(D,s)\left[2^{s-\frac{D}{2}-2}\Gamma(s-\frac{D}{2})m^{D-2s}\right.$$
$$+\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_i n_i}\right)^{\frac{D}{2}-s} K_{\frac{D}{2}-s}(mL_i n_i)$$
$$+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}}\right)^{\frac{D}{2}-s}$$
$$\times\, K_{\frac{D}{2}-s}\left(m\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}\right) + \cdots$$
$$+ 2^{d-1}\sum_{n_1,...,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}}\right)^{\frac{D}{2}-s}$$
$$\left.\times\, K_{\frac{D}{2}-s}\left(m\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}\right)\right], \tag{20.9}$$

with

$$h(D,s) = \frac{1}{2^{D/2+s-1}\pi^{D/2}}\frac{(-1)^{s+1}}{s\Gamma(s)}\,. \tag{20.10}$$

Criticality is attained when the physical mass vanishes. The mass is obtained using the appropriate generalization of the condition Eq. (19.29),

$$\frac{\partial^2}{\partial\varphi_0^2}U(D,\{L_j\})\bigg|_{\varphi_0=0} = m^2(\{L_j\};T)\,, \tag{20.11}$$

together with Eq. (20.9). Remembering that at the large N limit it is enough to take the one-loop contribution to the mass, we obtain

$$
\begin{aligned}
m^2(\{L_j\};T) = \overline{m}_0^2(L_1,\ldots,L_d;T) \\
&+ \frac{24\lambda}{(2\pi)^{D/2}}\left[\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_i n_i}\right)^{\frac{D}{2}-1} K_{\frac{D}{2}-1}\left(mL_i n_i\right)\right. \\
&+ 2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}}\right)^{\frac{D}{2}-1} \\
&\times K_{\frac{D}{2}-1}\left(m\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}\right) + \cdots \\
&+ 2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}}\right)^{\frac{D}{2}-1} \\
&\left.\times K_{\frac{D}{2}-1}\left(m\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}\right)\right] . \qquad (20.12)
\end{aligned}
$$

where $m = m(L_1,\ldots,L_d;T)$ on the right-hand side. Notice that, in writing Eq. (20.12), the term proportional to $2^{-\frac{D}{2}-1}\Gamma(1-\frac{D}{2})m^{D-2}$, the first term in the square bracket of Eq. (20.9), is suppressed. This term, which does not depend on L_i, diverges for even D due to the poles of the gamma function; in this case, this part is subtracted to get a renormalized mass. For odd D, $\Gamma\left(1-\frac{D}{2}\right)$ is finite but we still subtract this term, corresponding to a finite renormalization, for the sake of uniformity; besides, for $D \geq 3$, the factor m^{D-2} does not contribute at criticality.

The vanishing of Eq. (20.12) defines criticality for the compactified system. It is to be emphasized that Eq. (20.12) is a self-consistent equation, the modified Dyson-Schwinger equation for the mass. For $d = 1$ Eq. (20.12) reduces to Eq. (19.31), corresponding to the case of a thin film. Taking $d = 2$ and $d = 3$, with $D = 3$, we describe respectively the critical behavior of samples of materials in the form of square wires and cubic grains. Equations for the critical temperature are derived as a function of the confining dimensions. We calculate the minimal system size (cross-section area or volume) below which the phase transition does not take place.

20.2 Critical behavior for wires

Now we focus on two spatial compactified dimensions. From Eq. (20.12), taking $d = 2$, we get,

$$m^2(L_1,L_2,T) = \overline{m}_0^2(L_1,L_2,T) + \frac{24\lambda}{(2\pi)^{D/2}} \times \left[\sum_{i=1}^{2} \sum_{n_i=1}^{\infty} \left(\frac{m}{n_i L_i}\right)^{\frac{D}{2}-1} K_{\frac{D}{2}-1}(n_i L_i m) + 2 \sum_{n_1,n_2=1}^{\infty} \left(\frac{m}{\sqrt{L_1^2 n_1^2 + L_2^2 n_2^2}}\right)^{\frac{D}{2}-1} \times K_{\frac{D}{2}-1}(m\sqrt{L_1^2 n_1^2 + L_2^2 n_2^2}) \right]. \tag{20.13}$$

Near criticality, $m^2 \approx 0$, taking both L_1 and L_2 sufficiently small, use of Eq. (19.32) gives,

$$m^2(L_1,L_2,T) \approx \overline{m}_0^2(L_1,L_2,T) + \frac{6\lambda}{\pi^{D/2}}\,\Gamma\left(\frac{D}{2}-1\right) \times \left[\left(\frac{1}{L_1^{D-2}} + \frac{1}{L_2^{D-2}} \right) \zeta(D-2) + 2\,E_2\left(\frac{D-2}{2}; L_1, L_2\right) \right], \tag{20.14}$$

where $E_2\left(\frac{D-2}{2}; L_1, L_2\right)$ is the two-variable Epstein zeta function,

$$E_2\left(\frac{D-2}{2}; L_1, L_2\right) = \sum_{n_1,\,n_2=1}^{\infty} \left[L_1^2 n_1^2 + L_2^2 n_2^2\right]^{-\left(\frac{D-2}{2}\right)}, \tag{20.15}$$

defined for $\mathrm{Re}D > 3$.

The Riemann zeta function, $\zeta(D-2)$, has an analytical extension to the whole complex D-plane, having an unique simple pole with a residue 1 at $D = 3$. Consider the analytical continuation of the Epstein-Hurwitz zeta function given by [284, 289]

$$\sum_{n=1}^{\infty} \left(n^2 + p^2\right)^{-\nu} = -\frac{1}{2}\,p^{-2\nu} + \frac{\sqrt{\pi}}{2p^{2\nu-1}\Gamma(\nu)} \times \left[\Gamma\left(\nu - \frac{1}{2}\right) + 4 \sum_{n=1}^{\infty} (\pi p n)^{\nu-\frac{1}{2}} K_{\nu-\frac{1}{2}}(2\pi p n) \right]. \tag{20.16}$$

As explained in Chapter 18, using this relation to perform one of the sums in Eq. (20.15), the manifest $L_1 \leftrightarrow L_2$ symmetry is lost in this equation. In order to preserve this symmetry, the multivariable Epstein-Hurwitz zeta function is redefined using a symmetrized summation,

$$E_d\left(\nu; L_1, ..., L_d\right) = \frac{1}{d!} \sum_{\sigma} \sum_{n_1=1}^{\infty} \cdots \sum_{n_d=1}^{\infty} \left[\sigma_1^2 n_1^2 + \cdots + \sigma_d^2 n_d^2\right]^{-\nu}, \tag{20.17}$$

where $\sigma_i = \sigma(L_i)$, with σ running in the set of all permutations of the parameters $L_1, ..., L_d$, and the summations over $n_1, ..., n_d$ being taken in the given order. Then

symmetrized analytic continuations and recurrence relations are obtained. Using Eq. (20.16) to perform the sum over n_d, gives

$$E_d\left(\nu; L_1, ..., L_d\right) = -\frac{1}{2\,d}\sum_{i=1}^{d} E_{d-1}\left(\nu; ..., \widehat{L_i}, ...\right) + \frac{\sqrt{\pi}}{2\,d\,\Gamma(\nu)}\Gamma\left(\nu-\frac{1}{2}\right)\sum_{i=1}^{d}\frac{1}{L_i}E_{d-1}\left(\nu-\frac{1}{2}; ..., \widehat{L_i}, ...\right) + \frac{2\sqrt{\pi}}{d\,\Gamma(\nu)}W_d\left(\nu-\frac{1}{2}, L_1, ..., L_d\right), \tag{20.18}$$

where the hat over the parameter L_i in the function E_{d-1} means that it is excluded from the set $\{L_1, ..., L_d\}$; the remaining being the $d-1$ parameters of E_{d-1}, and

$$W_d\left(\eta; L_1, ..., L_d\right) = \sum_{i=1}^{d}\frac{1}{L_i}\sum_{n_1,...,n_d=1}^{\infty}\left(\frac{\pi n_i}{L_i\sqrt{(\cdots+\widehat{L_i^2 n_i^2}+\cdots)}}\right)^{\eta} \times K_\eta\left(\frac{2\pi n_i}{L_i}\sqrt{(\cdots+\widehat{L_i^2 n_i^2}+\cdots)}\right), \tag{20.19}$$

with $(\cdots+\widehat{L_i^2 n_i^2}+\cdots)$ representing the sum $\sum_{j=1}^{d} L_j^2 n_j^2 - L_i^2 n_i^2$. In particular, for $d=2$ using $E_1\left(\nu; L_j\right) = L_j^{-2\nu}\zeta(2\nu)$, we get

$$E_2\left(\frac{D-2}{2}; L_1^2, L_2^2\right) = -\frac{1}{4}\left(\frac{1}{L_1^{D-2}}+\frac{1}{L_2^{D-2}}\right)\zeta(D-2) + \frac{\sqrt{\pi}\Gamma(\frac{D-3}{2})}{4\Gamma(\frac{D-2}{2})}\left(\frac{1}{L_1 L_2^{D-3}}+\frac{1}{L_1^{D-3}L_2}\right)\zeta(D-3) + \frac{\sqrt{\pi}}{\Gamma(\frac{D-2}{2})}W_2\left(\frac{D-3}{2}; L_1, L_2\right). \tag{20.20}$$

Then Eq. (20.14) is written as

$$m^2(L_1, L_2, T) \approx \overline{m}_0^2(L_1, L_2, T) + \frac{3\lambda}{\pi^{D/2}} \times \left[\left(\frac{1}{L_1^{D-2}}+\frac{1}{L_2^{D-2}}\right)\Gamma\left(\frac{D-2}{2}\right)\zeta(D-2) + \sqrt{\pi}\left(\frac{1}{L_1 L_2^{D-3}}+\frac{1}{L_1^{D-3}L_2}\right)\Gamma\left(\frac{D-3}{2}\right)\zeta(D-3) + 2\sqrt{\pi}W_2\left(\frac{D-3}{2}; L_1, L_2\right)\right]. \tag{20.21}$$

For $D=3$, the first and second terms in square brackets in Eq. (20.21) are divergent due to the ζ- and Γ-functions, respectively. These divergences are dealt with by using the Laurent expansion of $\zeta(z)$, Eq. (19.35), and considering the expansion of $\Gamma(z)$ around $z=0$,

$$\Gamma(z) = \frac{1}{z} - \gamma_0 + \left(\gamma_0 + \frac{\pi^2}{6}\right) z + \cdots , \tag{20.22}$$

with $\zeta(0) = -\frac{1}{2}$ and $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. The two divergent terms cancel exactly, unlike in the case of a film. No renormalization is needed. For $D = 3$, taking the bare mass given by $\overline{m}_0^2(L_1, L_2, T) = \alpha\,(T - T_0)$, the physical mass has the form,

$$m^2(L_1, L_2, T) \approx \alpha\,(T - T_c(L_1, L_2))\,, \tag{20.23}$$

with the boundary-dependent critical temperature being

$$T_c(L_1, L_2) = T_0 - \frac{9\lambda\gamma}{2\pi\alpha}\left(\frac{1}{L_1} + \frac{1}{L_2}\right) - \frac{6\lambda}{\pi\alpha}\, W_2(0; L_1, L_2), \tag{20.24}$$

where

$$W_2(0; L_1, L_2) = \sum_{n_1, n_2 = 1}^{\infty} \left\{ \frac{1}{L_1} K_0\left(2\pi \frac{L_2}{L_1} n_1 n_2\right) + \frac{1}{L_2} K_0\left(2\pi \frac{L_1}{L_2} n_1 n_2\right) \right\}. \tag{20.25}$$

The function $W_2(0; L_1, L_2)$ involves double sums, which are difficult to handle for $L_1 \neq L_2$; in particular, it is not possible to take limits such as $L_i \to \infty$ analytically. Therefore we restrict ourselves to the case $L_1 = L_2$. For a wire with square cross-section, $L_1 = L_2 = L = \sqrt{A}$, Eq. (20.24) reduces to

$$T_c(A) = T_0 - C_2 \frac{\lambda}{\alpha\sqrt{A}}\,, \tag{20.26}$$

where C_2 is a constant given by

$$C_2 = \frac{9\gamma}{\pi} + \frac{12}{\pi} \sum_{n_1, n_2 = 1}^{\infty} K_0(2\pi n_1 n_2) \approx 1.6571\,. \tag{20.27}$$

The critical temperature of the square wire depends on the bulk critical temperature, on the area of its cross-section and the Ginzburg-Landau parameters α and λ, characteristics of the material constituting the wire, Since T_c decreases linearly with the inverse of the square root of cross-section, this implies that there is a minimal area for which $T_c(A_{\min}) = 0$,

$$A_{\min} = \left(C_2 \frac{\lambda}{\alpha T_0}\right)^2 . \tag{20.28}$$

For square wires of cross-section areas smaller than this value, superconductivity is suppressed. On topological grounds, we expect that our results would be independent of the cross-section shape of the wire.

20.3 Critical behavior for grains

Now consider the case where all three spatial dimensions are compactified, corresponding to the system confined in a box of sides L_1, L_2, L_3. Taking $d = 3$ in

Eq. (20.12) and using Eq. (19.25), for sufficiently small L_1, L_2, L_3, in the neighborhood of criticality, $m^2 \approx 0$, we obtain

$$m^2(L_1,L_2,L_3,T) \approx \overline{m}_0^2(L_1,L_2,L_3,T) + \frac{6\lambda}{\pi^{D/2}}\Gamma\left(\frac{D-2}{2}\right) \times \left[\sum_{i=1}^{3}\frac{\zeta(D-2)}{L_i^{D-2}} + 2\sum_{i<j=1}^{3} E_2\left(\frac{D-2}{2};L_i,L_j\right) + 4E_3\left(\frac{D-2}{2};L_1,L_2,L_3\right)\right], \tag{20.29}$$

where

$$E_3(\nu;L_1,L_2,L_3) = \sum_{n_1,n_2,n_3=1}^{\infty}\left[L_1^2n_1^2 + L_2^2n_2^2 + L_3^2n_3^2\right]^{-\nu} \tag{20.30}$$

and the function E_2 is given by Eq. (20.15).

The analytical structure of the function $E_3\left(\frac{D-2}{2};L_1,L_2,L_3\right)$ is obtained from the general symmetrized recurrence relation given by Eqs. (20.17) and (20.18); explicitly we have,

$$E_3\left(\frac{D-2}{2};L_1,L_2,L_3\right) = -\frac{1}{6}\sum_{i<j=1}^{3} E_2\left(\frac{D-2}{2};L_i,L_j\right) + \frac{\sqrt{\pi}\Gamma(\frac{D-3}{2})}{6\Gamma(\frac{D-2}{2})} \times \sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{1}{L_i}E_2\left(\frac{D-2}{2};L_j,L_k\right) + \frac{2\sqrt{\pi}}{3\Gamma(\frac{D-2}{2})}W_3\left(\frac{D-3}{2};L_1,L_2,L_3\right), \tag{20.31}$$

where ε_{ijk} is the totally antisymmetric symbol and the function W_3 is a particular case of Eq. (20.18). Using Eqs. (20.20) and (20.31), the boundary dependent mass is written as

$$m^2(\{L_i\},T) \approx \overline{m}_0^2(L_1,L_2,L_3,T) + \frac{6\lambda}{\pi^{D/2}} \times \left[\frac{1}{3}\Gamma\left(\frac{D-2}{2}\right)\sum_{i=1}^{3}\frac{1}{L_i^{D-2}}\zeta(D-2) + \frac{\sqrt{\pi}}{6}\zeta(D-3) \times \Gamma\left(\frac{D-3}{2}\right)\sum_{i<j=1}^{3}\left(\frac{1}{L_i^{D-3}L_j} + \frac{1}{L_j^{D-3}L_i}\right) + \frac{4\sqrt{\pi}}{3} \times \sum_{i<j=1}^{3} W_2\left(\frac{D-3}{2};L_i,L_j\right) + \frac{\pi}{6}\zeta(D-4)\Gamma\left(\frac{D-4}{2}\right)$$

$$\times \sum_{i,j,k=1}^{3} \frac{(1+\varepsilon_{ijk})}{2} \frac{1}{L_i} \left(\frac{1}{L_j^{D-4} L_k} + \frac{1}{L_k^{D-4} L_j} \right)$$
$$+ \frac{2\pi}{3} \sum_{i,j,k=1}^{3} \frac{(1+\varepsilon_{ijk})}{2} \frac{1}{L_i} W_2 \left(\frac{D-4}{2}; L_j, L_k \right)$$
$$+ \frac{8\sqrt{\pi}}{3} W_3 \left(\frac{D-3}{2}; L_1, L_2, L_3 \right) \Bigg] \tag{20.32}$$

The first two terms in the square bracket diverge as $D \to 3$ due to the poles of the ζ and Γ functions. However, as in the case of wires, using Eqs. (19.35) and (20.22) these divergences cancel exactly. For $D = 3$, the boundary dependent mass, Eq. (20.32) becomes

$$m^2(\{L_i\}, T) \approx \overline{m}_0^2(L_1, L_2, L_3, T) + \frac{6\lambda}{\pi} \left[\frac{\gamma}{2} \sum_{i=1}^{3} \frac{1}{L_i} \right.$$
$$+ \frac{4}{3} \sum_{i<j=1}^{3} W_2(0; L_i, L_j) + \frac{\pi}{18} \sum_{i,j,k=1}^{3} \frac{(1+\varepsilon_{ijk})}{2} \frac{L_i}{L_j L_k}$$
$$+ \frac{2\sqrt{\pi}}{3} \sum_{i,j,k=1}^{3} \frac{(1+\varepsilon_{ijk})}{2} \frac{1}{L_i} W_2 \left(-\frac{1}{2}; L_j, L_k \right)$$
$$\left. + \frac{8}{3} W_3(0; L_1, L_2, L_3) \right] . \tag{20.33}$$

Since no divergences need to be suppressed, we can take the bare mass given by $\overline{m}_0^2(L_1, L_2, L_3, T) = \alpha(T - T_0)$ and write the physical mass as $m^2(L_1, L_2, L_3, T) \approx \alpha\,(T - T_c(L_1, L_2, L_3))$. The expression for $T_c(L_1, L_2, L_3)$ is obtained from Eq. (20.33), but involves multiple sums, which makes almost impossible a general analytical study for arbitrary parameters L_1, L_2, L_3. Thus, we consider the case where $L_1 = L_2 = L_3 = L$, corresponding to a cubic box of volume $V = L^3$. Then the boundary dependent critical temperature reduces to

$$T_c(V) = T_0 - C_3 \frac{\lambda}{\alpha V^{1/3}} , \tag{20.34}$$

where the constant C_3 is given by

$$C_3 = 1 + \frac{9\gamma}{\pi} + \frac{12}{\pi} \sum_{n_1,n_2=1}^{\infty} \frac{e^{-2\pi n_1 n_2}}{n_1} + \frac{48}{\pi} \sum_{n_1,n_2=1}^{\infty} K_0(2\pi n_1 n_2)$$
$$+ \frac{48}{\pi} \sum_{n_1,n_2,n_3=1}^{\infty} K_0 \left(2\pi n_1 \sqrt{n_2^2 + n_3^2} \right) \approx 2.7657 . \tag{20.35}$$

Thus, the minimal volume of the cubic grain sustaining the superconducting phase is

$$V_{\min} = \left(C_3 \frac{\lambda}{\alpha T_0} \right)^3 . \tag{20.36}$$

20.4 Boundary effects on the coupling constant

In the following, we consider the four-point function at zero external momenta, which we take as the basic object for our definition of the renormalized coupling constant. At leading order in $\frac{1}{N}$, it is given by the sum of all chains of one-loop diagrams, which has the formal expression,

$$\Gamma_D^{(4)}(\mathbf{p}=0,m,\{L_i\}) = \frac{u}{1+Nu\Pi(D,m,\{L_i\})}\,, \tag{20.37}$$

where, after making use of the generalized Matsubara prescription (Chapter 15) and the dimensional regularization formula (Chapter 10), $\Pi(D,m,\{L_i\}) = \Pi(\mathbf{p}=0,D,m,\{L_i\})$ corresponds to the single bubble four-point diagram with compactification of a d-dimensional subspace.

To proceed we use the renormalization condition given in Eq. (18.21), from which we deduce formally that the single bubble function $\Pi(D,m,\{L_i\})$ is obtained from the coefficient of the fourth power of the field ($s=2$) in Eq. (20.9). Then we can write $\Pi(D,m,\{L_i\})$ in the form

$$\Pi(D,m,\{L_i\}) = H(D,m) + \Pi_R(D,m,\{L_i\})\,, \tag{20.38}$$

where the $\{L_i\}$-dependent term $\Pi_R(D,m,\{L_i\})$ comes from the second term between brackets in Eq. (20.9),

$$\begin{aligned}\Pi_R(D,m;\{L_i\}) = \frac{1}{(2\pi)^{D/2}}\Bigg[&\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_i n_i}\right)^{\frac{D-4}{2}} K_{\frac{D-4}{2}}(mL_i n_i)\\ &+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}}\right)^{\frac{D-4}{2}}\\ &\times K_{\frac{D-4}{2}}\left(m\sqrt{L_i^2n_i^2+L_j^2n_j^2}\right)+\cdots+\\ &+2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\right)^{\frac{D-4}{2}}\\ &\times K_{\frac{D-4}{2}}\left(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}\right)\Bigg]\end{aligned} \tag{20.39}$$

and $H(D,m)$ is a polar term coming from the first term between brackets in Eq. (20.9),

$$H(D,m) \propto \Gamma\left(2-\frac{D}{2}\right) m^{D-4}\,. \tag{20.40}$$

We see from Eq. (20.40) that for even dimensions $D \geq 4$, $H(D,m)$ is divergent, due to the pole of the Γ-function. Accordingly this term must be subtracted to give the renormalized single bubble function $\Pi_R(D,m,\{L_i\})$. In order to have a coherent procedure for a generic dimension D, the subtraction of the term $H(D,m)$ should

be performed even in the case of odd dimensions, where no poles of Γ-functions are present (finite renormalization). From the properties of Bessel functions, it can be seen from Eq. (20.39) that for any dimension D, $\Pi_R(D, m, \{L_i\})$ satisfies the conditions

$$\lim_{L_i \to \infty} \Pi_R(D, m, \{L_i\}) = 0 \,, \qquad \lim_{L_i \to 0} \Pi_R(D, m, \{L_i\}) \to \infty \,. \tag{20.41}$$

We also conclude that $\Pi_R(D, m, \{L_i\})$ is positive for all values of D and $\{L_i\}$.

Taking inspiration from Eq. (19.42), let us define the $\{L_i\}$-dependent renormalized coupling constant $\lambda_R(m, D, \{L_i\})$, at the leading order in $1/N$, as

$$N\Gamma^{(4)}_{D,R}(\mathbf{p} = 0, m, \{L_i\}) \equiv \lambda_R(D, m, \{L_i\}) = \frac{\lambda}{1 + \lambda \Pi_R(D, m, \{L_i\})}, \tag{20.42}$$

where as before, $\lambda - Nu$ fixed in the limit $N \to \infty$ $u \to 0$. Let $\lambda_R(D, m)$, the renormalized coupling constant in the absence of constraints be defined by,

$$\frac{\lambda_R(D, m)}{N} = \lim_{L_i \to \infty} \Gamma^{(4)}_{D,R}(\mathbf{p} = 0, m, \{L_i\}) \,. \tag{20.43}$$

From Eqs. (20.43), (20.42) and (20.41) we get simply $\lambda_R(D, m) = \lambda$. In other words we have done a choice of renormalization scheme such that the constant λ introduced in the Hamiltonian corresponds to the *renormalized* coupling constant in absence of boundaries. From Eqs. (20.42) and (20.43) we obtain the $\{L_i\}$-dependent renormalized coupling constant

$$\lambda_R(D, m, \{L_i\}) = \frac{\lambda}{1 + \lambda \Pi_R(D, m, \{L_i\})} \,. \tag{20.44}$$

20.5 Effects of the boundary-corrected coupling constant on the critical behavior

Criticality is attained from the ordered phase, when the inverse squared correlation length, $\xi^{-2}(\{L_i\}, \phi_0)$, vanishes in the large N gap equation,

$$\xi^{-2}(\{L_i\}, \varphi_0) = \overline{m}_0^2 + 12\lambda_R(D, \{L_i\})\varphi_0^2 + \frac{24\lambda_R(D, \{L_i\})}{L_1 \cdots L_d} \times \sum_{\{n_j\}=-\infty}^{\infty} \int \frac{d^{D-d}q}{(2\pi)^{D-d}} \times \frac{1}{\mathbf{q}^2 + \sum_{j=1}^{d} (\frac{2\pi n_j}{L_j})^2 + \xi^{-2}(\{L_i\}, \varphi_0)} \tag{20.45}$$

In the ordered-disordered border, φ_0 vanishes and the inverse correlation length equals the physical mass. The physical mass is obtained at the one-loop order from Eqs. (20.9) and (18.20), after performing the change $\lambda \to \lambda_R(D, m, \{L_i\})$ where

$\lambda_R(D, m, \{L_i\})$ is the renormalized $\{L_i\}$-dependent coupling constant; we get,

$$
\begin{aligned}
m^2(D,T,\{L_i\}) = \overline{m}_0^2(\{L_i\}) + \frac{24\lambda_R(D,m,\{L_i\})}{(2\pi)^{D/2}} \\
\times \left[\sum_{i=1}^{d} \sum_{n_i=1}^{\infty} \left(\frac{m}{L_i n_i} \right)^{\frac{D}{2}-1} K_{\frac{D}{2}-1}(mL_i n_i) \right. \\
+ 2 \sum_{i<j=1}^{d} \sum_{n_i,n_j=1}^{\infty} \left(\frac{m}{\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}} \right)^{\frac{D}{2}-1} \\
\times K_{\frac{D}{2}-1}\left(m\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2} \right) + \cdots \\
+ 2^{d-1} \sum_{n_1,\ldots,n_d=1}^{\infty} \left(\frac{m}{\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}} \right)^{\frac{D}{2}-1} \\
\left. \times K_{\frac{D}{2}-1}\left(m\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2} \right) \right] .
\end{aligned}
\tag{20.46}
$$

But $\lambda_R(D, m, \{L_i\})$ is itself a function of $m = m(D, T, \{L_i\})$, as given by appropriate versions of Eqs. (20.44) and (19.48), i.e.

$$
\lambda_R(D, m, \{L_i\})) = \frac{\lambda}{1 + \lambda \Pi_R(D, m(D,T,\{L_i\}), \{L_i\})} , \tag{20.47}
$$

with

$$
\begin{aligned}
\Pi_R(D, m(D,T,\{L_i\}); \{L_i\}) = \frac{1}{(2\pi)^{D/2}} \left[\sum_{i=1}^{d} \sum_{n_i=1}^{\infty} \left(\frac{m(D,T,\{L_i\})}{L_i n_i} \right)^{\frac{D-4}{2}} \right. \\
\times K_{\frac{D-4}{2}}(m(D,T,\{L_i\}) L_i n_i) \\
+ 2 \sum_{i<j=1}^{d} \sum_{n_i,n_j=1}^{\infty} \left(\frac{m(D,T,\{L_i\})}{\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}} \right)^{\frac{D-4}{2}} \\
\times K_{\frac{D-4}{2}}\left(m(D,T,\{L_i\}) \sqrt{L_i^2 n_i^2 + L_j^2 n_j^2} \right) + \cdots + \\
+ 2^{d-1} \sum_{n_1,\ldots,n_d=1}^{\infty} \left(\frac{m(D,T,\{L_i\})}{\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}} \right)^{\frac{D-4}{2}} \\
\left. \times K_{\frac{D-4}{2}}\left(m(D,T,\{L_i\}) \sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2} \right) \right] .
\end{aligned}
\tag{20.48}
$$

Therefore $m(D,T,\{L_i\})$ is given by a complicated set of coupled equations, Eqs. (20.46), (20.47) and (20.48), since $\lambda_R(D,m,\{L\})$ depends on $m(D,T,\{L_i\})$. This set of equations has no analytical solutions, in general. Nevertheless, limiting ourselves to the neighborhood of criticality, $m^2(D,T,\{L_i\}) \approx 0$, we may investigate the behavior of the system by using in Eq. (20.46), Eq. (20.47) and (20.48) the asymptotic formula for small values of the argument of the Bessel function,

$$K_\nu(z) \approx \frac{1}{2}\Gamma(\nu)\left(\frac{z}{2}\right)^{-\nu} \quad (z \sim 0\,; \quad Re(\nu) > 0)\,. \tag{20.49}$$

At criticality, using this equation in all the sums of Bessel functions present in Eqs. (20.48) and (20.46) the terms $m(D,T,\{L_i\})$ present in the coefficients and the arguments of the Bessel functions cancel out, giving for $m(D,T,\{L_i\}) \approx 0$, mass independent expressions of the form,

$$\frac{1}{2}\Gamma(\frac{D-s}{2})E_p\left(\frac{D-s}{2}; L_1, ..., L_p\right) \tag{20.50}$$

where $s = 2$ and $s = 4$ for respectively the mass in Eq. (20.46) and the renormalized one-loop bubble function in Eq. (20.48). In both cases, $p = 1, 2, \ldots, d$ and $E_p\left(\frac{D-s}{2}; L_1, ..., L_p\right)$ is one of the generalized Epstein-Hurwitz zeta functions defined in symmetric form in Eq. (20.17). Notice that, for $p = 1$, E_p reduces to the Riemann zeta function.

Inserting the appropriate versions of Eq. (20.50) in Eqs. (20.46) and (20.48), we obtain expressions for the physical mass and the renormalized coupling constant at criticality $m^2(D,T,\{L_i\}) \approx 0$,

$$\begin{aligned} m^2(D,T,\{L_i\}) \approx \overline{m}_0^2(L_1,...,L_d) + \frac{24\lambda_R(D,\{L_i\})}{(2\pi)^{D/2}} \\ \times \left[\sum_{i=1}^{d}\frac{1}{2}\Gamma(\frac{D-2}{2})E_1\left(\frac{D-2}{2}; L_i\right)\right. \\ + 2\sum_{i<j=1}^{d}\frac{1}{2}\Gamma(\frac{D-2}{2})E_2\left(\frac{D-2}{2}; L_i, L_j\right) + \cdots \\ \left. + 2^{d-1}\frac{1}{2}\Gamma(\frac{D-2}{2})E_d\left(\frac{D-s}{2}; L_1, ..., L_d\right)\right], \end{aligned} \tag{20.51}$$

and

$$\lambda_R(D,\{L_i\}) \approx \frac{\lambda}{1 + \lambda C(D) F_{Dd}(\{L_i\})}, \tag{20.52}$$

where

$$F_{Dd}(\{L_i\}) = \sum_{i=1}^{d} L_i^{4-D}\zeta(D-4) + 2\sum_{i<j=1}^{d} E_2\left(\frac{D-4}{2}; L_i, L_j\right) + \cdots + 2^{d-1}E_d\left(\frac{D-4}{2}; L_1, \ldots, L_d\right) \tag{20.53}$$

and $C(D) = \frac{1}{8\pi^{D/2}}\Gamma\left(\frac{D-4}{2}\right)$. Replacing Eq. (20.52) in Eq. (20.51) and taking $m^2(D,T,\{L_i\}) = 0$, gives the critical temperature as a function of the distances between the boundaries, $\{L_i\}$. This will be done in the following for $D = 3$. Then the physically interesting situations of $d = 1$ (a film), $d = 2$ (an infinitely long wire) and $d = 3$ (a cubic grain) are considered. For the situation without boundary corrections to the coupling constant we refer to [100].

20.5.1 *Effects of the boundary-corrected coupling constant on the phase transition for wires*

We now focus on the situation where two spatial dimensions are compactified. . From Eq. (20.51), taking $d = 2$, we get for $m^2(D,T,L_1,L_2) \approx 0$,

$$m^2(D,T,L_1,L_2) \approx \overline{m}_0^2(L_1,L_2) + \frac{6\lambda_R(D,m(D,T,L_1,L_2)}{\pi^{D/2}}\Gamma\left(\frac{D}{2}-1\right) \times \left[\left(\frac{1}{L_1^{D-2}} + \frac{1}{L_2^{D-2}}\right)\zeta(D-2) + 2E_2\left(\frac{D-2}{2}; L_1, L_2\right)\right], \tag{20.54}$$

where $E_2\left(\frac{D-2}{2}; L_1, L_2\right)$ is the generalized (twodimensional) Epstein zeta function obtained from Eq. (20.17),

$$E_2\left(\frac{D-2}{2}; L_1, L_2\right) = \sum_{n_1,\, n_2=1}^{\infty}\left[L_1^2 n_1^2 + L_2^2 n_2^2\right]^{-\left(\frac{D-2}{2}\right)}, \tag{20.55}$$

for $\mathrm{Re}\{D\} > 3$.

In particular, noticing that $E_1(\nu; L_j) = L_j^{-2\nu}\zeta(2\nu)$, we find

$$E_2\left(\frac{D-2}{2}; L_1, L_2\right) = -\frac{1}{4}\left(\frac{1}{L_1^{D-2}} + \frac{1}{L_2^{D-2}}\right)\zeta(D-2) + \frac{\sqrt{\pi}\Gamma(\frac{D-3}{2})}{4\Gamma(\frac{D-2}{2})}\left(\frac{1}{L_1 L_2^{D-3}} + \frac{1}{L_1^{D-3}L_2}\right)\zeta(D-3) + \frac{\sqrt{\pi}}{\Gamma(\frac{D-2}{2})}W_2\left(\frac{D-3}{2}; L_1, L_2\right), \tag{20.56}$$

which is a meromorphic function of D, symmetric in the parameters L_1 and L_2. The function $W_2\left(\frac{D-3}{2}; L_1, L_2\right)$ in Eq. (20.56) is the particular case of Eq. (20.19) for $p = 2$.

Using the above expression, Eq. (20.54) can be rewritten as

$$\begin{aligned} m^2(L_1, L_2) \approx \overline{m}_0^2(L_1, L_2) + \frac{3\lambda_R(D, m(D, T, L_1, L_2)}{\pi^{D/2}} \\ \times \left[\left(\frac{1}{L_1^{D-2}} + \frac{1}{L_2^{D-2}} \right) \Gamma\left(\frac{D-2}{2} \right) \zeta(D-2) \right. \\ + \sqrt{\pi} \left(\frac{1}{L_1 L_2^{D-3}} + \frac{1}{L_1^{D-3} L_2} \right) \Gamma\left(\frac{D-3}{2} \right) \zeta(D-3) \\ \left. + 2\sqrt{\pi} W_2\left(\frac{D-3}{2}; L_1, L_2 \right) \right] . \end{aligned} \tag{20.57}$$

This equation presents no problems for $3 < D < 4$ but, for $D = 3$, the first and second terms between brackets of Eq. (20.21) are divergent due to the ζ function and Γ function, respectively. However, these two divergences cancel out. No regularization is needed as in the case of films. This can be seen remembering the property in Eq. (19.35) and using the expansion of $\Gamma(\frac{D-3}{2})$ around $D = 3$,

$$\Gamma(\frac{D-3}{2}) \approx \frac{2}{D-3} + \Gamma'(1)\,, \tag{20.58}$$

$\Gamma'(z)$ standing for the derivative of the Γ function with respect to z. For $z = 1$ it coincides with the Euler digamma function $\psi(1)$, which has the particular value $\psi(1) = -\gamma$. The two divergent terms generated by the use of Eqs. (19.35) and (20.58) cancel exactly between them.

A similar formula can be obtained from Eq. (20.52), leading at criticality to,

$$\lambda_R(D, L_1, L_2) \approx \frac{\lambda}{1 + \lambda C(D) \left[\sum_{i=1}^{2} L_i^{4-D} \zeta(D-4) + 2E_2\left(\frac{D-4}{2}; L_1, L_2 \right) \right]} \tag{20.59}$$

Then we can replace Eq. (20.59) in (20.57) and take $D = 3$, in which case the function $W_2\left(\frac{D-3}{2}; L_1, L_2\right)$, becomes,

$$W_2(0; L_1, L_2) = \sum_{n_1, n_2 = 1}^{\infty} \left\{ \frac{1}{L_1} K_0\left(2\pi \frac{L_2}{L_1} n_1 n_2 \right) + \frac{1}{L_2} K_0\left(2\pi \frac{L_1}{L_2} n_1 n_2 \right) \right\}. \tag{20.60}$$

The quantity $W_2(0; L_1, L_2)$ involves complicated double sums, very difficult to handle for $L_1 \neq L_2$, but it has a summable expression for $L_1 = L_2 = L = \sqrt{A}$, which leads to Eq. (20.62) below. Next since we have no regularization to perform in this

case, we can take $\overline{m}_0^2 = \alpha(T - T_0)$. After using tabulated values for the special functions, we get for a wire with a square transversal section, $L_1 = L_2 = L = \sqrt{A}$,

$$T_c^{wire}(A) = T_0 - \frac{48\pi C_2 \lambda}{48\pi\alpha\sqrt{A} + C_1\alpha\lambda(\sqrt{A})^2} \tag{20.61}$$

where

$$C_1 = 1 + \frac{24}{\pi}\sum_{n_1,n_2=1}^{\infty}\frac{n_1}{n_2}K_1(2\pi n_1 n_2), \tag{20.62}$$

and

$$C_2 = \frac{9\gamma}{\pi} + \frac{12}{\pi}\sum_{n_1,n_2=1}^{\infty}K_0(2\pi n_1 n_2) \approx 1.6571\,. \tag{20.63}$$

As in the preceding subsection, we have from Eq. (20.61) a minimal transversal section sustaining the transition,

$$A'_{min} = \left[\frac{24\pi}{C_1\lambda}\left(\sqrt{1 + \frac{C_1\lambda(A_{min})^{1/2}}{12\pi}} - 1\right)\right]^2 \tag{20.64}$$

where A_{min} is the corresponding quantity with no boundary corrections to the coupling constant [100].

20.5.2 *Effects of the boundary-corrected coupling constant on the phase transition for grains*

We now turn our attention to the case where all three spatial dimensions are compactified, corresponding to the system confined in a box of sides L_1, L_2, L_3. Taking $d = 3$ in Eq. (20.51) and using Eq. (20.49), we obtain in the neighborhood of criticality, $m^2(D, T, L_1, L_2, L_3) \approx 0$,

$$\begin{aligned} m^2(D,T,L_1,L_2,L_3) \approx\ & \overline{m}_0^2(L_1,L_2,L_3) \\ & + \frac{6\lambda_R(D, m(D,T,L_1,L_2,L_3)}{\pi^{D/2}}\Gamma\left(\frac{D-2}{2}\right) \\ & \times\left[\sum_{i=1}^{3}\frac{\zeta(D-2)}{L_i^{D-2}} + 2\sum_{i<j=1}^{3}E_2\left(\frac{D-2}{2}; L_i, L_j\right)\right. \\ & \left. + 4E_3\left(\frac{D-2}{2}; L_1, L_2, L_3\right)\right]\,, \end{aligned} \tag{20.65}$$

where $E_3(\nu; L_1, L_2, L_3) = \sum_{n_1,n_2,n_3=1}^{\infty}\left[L_1^2 n_1^2 + L_2^2 n_2^2 + L_3^2 n_3^2\right]^{-\nu}$ and the functions E_2 are given by Eq. (20.56).

The analytical structure of the function $E_3\left(\frac{D-2}{2}; L_1, L_2, L_3\right)$ can be obtained from the general symmetrized recurrence relation given by Eqs. (20.17) and (20.18); explicitly, we have,

$$
\begin{aligned}
E_3\left(\frac{D-2}{2}; L_1, L_2, L_3\right) = & -\frac{1}{6}\sum_{i<j=1}^{3} E_2\left(\frac{D-2}{2}; L_i, L_j\right) \\
& + \frac{\sqrt{\pi}\Gamma(\frac{D-3}{2})}{6\Gamma(\frac{D-2}{2})}\sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{1}{L_i}E_2\left(\frac{D-2}{2}; L_j, L_k\right) \\
& + \frac{2\sqrt{\pi}}{3\Gamma(\frac{D-2}{2})}W_3\left(\frac{D-3}{2}; L_1, L_2, L_3\right),
\end{aligned}
\tag{20.66}
$$

where ε_{ijk} is the totally antisymmetric symbol and the function W_3 is a particular case of Eq. (20.18). Using Eqs. (20.56) and (20.66), the boundary dependent mass can be written as

$$
\begin{aligned}
m^2(D, T, \{L_i\}) \approx & \overline{m}_0^2(L_1, L_2, L_3) + \frac{6\lambda_R(D, m(D, T, L_1, L_2, L_3)}{\pi^{D/2}} \\
& \times \left[\frac{1}{3}\Gamma\left(\frac{D-2}{2}\right)\sum_{i=1}^{3}\frac{1}{L_i^{D-2}}\zeta(D-2)\right. \\
& + \frac{\sqrt{\pi}}{6}\zeta(D-3)\sum_{i<j=1}^{3}\left(\frac{1}{L_i^{D-3}L_j} + \frac{1}{L_j^{D-3}L_i}\right)\Gamma\left(\frac{D-3}{2}\right) \\
& + \frac{4\sqrt{\pi}}{3}\sum_{i<j=1}^{3}W_2\left(\frac{D-3}{2}; L_i, L_j\right) \\
& + \frac{\pi}{6}\zeta(D-4)\Gamma\left(\frac{D-4}{2}\right)\sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{1}{L_i}\left(\frac{1}{L_j^{D-4}L_k}\right. \\
& \left. + \frac{1}{L_k^{D-4}L_j}\right) \\
& + \frac{2\pi}{3}\sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{1}{L_i}W_2\left(\frac{D-4}{2}; L_j, L_k\right) \\
& \left. + \frac{8\sqrt{\pi}}{3}W_3\left(\frac{D-3}{2}; L_1, L_2, L_3\right)\right]
\end{aligned}
\tag{20.67}
$$

The first two terms in the square bracket of Eq. (20.67) diverge as $D \to 3$ due to the poles of the Γ and ζ functions. However, as it happens in the case of wires,

it can be shown that these divergences cancel exactly one another. For $D = 3$, the boundary dependent mass (20.67) becomes,

$$m^2(D,T,L_1,L_2,L_3) \approx \overline{m}_0^2(L_1,L_2,L_3) + \frac{6\lambda_R(D,m(D,T,L_1,L_2,L_3)}{\pi} \left[\frac{\gamma}{2}\sum_{i=1}^{3}\frac{1}{L_i} + \frac{4}{3}\sum_{i<j=1}^{3} W_2(0;L_i,L_j) + \frac{\pi}{18}\sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{L_i}{L_jL_k} + \frac{2\sqrt{\pi}}{3}\sum_{i,j,k=1}^{3}\frac{(1+\varepsilon_{ijk})}{2}\frac{1}{L_i}W_2\left(-\frac{1}{2};L_j,L_k\right) + \frac{8}{3}W_3(0;L_1,L_2,L_3)\right] . \tag{20.68}$$

As in the case of films and wires, it is possible to get the boundary dependence of the renormalized coupling constant. We obtain from Eq. (20.52) that,

$$\lambda_R(D,L_1,L_2,L_3) \approx \frac{\lambda}{1+\lambda C(D)F_{D3}(L_1,L_2,L_3)} \tag{20.69}$$

where

$$F_{D3}(L_1,L_2,L_3) = \sum_{i=1}^{3} L_i^{4-D}\zeta(D-4) + 2\sum_{i<j=1}^{3} E_2\left(\frac{D-4}{2};L_i,L_j\right) + 2^2 E_3\left(\frac{D-4}{2};L_1,L_2,L_3\right), \tag{20.70}$$

which is to be replaced in Eq. (20.68). As before, since no divergences need to be suppressed, we can take the bare mass given by $\overline{m}_0^2(L_1,L_2,L_3) = \alpha(T - T_0)$. The expression of $T_c(L_1,L_2,L_3)$ can be obtained from Eqs. (20.68) and (20.69), but it is a complicated formula, involving multiple sums, which makes almost impossible a general analytical study for arbitrary parameters L_1, L_2, L_3; thus, as before, we restrict ourselves to the situation where $L_1 = L_2 = L_3 = L$, corresponding to a cubic box of volume $V = L^3$. In this case, using Eqs. (20.68) and (20.69), the boundary dependent critical temperature is given by,

$$T_c(V) = T_0 - \frac{48\pi C_3\lambda}{48\pi\alpha\, V^{1/3} + C_4\alpha\lambda(V^{1/3})^2} \tag{20.71}$$

where

$$C_4 = 1 + \frac{\pi}{15} + \frac{24}{\pi} \sum_{n_1,n_2=1}^{\infty} \left(\frac{n_1}{n_2}\right)^{3/2} K_{3/2}(2\pi n_1 n_2) + \frac{48}{\pi} \sum_{n_1,n_2=1}^{\infty} \frac{n_1}{n_2} K_1(2\pi n_1 n_2)$$
$$+ \frac{48}{\pi} \sum_{n_1,n_2,n_3=1}^{\infty} \frac{\sqrt{n_1^2+n_2^2}}{n_3} K_1\left(2\pi n_3 \sqrt{n_1^2+n_2^2}\right) \approx 1.2246\,, \tag{20.72}$$

and

$$C_3 = 1 + \frac{9\gamma}{\pi} + \frac{12}{\pi} \sum_{n_1,n_2=1}^{\infty} \frac{e^{-2\pi n_1 n_2}}{n_1} + \frac{48}{\pi} \sum_{n_1,n_2=1}^{\infty} K_0(2\pi n_1 n_2)$$
$$+ \frac{48}{\pi} \sum_{n_1,n_2,n_3=1}^{\infty} K_0\left(2\pi n_1 \sqrt{n_2^2+n_3^2}\right) \approx 2.7657 \tag{20.73}$$

The minimal allowed volume of the grain, in this case, is

$$V'_{min} = \left[\frac{24\pi}{C_4\lambda}\left(\sqrt{1 + \frac{C_4\lambda (V_{min})^{1/3}}{12\pi}} - 1\right)\right]^3, \tag{20.74}$$

where V_{min} corresponds to the minimal volume for the situation where boundary corrections to the coupling constant are ignored [100].

20.6 Universal behavior of size-effects in second-order phase transitions

We now gather together the results presented so far. Define the reduced transition temperature by

$$t_c = \frac{T_c}{T_0}\,,$$

and consider the reduced length, defined in units of $L_{\min} = C_1\lambda/(\alpha T_0)$ (Eq. (19.41), the minimal thickness for a film, without coupling-constant correction),

$$l = \frac{L}{L_{\min}}\,.$$

Collecting the results of the present and the last chapters, we can write the reduced transition temperature as a function of the reduced length, in the case where no correction to the coupling constant is included, for films, square wires and cubic grains ($d = 1, 2, 3$, respectively), as

$$t_c^{(d)}(l) = 1 - \frac{\mathcal{C}_d}{l}\,, \tag{20.75}$$

with $\mathcal{C}_1 = 1$, $\mathcal{C}_2 = C_2/C_1 \simeq 1.5032$ and $\mathcal{C}_3 = C_3/C_1 \simeq 2.5088$; that is, for all values of d, the reduced temperature, t_c, scales with the inverse of the reduced length, l^{-1}. In other words, the overall behavior of the reduced temperature does not depend on the number of compactified dimensions but only on the dimension of the Euclidian space, here $D = 3$.

Considering the coupling-constant correction, the reduced transition temperature is written as

$$t_c^{(d)}(l) = 1 - \frac{48\pi\mathcal{C}_d}{48\pi l + \mathcal{E}_d \xi l^2}\,, \tag{20.76}$$

where $\mathcal{E}_1 = 1$, $\mathcal{E}_2 = C_1 \simeq 1.1024$, $\mathcal{E}_3 = C_4 \simeq 1.2246$ and $\xi = \lambda L_{\min}$. In Fig. 20.1, we plot the reduced transition temperature as a function of the reduced length for all cases (films, square wires and cubic grains), fixing $\xi = 30$.

Summarizing, in this chapter we have generalized the phenomenological approach to second-order phase transitions in films, discussed in Chapter 19. We have presented a general formalism which, in the framework of the Ginzburg–Landau model, is able to describe phase transitions for systems defined in spaces of arbitrary dimension, some of them being compactified. We have focused on the situations with $D = 3$ and $d = 2, 3$, corresponding to wires and grains, respectively. Such a generalization is not trivial, since it involves the extension to several dimensions of the one-dimensional mode-sum regularization procedure. This extension requires, in particular, the definition of symmetrized multidimensional Epstein–Hurwitz functions with no analog in the one-dimensional case. When combined with the boundary dependent coupling constant, this generates sets of coupled equations for the renormalized mass, which can be solved only at criticality. In this kind of mathematical framework the general formulas are obtained, and then applied to the

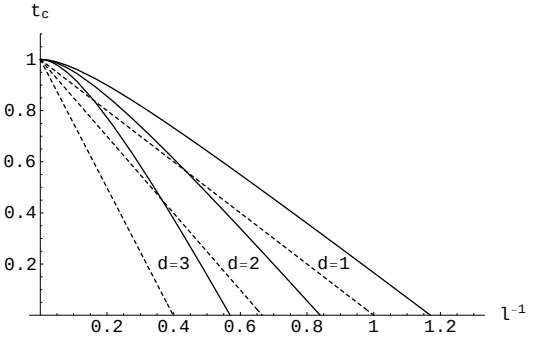


Fig. 20.1 Reduced transition temperature as a function of the inverse of the reduced compactification length, for films ($d = 1$), square wires ($d = 2$) and cubic grains ($d = 3$). The full and dashed lines correspond to results with and without correction of the coupling constant, respectively.

particular of films, wires and grains. This leads to specific forms of the critical temperature as a function of the size of the system. These examples provide a strong justification for the ideas of compactification enunciated in Chapter 15. In the next chapter, these ideas will be applied to first-order phase transitions.

Chapter 21

First-Order Phase Transitions in Confined Systems

In previous chapters a study of second-order phase transitions in a D-dimensional system described by the Ginzburg-Landau model in the absence of gauge fluctuations, has been carried out. We have assumed that d of the cartesian coordinates are compactified and we have found the critical temperature as a function of the size of compactified dimensions. This model describes first-order phase transitions. We calculate the transition temperature as a function of the size of compactification, using methods of quantum field theory. In this chapter we stay in a general framework, the Euclidean D-dimensional $\lambda|\varphi|^4+\eta|\varphi|^6$ model with d ($d \leq D$) compactified dimensions. We start from the effective potential, which gives the physical mass through a renormalization relation. This condition, however, reduces considerably the number of relevant Feynman diagrams contributing to the mass, if we consider only first-order terms in both coupling constants. In fact, just two diagrams need to be considered in this approximation: a tadpole graph with the ϕ^4 coupling (1 loop) and a "shoestring" graph with the ϕ^6 coupling (2 loops). No diagram with both couplings appear. The size-dependence appears as before, from the treatment of the loop integrals.

21.1 Effective potential with compactification of a d-dimensional subspace

We consider the model described by the Ginzburg-Landau Hamiltonian density in a Euclidian D-dimensional space,

$$\mathcal{H} = \frac{1}{2}\left|\partial_\mu\varphi\right|\left|\partial^\mu\varphi\right| + \frac{1}{2}m_0^2\left|\varphi\right|^2 - \frac{\lambda}{4!}\left|\varphi\right|^4 + \frac{\eta}{6!}\left|\varphi\right|^6, \tag{21.1}$$

where $\lambda > 0$ and $\eta > 0$ are the *renormalized* quartic and sextic self-coupling constants. Here the sign of quartic term is the opposite to that of the second-order phase transition. The field, $\varphi(x)$ is a complex field (two components). The bare mass is given by $m_0^2 = \alpha(T/T_0 - 1)$, with $\alpha > 0$ and T_0 being a temperature parameter, which is smaller than the critical temperature for a first-order phase transition. We consider the system in D dimensions confined to a d-dimensional

subspace, a parallelepiped box with edges $L_1, \dots L_d$. The general ideas presented in Chapter 15 provide arguments for using this procedure as a consequence of topological considerations. We use cartesian coordinates $\mathbf{r} = (x_1, ..., x_d, \mathbf{z})$, where $\mathbf{z}$ is a $(D-d)$-dimensional vector, with corresponding momentum $\mathbf{k} = (k_1, ..., k_d, \mathbf{q})$, $\mathbf{q}$ being a $(D-d)$-dimensional vector in momentum space. The field $\varphi(x_1, ..., x_d, \mathbf{z})$ satisfies periodic boundary conditions $\varphi(x_1 + L_1, \dots x_d + L_d) = \varphi(x_1, \dots, x_d)$. We introduce the generalized Matsubara prescription Eq. (19.7) for the Feynman rules. The effective potential is obtained [308], as an expansion in the number of loops in Feynman diagrams. Accordingly, to the free propagator and to the no-loop (tree) diagrams for both couplings, radiative corrections are added, with increasing number of loops. Thus, at the 1-loop approximation, we get the infinite series of 1-loop diagrams with all numbers of insertions of the φ^4 vertex (two external legs in each vertex), plus the infinite series of 1-loop diagrams with all numbers of insertions of the φ^6 vertex (four external legs in each vertex), plus the infinite series of 1-loop diagrams with all kinds of mixed numbers of insertions of φ^4 and φ^6 vertices. Analogously, there are insertions in diagrams with 2 loops, etc. However, to get the renormalized mass we restrict ourselves to the lowest order terms in the loop expansion, as given by Eq. (19.29).

(a) *The tadpole contribution to the mass*

To 1-loop approximation, the procedure follows along the same lines as in the previous chapters, starting from the expression for the one-loop contribution to the effective potential in unbounded space given by Eq. (4.21),

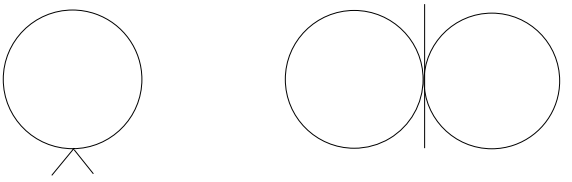
$$U_1(\varphi_0) = \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s} \left[\frac{\lambda|\varphi_0|^2}{2}\right]^s \int \frac{d^D k}{(k^2 + m^2)^s}, \tag{21.2}$$

where m is the physical mass. To deal with dimensionless quantities in the regularization procedures, we introduce parameters $c^2 = m^2/4\pi^2\mu^2$, $(L_i\mu)^2 = a_i^{-1}$, $g_1 = (-\lambda/4\pi^2\mu^{4-D})$, $|\varphi_0/\mu^{(D-2)/2}|^2 = |\phi_0|^2$, $q = k/2\pi\mu$, where φ_0 is the normalized vacuum expectation value of the field (the classical field) and μ is a mass scale. In terms of these parameters and performing the Matsubara replacements Eq. (19.7), the one-loop contribution to the effective potential is written as

$$U_1(\phi_0, a_1, ..., a_d) = \mu^D \sqrt{a_1 \cdots a_d} \sum_{s=1}^{\infty} \frac{(-1)^{s+1}}{2s} g_1^s |\phi_0|^{2s} \times \sum_{n_1,\dots,n_d=-\infty}^{+\infty} \int \frac{d^{D-d} q}{(a_1 n_1^2 + \cdots + a_d n_d^2 + c^2 + \mathbf{q}^2)^s}. \tag{21.3}$$

The parameter s counts the number of vertices on the loop. It is clear that only the $s = 1$ term contributes to the renormalization condition, Eq. (18.20). It corresponds to the tadpole diagram, Fig. 21.1a. It is also clear that all $|\phi_0|^6$-vertex and mixed $|\phi_0|^4$- and $|\phi_0|^6$-vertex insertions on the 1-loop diagrams do not contribute

when one computes the second derivative of similar expressions with respect to the classical field at zero value: only diagrams with two external legs would survive. This is impossible for a $|\phi_0|^6$-vertex insertion at the 1-loop approximation. The first contribution from the $|\phi_0|^6$ coupling must come from a higher-order term in the loop expansion. Two-loop diagrams with two external legs and only $|\phi_0|^4$ vertices are of second-order in its coupling constant, as well as all possible diagrams with vertices of mixed type are neglected. However, the 2-loop shoestring diagram, Fig. 21.1(b), with only one $|\phi_0|^6$ vertex and two external legs is a first-order (in η) contribution to the effective potential, according to our approximation.



(a) Tadpole diagram (b) Shoestring diagram

Fig. 21.1 Contributions to the effective potential.

In short, we consider the physical mass as defined to first-order in both coupling constants, by the contributions of radiative corrections from only two diagrams: the tadpole and the shoestring diagram.

The tadpole contribution is

$$U_1(\phi_0, a_1, ..., a_d) = \mu^D \sqrt{a_1 \cdots a_d} \frac{1}{2} g_1 |\phi_0|^2 \times \sum_{n_1,...,n_d=-\infty}^{+\infty} \int \frac{d^{D-d}q}{\mathbf{q}^2 + a_1 n_1^2 + \cdots + a_d n_d^2 + c^2}. \quad (21.4)$$

The integral over the $D - d$ non-compactified variables is performed using Eq. (10.12); leading to

$$U_1(\phi_0, a_1, ..., a_d) = \mu^D \sqrt{a_1 \cdots a_d} \sum_{s=1}^{\infty} f(D,d) g_1 |\phi_0|^2 A_d^{c^2}(\frac{2 - D + d}{2}; a_1, ..., a_d), \quad (21.5)$$

where

$$f(D,d) = \pi^{(D-d)/2} \frac{1}{2} \Gamma\left(1 - \frac{D-d}{2}\right) \quad (21.6)$$

and $A_d^{c^2}(\nu; a_1, ..., a_d)$ are Epstein–Hurwitz zeta functions, valid for $\mathrm{Re}(\nu) > d/2$, defined by

$$A_d^{c^2}(\nu; a_1, ..., a_d) = \sum_{n_1,...,n_d=-\infty}^{+\infty} (a_1 n_1^2 + \cdots + a_d n_d^2 + c^2)^{-\nu}. \quad (21.7)$$

As noted in Chapter 19, the multivariable Epstein–Hurwitz function has an analytic extension to the whole complex ν-plane, given by Eq. (18.16). Thus taking $\nu = (2-D+d)/2$ in Eq. (20.8), the tadpole part of the effective potential in D dimensions with a compactified d-dimensional subspace is:

$$\begin{aligned} U_1(\varphi_0, L_1, ..., L_d) = \frac{\lambda|\varphi_0|^2}{2\ (2\pi)^{D/2}} \Bigg[& 2^{-D/2-1} m^{D-2} \Gamma\left(\frac{2-D}{2}\right) \\ & + \sum_{i=1}^{d} \sum_{n_i=1}^{\infty} \left(\frac{m}{L_i n_i}\right)^{D/2-1} K_{D/2-1}(m L_i n_i) \\ & + 2 \sum_{j<i=1}^{d} \sum_{n_i, n_j=1}^{\infty} \left(\frac{m}{\sqrt{L_i^2 + L_j^2}}\right)^{D/2-1} K_{D/2-1}(m\sqrt{L_i^2 + L_j^2}) \\ & + \cdots + 2^{d-1} \sum_{n_1,\ldots,n_d=1}^{\infty} \left(\frac{m}{\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}}\right)^{D/2-1} \\ & \times K_{D/2-1}(m\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}) \Bigg], \end{aligned} \tag{21.8}$$

where the original variables, φ_0, λ, and L_i are reintroduced.

(b) *The shoestring diagram contribution to the effective potential*

The 2-loop shoestring diagram contribution to the effective potential in unbounded space ($L_i = \infty$) is given as [133],

$$U_2(\phi_0) = \frac{\eta|\phi_0|^2}{16} \left[\int \frac{d^D q}{(2\pi)^D} \frac{1}{q^2 + m^2} \right]^2. \tag{21.9}$$

After the compactification of d dimensions with lengths L_i, $i = 1, \ldots, d$ and integration over the non-compactified variables, U_2 becomes

$$\begin{aligned} U_2(\phi_0, a_1, \ldots, a_d) = & \frac{1}{2} g_2 |\phi_0|^2 \mu^{2D-2} a_1 \cdots a_d \pi^{D-d} \\ & \times \left[\Gamma\left(\frac{2-D+d}{2}\right) \right. \\ & \left. \sum_{n_1,\ldots,n_d=-\infty}^{\infty} \frac{1}{(a_1 n_1^2 + \cdots + a_d n_d^2 + c^2)^{(2-D+d)/2}} \right]^2, \end{aligned} \tag{21.10}$$

where ϕ_0 and a_i are already defined and the dimensionless quantity $g_2 = (\eta/8 \cdot 16\pi^4 \mu^{6-2D})$ is used. The multiple sum is again the Epstein–Hurwitz zeta function, $A_d^{c^2}(\frac{2-D+d}{2}; a_1, \ldots, a_d)$ given by Eq. (18.7), for $\nu = (2 - D + d)/2$. In terms of the original variables, φ, η, and L_i,and using the analytical continuation of the

Epstein-Hurwitz function, we have

$$U_2(\varphi_0, L_1, \ldots, L_d) = \frac{\eta|\varphi_0|^2}{4\ (2\pi)^D}\left[2^{-1-D/2}m^{D-2}\Gamma\left(\frac{2-D}{2}\right)\right.$$
$$+\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_i n_i}\right)^{D/2-1}K_{D/2-1}(mL_i n_i)+\cdots$$
$$+2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\right)^{D/2-1}$$
$$\left.K_{D/2-1}(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2})\right]^2. \tag{21.11}$$

In both Eqs. (21.8) and (21.11), there is a term proportional to $\Gamma\left(\frac{2-D}{2}\right)$ which as stated before, is divergent for even dimensions $D \geq 2$ and should be subtracted in order to obtain finite physical parameters. For odd D, the gamma function is finite, but we also subtract it (corresponding to a finite renormalization) for the sake of uniformity. After subtraction we get

$$U_1^{(\mathrm{Ren})}(\varphi_0, L_1, \ldots, L_d) = \frac{\lambda|\varphi_0|^2}{2\ (2\pi)^{D/2}}\left[\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_i n_i}\right)^{D/2-1}K_{D/2-1}(mL_i n_i)\right.$$
$$+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}}\right)^{D/2-1}$$
$$\times K_{D/2-1}(m\sqrt{L_i^2n_i^2+L_j^2n_j^2})+\cdots$$
$$+2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\right)^{D/2-1}$$
$$\left.\times K_{D/2-1}(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2})\right] \tag{21.12}$$

and

$$U_2^{(\mathrm{Ren})}(\varphi_0, L_1, \ldots, L_d) = \frac{\eta|\varphi_0|^2}{4\,(2\pi)^D}\left[\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_i n_i}\right)^{D/2-1}K_{D/2-1}(mL_i n_i)\right.$$
$$+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}}\right)^{D/2-1}$$
$$\left.\times K_{D/2-1}(m\sqrt{L_i^2n_i^2+L_j^2n_j^2})+\cdots\right.$$

$$+2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\right)^{D/2-1}$$
$$\times K_{D/2-1}(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2})\Bigg]^2. \tag{21.13}$$

Then the physical mass with both contributions is obtained from Eq. (19.29), using Eqs. (21.12), (21.13) and also taking into account the contribution at the tree level; it satisfies a generalized Dyson–Schwinger equation depending on the lengths L_i of the confining box:

$$\begin{aligned}
m^2(\{L_i\}) = m_0^2 - \frac{\lambda}{(2\pi)^{D/2}}\Bigg[&\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_in_i}\right)^{D/2-1}\times K_{D/2-1}(mL_in_i)\\
&+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}}\right)^{D/2-1}\\
&\times K_{D/2-1}(m\sqrt{L_i^2n_i^2+L_j^2n_j^2})+\cdots\\
&+2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots L_d^2n_d^2}}\right)^{D/2-1}\\
&\times K_{D/2-1}(m\sqrt{L_1^2n_1^2+\cdots L_d^2n_d^2})\Bigg]\\
+\frac{\eta}{2(2\pi)^D}\Bigg[&\sum_{i=1}^{d}\sum_{n_i=1}^{\infty}\left(\frac{m}{L_in_i}\right)^{D/2-1}K_{D/2-1}(mL_in_i)\\
&+2\sum_{i<j=1}^{d}\sum_{n_i,n_j=1}^{\infty}\left(\frac{m}{\sqrt{L_i^2n_i^2+L_j^2n_j^2}}\right)^{D/2-1}K_{D/2-1}(m\sqrt{L_i^2n_i^2+L_j^2n_j^2})\\
&+\cdots+2^{d-1}\sum_{n_1,\ldots,n_d=1}^{\infty}\left(\frac{m}{\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2}}\right)^{D/2-1}\\
&\times K_{D/2-1}(m\sqrt{L_1^2n_1^2+\cdots+L_d^2n_d^2})\Bigg]^2.
\end{aligned} \tag{21.14}$$

A first-order transition occurs when all the three minima of the potential

$$U(\varphi_0)=\frac{1}{2}m^2(\{L_i\})|\varphi_0|^2-\frac{\lambda}{4}|\varphi_0|^4+\frac{\eta}{6}|\varphi_0|^6, \tag{21.15}$$

where $m(\{L_i\})$ is the renormalized mass defined above, are simultaneously on the line $U(\varphi_0)=0$. This gives the condition

$$m^2(\{L_i\})=\frac{3\lambda^2}{16\eta}. \tag{21.16}$$

For $D = 3$, the Bessel functions have an explicit form, $K_{1/2}(z) = \sqrt{\pi}e^{-z}/\sqrt{2z}$; replacing this formula in Eq. (21.14), remembering $m_0^2 = \alpha(T/T_0 - 1)$ and using the condition Eq. (21.16), we get the critical temperature,

$$
\begin{aligned}
T_c(\{L_i\}) = T_c^{\text{bulk}} \Bigg\{ 1 - \left(1 + \frac{3\lambda^2}{16\eta\alpha}\right)^{-1} \\
\times \Bigg\{ \frac{\lambda}{8\pi\alpha} \Bigg[\sum_{i=1}^{d} \frac{1}{L_i} \ln(1 - e^{-\sqrt{3\lambda^2/16\eta}L_i}) \\
+ 2 \sum_{j<i=1}^{d} \sum_{n_i,n_j=1}^{\infty} \frac{e^{-\sqrt{3\lambda^2/16\eta}\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}}}{\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}} + \cdots \\
+ 2^{d-1} \sum_{n_1,\ldots,n_d=1}^{\infty} \frac{e^{-\sqrt{3\lambda^2/16\eta}\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}}}{\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}} \Bigg] \\
- \frac{\eta}{64\pi^2\alpha} \Bigg[\sum_{i=1}^{d} \frac{1}{L_i} \ln(1 - e^{-\sqrt{3\lambda^2/16\eta}L_i}) \\
+ 2 \sum_{j<i=1}^{d} \sum_{n_i,n_j=1}^{\infty} \frac{e^{-\sqrt{3\lambda^2/16\eta}\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}}}{\sqrt{L_i^2 n_i^2 + L_j^2 n_j^2}} + \cdots \\
+ 2^{d-1} \sum_{n_1,\ldots,n_d=1}^{\infty} \frac{e^{-\sqrt{3\lambda^2/16\eta}\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}}}{\sqrt{L_1^2 n_1^2 + \cdots + L_d^2 n_d^2}} \Bigg]^2 \Bigg\} \Bigg\}, \qquad (21.17)
\end{aligned}
$$

where

$$
T_c^{\text{bulk}} = T_0 \left(1 + \frac{3\lambda^2}{16\eta\alpha}\right) \qquad (21.18)
$$

is the bulk ($L_i \to \infty$) critical temperature for the first-order phase transition.

21.2 The film, the wire and the grain

Having developed the general case of a d-dimensional compactified subspace, it is now easy to obtain the specific formulas for particular values of d. If we choose $d = 1$, the compactification of just one dimension, let us say, along the x_1-axis, we are considering that the system is confined between two planes, separated by a distance $L_1 = L$. Physically, this corresponds to the situation explored in [309], and the transition occurs at the critical temperature $T_c^{\text{film}}(L)$ given by

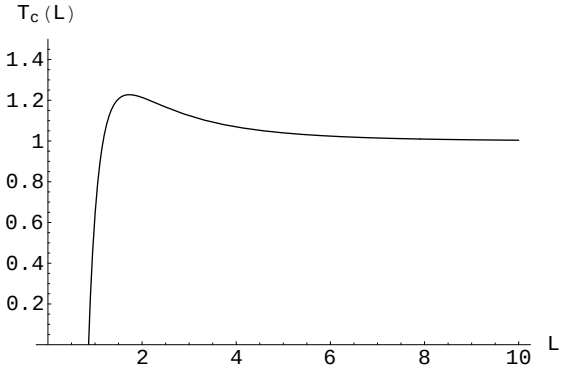


Fig. 21.2 Critical temperature for a superconducting film, undergoing a first-order phase-transition, as function of the thickness.

$$T_c^{\rm film}(L) = T_c \left\{ 1 - \left(1 + \frac{3\lambda^2}{16\eta\alpha} \right)^{-1} \left[\frac{\lambda}{8\pi\alpha L} \ln(1 - e^{-\sqrt{3\lambda^2/16\eta}L}) \right.\right.$$
$$\left.\left. - \frac{\eta}{64\pi^2\alpha L^2} \left(\ln(1 - e^{-\sqrt{3\lambda^2 16\eta}L}) \right)^2 \right] \right\}. \tag{21.19}$$

The behavior of $T_c^{\rm film}$ as a function of L is shown Fig. 21.2.

Let us now take the case $d = 2$. To simplify matters, we take $L_1 = L_2 = L$ in Eq. (21.17) with $d = 2$, the critical temperature is written in terms of L as

$$T_c^{\rm wire}(L) = T_c \left\{ 1 - \left(1 + \frac{3\lambda^2}{16\eta\alpha} \right)^{-1} \left[\frac{\lambda}{4\pi\alpha L} \right.\right.$$
$$\times \left[2\ln(1 - e^{-L\sqrt{3\lambda^2/16\eta}}) + 2\ln(1 - e^{-L\sqrt{3\lambda^2/16\eta}}) \right.$$
$$\left. + 2 \sum_{n_1,n_2=1}^{\infty} \frac{e^{-L\sqrt{3\lambda^2 16\eta}\sqrt{n_1^2+n_2^2}}}{\sqrt{n_1^2+n_2^2}} \right]$$
$$- \frac{\eta}{32\pi^2\alpha L^2} \left(\ln(1 - e^{-L\sqrt{3\lambda^2/16\eta}}) \right.$$
$$\left.\left.\left. + \ln(1 - e^{-L\sqrt{3\lambda^2/16\eta}}) + 2 \sum_{n_1,n_2=1}^{\infty} \frac{e^{-L\sqrt{3\lambda^2/16\eta}}\sqrt{n_1^2+n_2^2}}{\sqrt{n_1^2+n_2^2}} \right)^2 \right] \right\}. \tag{21.20}$$

Finally, we compactify all three dimensions, which leaves us with a system in the form of a cubic grain. The dependence of the critical temperature on its linear

dimension $L_1 = L_2 = L_3 = L$, is given by taking $d = 3$ in Eq. (21.17):

$$T_c^{\rm grain}(L) = T_c \left\{ 1 - \left(1 + \frac{3\lambda^2}{16\eta\alpha} \right)^{-1} \left\{ \frac{\lambda}{4\pi\alpha L} \left[3 \ln(1 - e^{-L\sqrt{3\lambda^2/16\eta}}) \right.\right.\right.$$
$$+2 \sum_{j<i=1}^{3} \sum_{n_i,n_j=1}^{\infty} \frac{e^{-\sqrt{3\lambda^2/16\eta} L \sqrt{n_i^2+n_j^2}}}{\sqrt{n_i^2+n_j^2}}$$
$$\left. +4 \sum_{n_1,\ldots,n_3=1}^{\infty} \frac{e^{-L\sqrt{3\lambda^2 16\eta}\sqrt{n_1^2+\cdots+n_3^2}}}{\sqrt{n_1^2+\cdots+n_3^2}} \right]$$
$$-\frac{\eta}{32\pi^2\alpha L^2} \left[3 \ln(1 - e^{-L\sqrt{3\lambda^2/16\eta}}) \right.$$
$$+2 \sum_{j<i=1}^{3} \sum_{n_i,n_j=1}^{\infty} \frac{e^{-\sqrt{3\lambda^2/16\eta} L \sqrt{n_i^2+n_j^2}}}{\sqrt{n_i^2+n_j^2}}$$
$$\left.\left.\left. +4 \sum_{n_1,\ldots,n_3=1}^{\infty} \frac{e^{-L\sqrt{3\lambda^2/16\eta}\sqrt{n_1^2+\cdots+n_3^2}}}{\sqrt{n_1^2+\cdots+n_3^2}} \right]^2 \right\} \right\} . \tag{21.21}$$

It is interesting to compare the above formulas to those for a *second-order* transition in either films, wires or grains, obtained by the similar methods from the $\lambda\phi^4$ Ginzburg–Landau model in Chapters 19 and 20. All of them have the same functional dependence on the linear dimension L. In all cases studied there, it is found that the boundary-dependent critical temperature decreases linearly with the inverse of the linear dimension L, according to the results of Chapter 20. It is to be noted that in order to get the transition temperature for a film, a mass renormalization is needed in second-order phase transitions, which is not the case for first-order ones.

We have discussed here the $\left(\lambda|\varphi|^4 + \eta|\varphi|^6\right)_D$ theory compactified in $d \leq D$ Euclidean dimensions, extending for first-order transitions in arbitrary dimension some results for second-order transitions [309]. The bare mass term has been parametrized in the form $m_0^2 = \alpha(T/T_0 - 1)$, with $\alpha > 0$ and T_0 being a parameter with the dimension of temperature, thus placing the analysis within the Ginzburg–Landau framework. We have presented a general formalism and we have focused on the situations with $D = 3$ and $d = 1, 2, 3$, corresponding (in the context of condensed matter systems) to films, wires and grains, respectively, undergoing phase transitions which may be described by (mean field) Ginzburg–Landau models. This generalizes to more compactified dimensions previous investigations on first-order superconducting transitions in films [309].

It should be observed the very different form of Eqs. (21.19), (21.20) and (21.21) when compared with the corresponding ones for second-order transitions given in the preceding chapters. In the particular case of a superconducting film, as we have seen above, the functional form Eq. (21.19) of the dependence of the critical temperature

$T_c(L)$ on the film thickness L, grows from zero at a non-null minimal allowed value of L above the bulk transition temperature T_c as the thickness is increased, reaching a maximum and afterwards starting to decrease, going asymptotically to T_c as $L \to \infty$. This is in qualitatively good agreement with measurements [310] taken for a superconducting aluminum film, especially for thin ones. This is a rather contrasting behavior with that of the critical temperature for materials displaying a second-order phase transition [311], for which the critical temperature increases monotonically from zero, again corresponding to a finite minimal film thickness, going to the bulk transition temperature as $L \to \infty$. We could say that the form of the dependence of the critical temperature on the size of the system, is indicative of the order of the transition. This is particularly striking for films, in which case experimental data are more easily available.

PART V

Applications to Open Systems

Chapter 22

Thermo-Algebras in Phase Space: Quantum and Classical Systems

We explore in this chapter representations of thermo-algebras in phase space. We begin by presenting a derivation of the Wigner formalism for non-relativistic and relativistic fields based on symmetry. The basic result is the formulation of the quantum theory in phase space having as basic ingredients symmetry groups. The last part of the chapter is dedicated to study representations for classical systems, associated for instance with stochastic equations.

22.1 Wigner function for the Schrödinger field

The commutation relations for the thermo Galilei Lie-algebra in Chapter 7 show that we have different possibilities to define a frame in the Hilbert space $\mathcal{H}_T$. An interesting one is built with the operators $\underline{P}$ and $\underline{Q}$ defined by

$$\underline{P} = P - \frac{1}{2}\widehat{P},$$
$$\underline{Q} = Q - \frac{1}{2}\widehat{Q}.$$

Observe that $\underline{Q}$ and $\underline{P}$ satisfy the Galilei-boost conditions

$$U(\widehat{K})\ \underline{Q}\ U^{-1}(\widehat{K}) = \underline{Q} + vt\mathbf{1}, \tag{22.1}$$

and

$$U(\widehat{K})\ \underline{P}\ U^{-1}(\widehat{K}) = \underline{P} + mv\mathbf{1}, \tag{22.2}$$

where

$$U(\widehat{K}) = \exp(-imv\widehat{K}),$$

with $\widehat{K}$ being the boost operator (see Chapter 7). Therefore, $\underline{P}$ and $\underline{Q}$ might be taken as momentum and position operators, respectively. But despite this fact, $\underline{P}$ and $\underline{Q}$ cannot be considered as observables, for, in this representation, the hat operators are generators of symmetry, not observables. In addition, these operators commute with each other, i.e. $[\underline{P}, \underline{Q}] = 0$. Representative operators for the position

and momentum observables can be given, respectively, by Q and P, which satisfy the same relations for the Galilei boost as those given by Eqs. (22.1) and (22.2), while fulfilling the Heisenberg condition, that is

$$[Q_i, P_j] = i\delta_{ij}.$$

Since $\underline{P}$ and $\underline{Q}$ commute, they can be used in a diagonal representation, so as to define a quantum phase space. This phase-space frame is then introduced by

$$\underline{P}\,|q,p\rangle = p\,|q,p\rangle \text{ and } \underline{Q}\,|q,p\rangle = q\,|q,p\rangle,$$

where the kets $|q,p\rangle$ are an orthonormal basis in $\mathcal{H}_\alpha$, that is,

$$\langle q,p|q',p'\rangle = \delta(q-q')\delta(p-p') \text{ and } \int |q,p\rangle\langle q,p|dqdp = 1.$$

In this basis, we write the observables Q and P, and the generators $\widehat{P}$ and $\widehat{Q}$ as

$$Q_j = q_j + \frac{i}{2}\frac{\partial}{\partial p_j}, \quad \widehat{Q}_j = i\frac{\partial}{\partial p_j}\ ,$$
$$P_j = p_j - \frac{i}{2}\frac{\partial}{\partial q_j}, \quad \widehat{P}_j = -i\frac{\partial}{\partial q_j}\ .$$

These results show that $\mathcal{H}_\alpha$ is a reducible representation space for the observables Q_i and P_i [315–318].

The evolution equation for the states is then given by

$$i\partial_t\psi(q,p;t) \ = \int \langle q,p|\widehat{H}|q',p'\rangle\,\langle q',p'|\psi(t)\rangle dq'dp', \tag{22.3}$$

where $|\psi(t)\rangle$ is in $\mathcal{H}_\alpha$ and $\psi(q,p;t) = \langle q,p|\psi(t)\rangle$. Assuming

$$H(q,p;\frac{\partial}{\partial q},\frac{\partial}{\partial p}) = \delta(q-q')\delta(p-p')\langle q,p|\widehat{H}|q',p'\rangle,$$

We write

$$i\partial_t\psi(q,p;t) \ = H(q,p;\frac{\partial}{\partial q},\frac{\partial}{\partial p})\psi(q,p;t).$$

An observable operator, A, a function of Q and P, is such that

$$\langle q,p|A(Q,P)|q,p\rangle = A(q+\frac{i}{2}\frac{\partial}{\partial p},\, p-\frac{i}{2}\frac{\partial}{\partial q}), \tag{22.4}$$

whose average, $\langle A\rangle$, is defined as

$$\begin{aligned}\langle A\rangle &= \langle\psi|A|\psi\rangle \\ &= \int dqdp\,\psi^*(q,p;t)\,A(q+\frac{i}{2}\frac{\partial}{\partial p},\, p-\frac{i}{2}\frac{\partial}{\partial q})\psi(q,p;t).\end{aligned} \tag{22.5}$$

Considering that $\widehat{H} = H - \widetilde{H}$, in the phase space we have

$$\begin{aligned}\widehat{H} &= \langle q,p|H(Q,P)|q,p\rangle - \langle q,p|\widetilde{H}(Q,P)|q,p\rangle \\ &= H(q+\frac{i}{2}\frac{\partial}{\partial p},\, p-\frac{i}{2}\frac{\partial}{\partial q}) - H(q-\frac{i}{2}\frac{\partial}{\partial p},\, p+\frac{i}{2}\frac{\partial}{\partial q}),\end{aligned} \tag{22.6}$$

where $H = H(Q,P)$ is the Hamiltonian of the system written in terms of the position and momentum operators, Q and P, respectively. For instance, let us consider the Hamiltonian

$$H(Q,P) = \frac{P^2}{2m} + V(Q).$$

Then we have

$$\begin{aligned}\widehat{H} &= \langle q,p|H(Q,P)|q,p\rangle - \langle q,p|\widetilde{H}(Q,P)|q,p\rangle \\ &= \frac{1}{2m}(p - \frac{i}{2}\frac{\partial}{\partial q})^2 + V(q + \frac{i}{2}\frac{\partial}{\partial p}) \\ &- \frac{1}{2m}(p + \frac{i}{2}\frac{\partial}{\partial q})^2 - V(q - \frac{i}{2}\frac{\partial}{\partial p}).\end{aligned} \tag{22.7}$$

Using a Taylor series, we write $\widehat{H}$ as

$$\widehat{H} = i\{H(q,p),\cdot\}_M,$$

where $\{\cdot,\cdot\}_M$ is the Moyal bracket given by

$$\{g,f\}_M(q,p) = g(q,p)2\sin\left(\frac{1}{2}\left[\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}\right]\right) f(q,p),$$

and $H(q,p)$ is the Hamiltonian written in terms of the c-number variables q and p. As discussed in Chapter 2, $H(q,p)$ is associated with a classical Hamiltonian. We consider such an interpretation only after an analysis of the classical limit of $\widehat{H}$ in the phase space representation. This aspect can be made clear if we include explicitly the Planck's constant in the definition of Q and P, writing $Q = q + i\hbar\partial/\partial p$ and $P = p + i\hbar\partial/\partial q$ and taking the formal limit $\hbar \to 0$.

As a second step, we associate the state $\psi(q,p)$ with the Wigner function. To do this, we use the $*$-product

$$(\psi \star \psi')(q,p) = \psi(q,p)\exp\left(\frac{\hbar}{2}\left[\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}\right]\right)\psi'(q,p). \tag{22.8}$$

The $\star$-product is associative and satisfies the following derivative rule

$$\widehat{H}(\psi \star \psi')(q,p) = (\widehat{H}\psi \star \psi')(q,p) + (\psi \star \widehat{H}\psi')(q,p). \tag{22.9}$$

Therefore, introducing the function

$$f(q,p) = (\psi \star \psi^\dagger)(q,p),$$

and using Eq. (22.9), we find that

$$\partial_t f(q,p;t) = \{H(q,p)\,,\, f(q,p;t)\}_M. \tag{22.10}$$

This is the Liouville-von Neumann equation in phase space as presented in Chapter 2. To avoid confusion with the star product, $\star$, in this section we denote the complex conjugate by †. Besides that, we have

$$\begin{aligned}\int dqdp\,\psi(q,p)\star\psi^{\dagger}(q,p) &= \int dqdp\,\psi(q,p)\psi^{\dagger}(q,p)\\ &= \int dqdp\,f(q,p;t)\ .\end{aligned}$$

The normalization of $\psi(q,p)$ is

$$\int dqdp\,\psi(q,p)\star\psi^{\dagger}(q,p)=1.$$

The average for the observables defined by Eq. (22.5) reduces to

$$\begin{aligned}\langle A\rangle &= \langle\psi|A|\psi\rangle\\ &= \int dqdp\,f(q,p;t)A(q,p).\end{aligned}\tag{22.11}$$

The integration over p (q) leads to a distribution of probability in q (p). Then the function $f(q,p)$ fulfills all the properties of the Wigner function. As a consequence the function $\psi(q,p)$ can be interpreted as a wave function associated with the quantum-mechanical Wigner function. It is worth noting that the derivation of Eq. (22.11) was possible since $A(q,p)$ is assumed to be an observable according to the thermo-Galilei algebra. However, this is not the case for more general operators, such as the hat-Hamiltonian. This shows that the formalism with the Wigner function amplitude is a generalization of the usual one.

Let us briefly investigate two other examples of representations for the phase space. The first one is defined by the operators $\widetilde{Q}=Q-\widehat{Q}$ and P such that $[\widetilde{Q},P]=0$; thus we introduce

$$\begin{aligned}P|q,p\rangle &= p|q,p\rangle,\quad \widetilde{Q}|q,p\rangle = q|q,p\rangle\,,\\ Q_j &= q_j+\frac{i}{2}\hbar\frac{\partial}{\partial p_j}\,,\\ \widetilde{P}_j &= p_j+\frac{i}{2}\hbar\frac{\partial}{\partial q_j}.\end{aligned}$$

In this case the $*$-product reduces to

$$(\psi\star\psi')(q,p)=\psi(q,p)\exp[i\frac{\hbar}{2}\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}]\psi'(q,p).\tag{22.12}$$

As a second example, we consider $[Q,\widetilde{P}]=0$, such that $\widetilde{P}\ |q,p\rangle=p|q,p\rangle$, and

$$\begin{aligned}Q\,|q,p\rangle &= q\,|q,p\rangle\ ,\\ \widetilde{Q}_j &= q_j-\frac{i}{2}\hbar\frac{\partial}{\partial p_j}\ ,\\ P_j &= p_j-\frac{i}{2}\hbar\frac{\partial}{\partial q_j}\,,\end{aligned}$$

resulting in

$$(\psi\star\psi')(q,p)=\psi(q,p)\exp[i\frac{\hbar}{2}\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}]\psi'(q,p).\tag{22.13}$$

22.2 Wigner function for the Klein-Gordon field

In this section we analyze the structure of the statistical mechanics and relativistic kinetic theory for bosons. First we deal with the system in thermal equilibrium. The basic equation is, as we have demonstrated in Chapter 7,

$$[\Box, \rho] = 0. \tag{22.14}$$

Consider an ensemble of quantum particles specified by the density matrix ρ, such that the entropy is

$$S = -k_B \mathrm{Tr}\rho \ln \rho. \tag{22.15}$$

In the stationary case the entropy is also an extremum; that is

$$\delta S = 0, \tag{22.16}$$

under the constraints

$$\mathrm{Tr}\rho = 1, \tag{22.17}$$

$$\mathrm{Tr}\rho N = \langle N \rangle, \tag{22.18}$$

$$\mathrm{Tr}\rho P^\nu = \langle P^\nu \rangle, \tag{22.19}$$

where $\langle N \rangle$, the macroscopic particle number, and $\langle P^\mu \rangle$, the macroscopic four momentum, are assumed to be constant. Then we obtain (see Chapter 2)

$$\alpha_0 + \alpha_\nu P^\nu + \alpha_N N - k_B - k_B \ln \rho = 0, \tag{22.20}$$

where α_0, α_μ and α_N are Lagrange multipliers, introduced to account for the constraints given by Eqs. (22.17)–(22.19), respectively. From Eq. (22.20), we get

$$\rho = \frac{1}{Z} \exp[\frac{1}{k_B}(\alpha_\nu P^\nu + \alpha_N N)], \tag{22.21}$$

where

$$Z = \exp(1 - \frac{\alpha_o}{k_B}). \tag{22.22}$$

The quantity ρ in Eq. (22.21) is a solution of Eq. (22.14) assuming that N and P commute with each other. Multiplying Eq. (22.20) by ρ, taking the trace and using Eqs. (22.17)–(22.19) and Eq. (22.22), we derive

$$k_B \ln Z + \alpha_\nu \langle P^\nu \rangle + \alpha_N \langle N \rangle + S = 0.$$

We obtain a physical interpretation of the Lagrange multipliers α_ν and α_N by taking

$$\alpha_\nu = -k_B \beta U_\nu, \text{ and } \alpha_N = k_B \mu_c \beta,$$

where μ_c is the chemical potential and U_ν is the macroscopic four-velocity field satisfying the relation $U_\nu U^\nu = 1$. Therefore, ρ in Eq. (22.21) is given as

$$\rho = \frac{1}{Z} \exp[-\beta(U_\nu P^\nu - \mu_c N)]. \tag{22.23}$$

The partition function, Z, is inferred from the normalization of ρ. Thus, Eq. (22.23) provides a general form of ρ for steady states. Let us analyze this from another point of view.

The Liouville-von Neumann equation, Eq. (22.14), is written as

$$(\partial^{\mu'}\partial_{\mu'} - \partial^{\mu}\partial_{\mu})\rho(x', x) = 0. \tag{22.24}$$

Introducing the linear transformation

$$\frac{\partial}{\partial x^{\mu}} = \frac{1}{\sqrt{2}}(\frac{\partial}{\partial q^{\mu}} - p^{\mu}) \text{ and } \frac{\partial}{\partial\, x'^{\mu}} = \frac{1}{\sqrt{2}}(\frac{\partial}{\partial q^{\mu}} + p^{\mu}) \ , \tag{22.25}$$

Eq. (22.24) becomes

$$p^{\mu}\frac{\partial}{\partial q^{\mu}}\,\rho(q, p) = 0. \tag{22.26}$$

This equation can be interpreted as the drift term of a collisionless Boltzmann equation for the one-particle Wigner distribution $\rho(q, p)$. To see that, let us explore the physical meaning of $\rho(q, p)$. First, note that $\rho(q, p\ )$ is a Lorentz scalar. Thus an invariant solution of Eq. (22.26) is

$$\rho(q, p) = \int d^4u\, \delta(u \cdot p) \exp[-u \cdot q] g(p, u). \tag{22.27}$$

The microscopic nature of $\rho(q, p\ )$ is specified through the definition

$$\begin{aligned} g(p, u) &= \langle a^{\dagger}(p - \frac{1}{2}u)\, a(p + \frac{1}{2}u)\rangle \\ &= \mathrm{Tr}[\rho a^{\dagger}(p - \frac{1}{2}u)\, a(p + \frac{1}{2}u)], \end{aligned} \tag{22.28}$$

where $a(p)$ and $a^{\dagger}(p)$ are boson operators, such that the number and momentum operators are introduced by

$$\begin{aligned} N &= \int \frac{d^3p}{p^o} a^{\dagger}(p)a(p), \\ P^{\mu} &= \int \frac{d^3p}{p^o} p^{\mu} a^{\dagger}(p)a(p). \end{aligned}$$

Notice that

$$\begin{aligned} g(p, u) &= \langle a^{\dagger}(p - \frac{1}{2}u)\, a(p + \frac{1}{2}u)\rangle_0 \\ &= \langle a(p + \frac{1}{2}u)a^{\dagger}(p - \frac{1}{2}u)\rangle_0 \exp(\beta\mu_c - p^{\nu}U_{\nu}), \end{aligned}$$

a result that is derived from the properties of the trace in the equilibrium average represented by $\langle \cdots \rangle_0$. With this result, and using Eq. (22.23) in Eq. (22.28) we obtain

$$\rho(p) = \frac{1}{\exp([\beta p^{\nu}U_{\nu} - \beta\mu_c\langle N\rangle] - 1}, $$

which is the Jüttiner distribution [18, 319]. Thus Eq. (22.28) is an appropriate choice for $g(q,p)$, that provides a physical interpretation of the theory in the case of bosons.

Including anti-particles, $g(q,p)$ in Eq. (22.27) is written as

$$g(p,u) = \langle a^\dagger(p-\frac{1}{2}u)\, a(p+\frac{1}{2}u)\rangle + \langle \overline{a}^\dagger(p-\frac{1}{2}u)\, \overline{a}(p+\frac{1}{2}u)\rangle,$$

where $\overline{a}(p)$ and $\overline{a}^\dagger(p)$ are anihilation and creation operators, respectively, for anti-bosons. The microscopic specification of the operators N and P^ν, in the momentum space, is

$$N = \int \frac{d^3p}{p^0}[a^\dagger(p)a(p) + \overline{a}^\dagger(p)\overline{a}(p)],$$

$$P^\nu = \int \frac{d^3p}{p^0}p^\nu[a^\dagger(p)a(p) + \overline{a}^\dagger(p)\overline{a}(p)].$$

The macroscopic current density, J^ν, and the energy-momentum tensor, $T^{\mu\nu}$, are respectively,

$$\langle J^\nu\rangle = \int d^3p \frac{1}{p^0}p^\mu \rho(q,p), \tag{22.29}$$

and

$$T^{\mu\nu} = \int d^3p \frac{1}{p^0}p^\mu p^\nu \rho(q,p). \tag{22.30}$$

Therefore, $\rho(q,p)$ is interpreted as a Wigner function density. In other words, this shows how to use representations of symmetry groups to derive relativistic statistical mechanics. Due to the symmetry properties, the simplicity is a noteworthy fact in this method, of the result that the distribution function $\rho(q,p)$ arises naturally in a covariant form.

22.3 Wigner function for the Dirac field

In order to derive a Wigner representation for the Dirac field we start with the density matrix equation for the Dirac field (see Chapter 7)

$$[\sigma\gamma\cdot\partial, \rho] = 0$$

written in the following general form

$$(\sigma^l\gamma^{l\mu}\frac{\partial}{\partial x^\mu} - \sigma^r\gamma^{r\mu}\frac{\partial}{\partial x'^\mu})\rho(x,x') = 0, \tag{22.31}$$

where $\gamma^{l\mu} = \gamma^\mu \otimes 1$, $\gamma^{r\mu} = 1 \otimes \gamma^\mu$ with γ^μ being the Dirac matrices; $\sigma^l = \sigma \otimes 1$ and $\sigma^r = 1 \otimes \sigma$; with σ an arbitrary Lorentz invariant, satisfying $\sigma^2 = 1$. The Dirac matrices, $\gamma^{r,l}$, fulfill two Clifford algebras,

$$\{\gamma^{l\mu}, \gamma^{l\nu}\} = \{\gamma^{r\mu}, \gamma^{r\nu}\} = 2g^{\mu\nu}; \tag{22.32}$$

such that $[\gamma^{l\mu}, \gamma^{r\nu}] = 0$. Observe that $\rho(x,x')$ is a 16-component object.

Multiplying Eq. (22.31) by $\left(\sigma^l\right)^{-1}$, it follows that

$$\Lambda(\kappa)\rho(x,x') = (\gamma^{l\mu}\frac{\partial}{\partial x^\mu} - \kappa\gamma^{r\mu}\frac{\partial}{\partial x'^\mu})\rho(x,x') = 0, \tag{22.33}$$

where $\kappa = (\sigma^l)^{-1}\sigma^r$. Using Eq. (22.25), the square of $\Lambda(\kappa)$ is

$$\Lambda^2(\kappa) = \Lambda_1^{\mu\nu}(\kappa)\frac{\partial^2}{\partial q^\mu \partial q^\nu} + \Lambda_2^{\mu\nu}(\kappa)\frac{\partial}{\partial q^\mu}\, p_\nu + \Lambda_3^{\mu\nu}(\kappa)\, p_\mu \frac{\partial}{\partial q^\mu} + \Lambda_2^{\mu\nu}(\kappa)p_\mu p_\nu, \tag{22.34}$$

where

$$\Lambda_1^{\mu\nu}(\kappa) = \frac{1}{2}(\gamma^{l\mu} - \kappa\gamma^{r\mu})(\gamma^{l\nu} - \kappa\gamma^{r\nu}),$$
$$\Lambda_2^{\mu\nu}(\kappa) = \frac{1}{2}(\gamma^{l\mu} + \kappa\gamma^{r\mu})(\gamma^{l\nu} - \kappa\gamma^{r\nu}),$$
$$\Lambda_3^{\mu\nu}(\kappa) = \frac{1}{2}(\gamma^{l\mu} - \kappa\gamma^{r\mu})(\gamma^{l\nu} + \kappa\gamma^{r\nu}),$$
$$\Lambda_4^{\mu\nu}(\kappa) = \frac{1}{2}(\gamma^{l\mu} + \kappa\gamma^{r\mu})(\gamma^{l\nu} + \kappa\gamma^{r\nu}).$$

From these expressions for $\Lambda_i^{\mu\nu}(\kappa)$, $(i = 1,..,4)$, the following operators are defined

$$a^{\mu+}(\kappa) = \frac{1}{\sqrt{2}}(\gamma^{l\mu} + \kappa\gamma^{r\mu}) \text{ and } a^{\mu-}(\kappa) = \frac{1}{\sqrt{2}}(\gamma^{l\mu} - \kappa\gamma^{r\mu}); \tag{22.35}$$

then Eq. (22.34) is written as

$$\Lambda^2(\kappa) = a^{\mu-}(\kappa)a^{\nu-}(\kappa)\frac{\partial^2}{\partial q^\mu \partial q^\nu} + a^{\mu+}(\kappa)a^{\nu-}(\kappa)\frac{\partial}{\partial q^\mu}\, p_\nu$$
$$+ a^{\mu-}(\kappa)a^{\nu+}(\kappa)\, p_\nu \frac{\partial}{\partial q^\mu} + a^{\mu+}(\kappa)a^{\nu+}(\kappa)p_\mu p_\nu.$$

For a suitable choice of the arbitrary invariant κ, two Grassmann algebras can be introduced with the operator $a^{\mu-}(\kappa)$ and $a^{\mu+}(\kappa)$. Indeed, if κ anti-commutes with the matrices $\gamma^{l\mu}$ and $\gamma^{r\mu}$, and since $\kappa^2 = 1$, it leads to

$$\{a^{\mu-}, a^{\nu-}\} = \{a^{\mu+}, a^{\nu+}\} = 0$$
$$\{a^{\mu+}, a^{\nu-}\} = g^{\mu\nu}.$$

Requirement of Lorentz invariance for κ can be achieved if, in Eq. (22.31), we define $\sigma^l = \gamma^{l5}$ and $\sigma^r = \gamma^{r5}$, where $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$. Using these results, we obtain [18]

$$\Lambda^2 = a^{\mu+}a^{\nu-}\frac{\partial}{\partial q^\mu}\, p_\nu + a^{\mu-}a^{\nu+}\, p_\mu \frac{\partial}{\partial q^\mu}$$
$$= p^\mu \frac{\partial}{\partial q^\mu}.$$

Therefore, from Eq. (22.33), we obtain

$$p^\mu \frac{\partial}{\partial q^\mu}\, \rho(q,p\,) = 0. \tag{22.36}$$

We can use Eq. (22.36) to study the kinetic theory of spin 1/2 particles similar to the case of the Klein-Gordon field. Then the definition of the energy-momentum tensor follows the definition given by Eq. (22.30) but including spinorial indices.

22.4 Representations for classical systems

In this section we study thermo-algebra representations for classical systems with emphasis in deriving structural elements of the classical kinetic theory from a group theory point of view. In this sense, classical analogues of elements of thermofield dynamics are specified. We first construct a representation using the Poisson brackets as the Lie product of the Galilei thermo-algebra. Later, we study unitary representations considering that operators describing classical observables have to commute with each other, in a thermo-algebra. In this case, the Lie product is the commutator, and the inner product in the representation space is defined on a set of complex functions in the phase space. Representations of Lie algebras for classical systems have been studied in the literature in different ways [320–325]. The first attempt to study classical systems using unitary representations and field operators defined in a Fock space is due to Shönberg [326]. This method has been explored a great deal [327–340]. The physical and the mathematical nature of such a formalism have also been analyzed with representations of Lie groups [80, 104] and in particular has been used to study stochastic problems, as in the reaction-diffusion and spin lattices [341–355]. Here we show the symmetry basis for these methods as a classical counterpart of TFD.

22.4.1 *Thermo-Lie groups for classical systems*

Let $\ell = \{a_i, |a_i \diamond a_j = C_{ijk} a_k\}$ be the Lie algebra associated with the usual dynamical physical variables, where $\diamond$ denotes the Lie product, and c_{ijk} are the structure constants. In order to construct the thermo-algebra representation we associate this algebra with an isomorphic hat-algebra denoted by $\widehat{\ell} = \{\widehat{A}_i, |\widehat{A}_i \diamond \widehat{A}_j = C_{ijk}\widehat{A}_k\}$, such that the thermo-algebra, designated by ℓ_T, is defined by

$$A_i \diamond A_j = E_{ijk} A_k, \tag{22.37}$$

$$A_i \diamond \widehat{A}_j = D_{ijk} A_k, \tag{22.38}$$

$$\widehat{A}_i \diamond \widehat{A}_j = C_{ijk} \widehat{A}_k. \tag{22.39}$$

The tilde operators, $\widetilde{A}$, that are isomorphic to the non-tilde operator A through the doubling process, are identified by $\widetilde{A} = A - \widehat{A}$. In general, however, such an association should not be assumed. Instead, the search for hat operators should be our primary goal.

The main characteristics of ℓ_T are the following (see Chapter 5): (i) As a vector space, ℓ_T is the direct sum of ℓ and $\widehat{\ell}$. (ii) ℓ is an ideal of ℓ_T. (iii) From the dynamical standpoint, the elements of the subalgebra $\widehat{\ell}$ are interpreted as dynamical generators of symmetry and elements of ℓ are the usual dynamical observables. Both are called dynamical variables. In the Lie algebra approach, infinitesimal transformations of dynamical variables are induced by the (Lie) product of the

generators. Then Eq. (22.38) dictates just how the dynamical generators act on the dynamical variables infinitesimally, as we have stated it in Chapter 5. (iv) The non-abelian nature of the dynamical observables, related to the measurement processes, is defined by Eq. (22.37).

We can define the concept of thermo-algebra for classical systems, using the interpretations of the non-hat operators given in property (iv) to write Eq. (22.37) as

$$A_i \diamond A_j \equiv [A_i, A_j] = 0,$$

where $[A, B] = AB - BA$, the commutator, is the Lie product. That is the observables are abelian. Then we assume that a unitary representation describing a classical system should be given by

$$[A_i, A_j] = 0, \tag{22.40}$$

$$[A_i, \widehat{A}_j] = iC_{ijk}A_k, \tag{22.41}$$

$$[\widehat{A}_i, \widehat{A}_j] = iC_{ijk}\widehat{A}_k. \tag{22.42}$$

In this case, the hat operators are a faithful representation of the symmetry operations.

On the other hand, one way to maintain Properties (i) to (iv) for abelian observables is to define the Lie product as Poisson brackets. Hence we write

$$\{A_i, A_j\} = C_{ijk}A_k, \tag{22.43}$$

$$\{A_i, \widehat{A}_j\} = C_{ijk}A_k, \tag{22.44}$$

$$\{\widehat{A}_i, \widehat{A}_j\} = C_{ijk}\widehat{A}_k. \tag{22.45}$$

(We are using the same notation for operators and c-number functions in the phase space since it will not create any confusion.) Introducing the tilde variables in the phase space as

$$\widetilde{A}_i = A_i - \widehat{A}_i, \tag{22.46}$$

the tilde and non-tilde variables satisfy the following relations:

$$\{A_i, \widetilde{A}_j\} = 0, \tag{22.47}$$

$$\{A_i, A_j\} = C_{ijk}A_k, \tag{22.48}$$

$$\{\widetilde{A}_i, \widetilde{A}_j\} = -C_{ijk}\widetilde{A}_k. \tag{22.49}$$

Representations of Lie groups through the Poisson brackets are, in general, projective representations. That is, given a symmetry group characterized by the Lie algebra $a_i \diamond a_j = C_{ijk}A_k$, realizations in terms of Poisson brackets are given by

$$\{A_i, A_j\} = C_{ijk}A_k + d_{ij},$$

where d_{ij} are c-numbers [325]. In this case, using the relations $\{A_i, A_j\} = C_{ijk}A_k + d_{ij}$ and $\{\widetilde{A}_i, \widetilde{A}_j\} = -C_{ijk}\widetilde{A}_k - d_{ij}$, the thermo-algebra is modified to assume the following relations

$$\{A_i, A_j\} = C_{ijk}A_k + d_{ij}, \tag{22.50}$$

$$\{A_i, \widehat{A}_j\} = C_{ijk}A_k + d_{ij}, \tag{22.51}$$

$$\{\widehat{A}_i, \widehat{A}_j\} = C_{ijk}\widehat{A}_k. \tag{22.52}$$

Note that the hat functions define a subalgebra of ℓ_T are still a faithful representation of the original Lie-symmetry.

The generators of symmetries acting on the dynamical variables are defined by the following relation

$$\bar{A}(\lambda) = e^{-\lambda\{\widehat{D},\ \cdot\ \}}\bar{A}(\lambda = 0), \tag{22.53}$$

where $\bar{A}$ stands for the dynamical variables A, $\widehat{A}$ or $\widetilde{A}$ (this notation will be used throughout); and, $\widehat{D}$ is a general generator defining a one parameter (λ) subgroup. In particular, if λ is the time parameter, we derive from Eq. (22.53) the equation of motion

$$\dot{\bar{A}} = \{\bar{A}, \widehat{H}\}. \tag{22.54}$$

When $\bar{A} = A$, Eq. (22.54) reduces to $\dot{A} = \{A, \widehat{H}\}$, and the usual classical formalism is obtained, where $\widehat{H}$ is the Hamiltonian written as a function in phase space.

An explicit form for the Poisson bracket in Eq. (22.54) is

$$\{A, B\} = \sum_{a=1}^{2}\left(\frac{\partial\ A}{\partial x_a}\frac{\partial B}{\partial\ p_a} - \frac{\partial A}{\partial\ p_a}\frac{\partial B}{\partial x_a}\right), \tag{22.55}$$

where $x_1 = q$, $x_2 = -\tilde{q}$, $p_1 = p$ and $p_2 = \tilde{p}$. Then we have a pair of Hamilton equations,

$$\dot{x}_a = \{x_a, \widehat{H}\} = \frac{\partial \widehat{H}}{\partial p_a}, \tag{22.56}$$

$$\dot{p}_a = \{p_a, \widehat{H}\} = -\frac{\partial \widehat{H}}{\partial x_a}, \tag{22.57}$$

where $a = 1, 2$. We have derived two possibilities to study representations in classical systems. In the following we explore both of these representations.

22.4.2 *SU*(1, 1) *and the thermal classical oscillator*

Considering the representation of the thermo-algebra in terms of the Poisson bracket [104], a realization of the rotation group in this doubled phase space is

$$\{L_i, L_j\} = \varepsilon_{ijk}L_k, \tag{22.58}$$

such that each component of L is a function of (x_r, p_s); $r, s = 1, 2$. The Casimir invariant is

$$\mathcal{C}^2 = {L_1}^2 + {L_2}^2 + {L_3}^2, \tag{22.59}$$

and we consider a system described by the following hat Hamiltonian (the generator of time translation)

$$\widehat{H} = N\mathcal{C} + ML_2, \tag{22.60}$$

where N and M are constants. Let us introduce the following set of variables

$$L_1 = \frac{i}{2}(L_- + L_+),$$
$$L_2 = \frac{1}{2}(L_+ - L_-),$$

with the inverse, $L_\pm = \mp(L_2 \pm iL_1)$. The algebra with elements $L_+, L_-$and L_3 is a representation of $su(1,1)$ for

$$\frac{1}{i}\{L_\pm, L_3\} = \mp L_\pm,$$
$$\frac{1}{i}\{L_-, L_+\} = -2L_3.$$

In terms of $L_+, L_-$and L_3, $\mathcal{C}$ is given by $\mathcal{C}^2 = {L_3}^2 - L_+L_-$.

Since we have an $su(1,1)$ algebra, we can define an algebra for oscillator-like operators. That is, we define variables a and b, such that

$$L_+ = \frac{1}{2}(a^2 - b^2), \tag{22.61}$$
$$L_- = \frac{1}{2}(a^{*2} - b^{*2}), \tag{22.62}$$
$$L_3 = \frac{1}{2}(aa^* + bb^*), \tag{22.63}$$

where a^* (b^*) is the complex conjugate of a (b). Then the algebra for the variables a, b and their complex conjugates is given by the relations

$$\{a, a^*\} = i,\ \{b, b^*\} = i,\ \ \{a, b\} = 0.$$

Other Poisson brackets are zero.

The basic variables x_r, p_r of the doubled phase space specified by Eq. (22.55) are introduced through a transformation defined by

$$a = \left(\frac{1}{2\Omega}\right)^{\frac{1}{2}}(p_1 - i\Omega x_1), \tag{22.64}$$
$$b = \left(\frac{1}{2\Omega}\right)^{\frac{1}{2}}(p_2 - i\Omega x_2), \tag{22.65}$$

and the constants: $N = 2\Omega$, $M = -i\gamma$ and $\Omega^2 = k - (\gamma/2m)^2$. Then, the Hamiltonian, Eq. (22.60), is

$$\widehat{H} = \frac{1}{2}p_1p_2 + \frac{1}{2}\Omega^2 x_1x_2 + \frac{\gamma}{4}(p_2x_2 - p_1x_1). \tag{22.66}$$

Using this and the Hamilton equations given by Eqs. (22.56) and (22.57), we have

$$m\ddot{x}_1 + \gamma\dot{x}_1 + kx_1 = 0, \tag{22.67}$$
$$m\ddot{x}_2 - \gamma\dot{x}_2 + kx_2 = 0. \tag{22.68}$$

These two equations describe a system of two oscillators: one is the usual dissipative harmonic oscillator, Eq. (22.67), and the other, Eq. (22.68), is a growing energy oscillator to which the energy of the dissipative oscillator flows. Such a classical system with two degrees of freedom was analysed by Feshbach and Tikochinsky [356–359]. In this case, the tilde variable describe the anti-dissipative system.

22.5 Classical unitary representations

Now we turn our attention to the unitary representations of the thermo-algebra describing classical systems. Following Eqs. (22.40)–(22.42), we write the thermal Galilei algebra, $\mathfrak{g}_T$, for a classical system as

$$\begin{aligned}
[J_i, J_j] &= 0, \qquad [\widehat{J}_i, \widehat{J}_j] = i\varepsilon_{ijk}\widehat{J}_k,\\
[J_i, P_j] &= 0, \qquad [\widehat{J}_i, \widehat{P}_j] = i\varepsilon_{ijk}\widehat{P}_k,\\
[J_i, K_j] &= 0, \qquad [\widehat{J}_i, \widehat{K}_j] = i\varepsilon_{ijk}\widehat{K}_k,\\
[K_i, H] &= 0, \qquad [\widehat{K}_i, \widehat{H}] = i\widehat{P}_i,\\
[P_i, K_j] &= 0, \qquad [\widehat{P}_i, \widehat{K}_j] = 0\\
[\widehat{J}_i, J_j] &= [J_i, \widehat{J}_j] = i\varepsilon_{ijk}J_k,\\
[\widehat{J}_i, P_j] &= [J_i, \widehat{P}_j] = i\varepsilon_{ijk}P_k,\\
[\widehat{J}_i, K_j] &= [J_i, \widehat{K}_j] = i\varepsilon_{ijk}K_k,\\
[\widehat{K}_i, H] &= [K_i, \widehat{H}] = iP_i,\\
[\widehat{P}_i, K_j] &= [P_i, \widehat{K}_j] = -iM\delta_{ij}
\end{aligned} \tag{22.69}$$

where the generators of the symmetries are $\widehat{P}$ for translations, $\widehat{J}$ for rotations, $\widehat{K}$ for the Galilei boost and $\widehat{H}$ for the time translations. These operators form a subalgebra of $\mathfrak{g}_T$, denoted by $\widehat{\mathfrak{g}}_T$, which is manifestly a faithful representation of the Galilei Lie-algebra. Moreover, there is the subalgebra $\mathfrak{g}$ of the dynamical observables (non-hat operators), which is an abelian algebra.

In the set of Eq. (22.69), we have $[\widehat{P}_i, \widehat{K}_j] = \widehat{M} = 0$ whilst in $[\widehat{P}_i, K_j] = [P_i, \widehat{K}_j] = -iM\delta_{ij}$, M is a constant operator, that is $M = m\mathbf{1}$. In order to define the Galilei boost for a point mass, m is considered real and positive. Thus let the operator of position (Q) be defined by

$$K = mQ - tP. \tag{22.70}$$

This relation among K, P and Q is similar to that used in quantum mechanics, but here Q and P commute with one another.

A representation where P and Q are diagonal is specified by:

$$P|p,q\rangle = p|p,q\rangle, Q|p,q\rangle = q|p,q\rangle,$$

so that $\langle q,p|\theta\rangle = \theta(p,q)$ is a vector in the representation space, which is a Hilbert space, $\mathcal{H}(\Gamma)$, on the phase space, Γ, of the (q,p)-points. Then, the other operators

of $\mathfrak{g}_T$ can be written as

$$J_i = L_i + S_i, \tag{22.71}$$

$$H = \frac{P^2}{2m} + C_1, \tag{22.72}$$

$$\widehat{J}_i = \widehat{L}_i + \widehat{S}_i, \tag{22.73}$$

$$\widehat{K}_i = im\frac{\partial}{\partial P_i} + it\frac{\partial}{\partial Q_i}, \tag{22.74}$$

$$\widehat{P}_i = -i\frac{\partial}{\partial Q_i}, \tag{22.75}$$

$$\widehat{H} = i\frac{\partial}{\partial t}. \tag{22.76}$$

where

$$\widehat{L}_i = i\varepsilon_{ijk}\left(Q_k\frac{\partial}{\partial Q_j} + P_k\frac{\partial}{\partial P_j}\right), \tag{22.77}$$

$$L_i = \varepsilon_{ijk}Q_jP_k, \tag{22.78}$$

$\widehat{S}_i$ are the spin operators (a representation of $SO(3)$ such that $\widehat{S}$ commutes with every operator defined on the space (p, q)), and C_1 is a c-number. Observe that in this representation $\widehat{H}$ is not a c-number in phase space, as it was the case studied in the previous section.

The operators P and Q can be interpreted as the momentum and position operators, since they satisfy the Galilei boost conditions, namely

$$\langle\theta|\exp(-iv\widehat{K})Q\exp(iv\widehat{K})|\phi\rangle = \langle\theta|Q|\phi\rangle + vt\langle\theta|\phi\rangle, \tag{22.79}$$

and

$$\langle\theta|\exp(-iv\widehat{K})P\exp(iv\widehat{K})|\phi\rangle = \langle\theta|P|\phi\rangle + mv\langle\theta|\phi\rangle. \tag{22.80}$$

where $|\theta\rangle$ and $|\phi\rangle$ ($\in \mathcal{H}$) are arbitrary states of the system. Besides, $\widehat{P}$ is the generator for spatial translation, since $[\widehat{P}_i, Q_j] = -i\delta_{ij}$. Then, L is the angular momentum, and H is the Hamiltonian.

In the case when $\widehat{S}_i = S_i = 0$, $\mathfrak{g}_T$ has two non-null invariants, which have fixed values within the irreducible representation, given by

$$C_1 = \frac{P^2}{2m} - H, \tag{22.81}$$

$$C_2 = \frac{\widehat{P}}{m}P - \widehat{H}. \tag{22.82}$$

Following the case of the Galilean quantum mechanics, the expectation value of a dynamical variable $\bar{A}$ in a state $|\theta\rangle$ is defined by

$$\langle\bar{A}\rangle = \langle\theta|\bar{A}|\theta\rangle. \tag{22.83}$$

On the other hand, the temporal evolution of $\bar{A}$ is given by

$$\langle\theta_0|\exp(it\widehat{H})\bar{A}\exp((-it\widehat{H})|\theta_0\rangle = \langle\theta_0|\bar{A}(t)|\theta_0\rangle. \tag{22.84}$$

Therefore, we have defined a Heisenberg picture for the temporal evolution of the dynamical variables, and from Eq. (22.84) we obtain

$$i\partial_t \bar{A} = [\bar{A}, \widehat{H}]. \tag{22.85}$$

Using Eq. (22.82), we have

$$i\partial_t \bar{A} = [\bar{A}, P\frac{\widehat{P}}{m}],$$

which shows that the value of C_2 does not play a special role in this case. That is

$$\widehat{H} = \frac{P}{m}\widehat{P}$$

In the Schrödinger picture, we derive the following equation for the evolution of the state

$$i\partial_t |\theta(t)\rangle = \widehat{H}|\theta(t)\rangle, \tag{22.86}$$

Using

$$\langle q,p|q',p'\rangle = \delta(q-q')\delta(p-p') \text{ and } \int |q,p\rangle\langle q,p|dqdp = 1,$$

we write in this phase space basis

$$i\partial_t \theta(q,p;t) \ = \int \langle q,p|\widehat{H}|q',p'\rangle \, \langle q',p'|\theta(t)\rangle dq'dp', \tag{22.87}$$

where $|\theta(t)\rangle$ is in $\mathcal{H}(\Gamma)$ and $\theta(q,p;t) = \langle q,p|\theta(t)\rangle$. Assuming

$$\langle q,p|\widehat{H}|q',p'\rangle = \delta(q-q')\delta(p-p')\langle q,p|\widehat{H}|q,p\rangle,$$

we have

$$i\partial_t \theta(q,p;t) \ = L_\Gamma(q,p)\theta(q,p;t), \tag{22.88}$$

and

$$\begin{aligned} L_\Gamma(q,p) &= \langle q,p|\widehat{H}|q,p\rangle = \langle q,p|\frac{P}{m}\widehat{P}|q,p\rangle \\ &= -i\frac{p}{m}\frac{\partial}{\partial q_i}, \end{aligned}$$

where we have used $\langle q,p|\widehat{H}|q,p\rangle$ given by Eq. (22.82) in the basis $|q,p\rangle$.

A formal solution of Eq. (22.88) is

$$\theta(q,p;t) = e^{-i(t-t_0)L_\Gamma}\theta(q,p;t_0).$$

Writing $\theta(q,p;t) = \psi(t)\phi(q,p)$, we have the eigenvalue equation.

$$L_\Gamma\phi(q,p) = \nu\phi(q,p) \quad and \quad \psi(t) = \psi(0)e^{-i\nu t}.$$

Notice that Eq. (22.88) is the the usual Liouville equation describing a free particle in classical mechanics; where $L_\Gamma(q,p)$ is the Liouvillian. However, here, $\theta(q,p;t)$ is a complex function. This fact points the way to find a physical interpretation for this representation.

By the definition, to every non-hat operator (say A) there is a hat operator (say $\widehat{A}$). This is a one-to-one mapping, which may be determined using the explicit representation of the thermo-algebra given by Eqs. (22.70)–(22.76). Then, we define the one-to-one hat mapping, $\widehat{\ } : A \longrightarrow \widehat{A}$, such that $\widehat{A} = i\{A, .\}$; explicitly

$$\widehat{A} = i\{A, .\} = i\frac{\partial A}{\partial q}\frac{\partial}{\partial p} - i\frac{\partial A}{\partial p}\frac{\partial}{\partial q}. \tag{22.89}$$

We have, hence, the following correspondence for the Lie algebra elements,

$$P \longrightarrow \widehat{P} = i\{P, .\}, \tag{22.90}$$
$$K \longrightarrow \widehat{K} = i\{K, .\}, \tag{22.91}$$
$$L \longrightarrow \widehat{L} = i\{L, .\}, \tag{22.92}$$
$$H \longrightarrow \widehat{H} = L_\Gamma = i\{H, .\}, \tag{22.93}$$
$$M \longrightarrow \widehat{M} = i\{M, .\} = 0. \tag{22.94}$$

Therefore, $\widehat{H} = L_\Gamma$ is the classical Liouvillian operator in the general form, written in terms of the Poisson bracket, from the observable Hamiltonian. To complete the physical meaning of the representation, we observe that $f(q, p; t) = |\theta(q, p; t)|^2$ is also a solution Eq. (22.88), i.e.

$$i\partial_t f(q, p; t) \ = L_\Gamma(q, p) f(q, p; t), \tag{22.95}$$

or

$$\partial_t f(q, p; t) = \{H, f(q, p; t)\},$$

and the average of an observable, given by Eq. (22.83), reduces to the usual average in the phase space for the non-hat operators; we have

$$\begin{aligned}\langle A\rangle = \langle\theta(t)|A|\theta(t)\rangle &= \int dpdq\theta^*(q, p; t)A(q, p)\theta(q, p; t)\\ &= \int dpdq\ f(q, p; t)A(q, p).\end{aligned}$$

For normalized functions, we have

$$\begin{aligned}\langle\theta(t)|A|\theta(t)\rangle &= \int dpdq\theta^*(q, p; t)\theta(q, p; t)\\ &= \int dpdq\ f(q, p; t) = 1.\end{aligned}$$

Then the complex functions are interpreted as amplitudes of probability in the phase space, associated with a probability density given by $f(q, p; t) = |\theta(q, p; t)|^2$. The conservation of probability is expressed by the same equation. This formalism was first proposed by Schönberg [326], as a generalization of the Liouville theorem.

From, $\mathfrak{g}_T$, given by Eqs. (22.40)–(22.42), we observe that the hat mapping ($\widehat{\ }$) satisfies the following properties [104]:

p.1 (linearity): $(A_1 + aA_2)^\wedge = \widehat{A}_1 + a\widehat{A}_2$.
p.2 (derivation): $(\prod_{i=1}^n A_i)^\wedge = \sum_{i=1}^n (A_1 \cdots A_{i-1}\widehat{A}_i A_{i+1} \cdots A_n)$.
Proposition 1: Given $C \in \mathfrak{g}$ (the abelian algebra of the observables) and $\{C, A\} = 0$, for every $A \in \mathfrak{g}$, then C and $\widehat{C}$ are two Casimir invariants of $\mathfrak{g}_T$.

Since we know the invariants of the Galilei group, considering Proposition 1, we write the Casimir invariants of $\mathfrak{g}_T$ in the general case when $S \neq 0$. These invariants are C_1 and C_2, given by Eqs. (22.81) and (22.82), respectively, and

$$C_3 = (J - L)^2, \tag{22.96}$$

$$C_4 = \left[(J - L)^2\right]^\wedge. \tag{22.97}$$

Both $C_4 = \widehat{C}_3$ and $C_2 = \widehat{C}_1$ have a fixed value in an irreducible representation. But in accordance with the properties of the hat mapping C_2 and C_4 are null constants. With the properties p.1 and p.2, and the Proposition 1, we verify that we cannot find a physical representation for $\mathfrak{g}_T$ for the case of $M = 0$. Therefore, we do not have classical particles of zero mass in this representation.

Similar to the quantum TFD, we can introduce in this classical formalism an arbitrary parameter ξ , by generalizing the average of observables given in Eq. (22.83) to

$$\begin{aligned}\langle \bar{A} \rangle &= \langle f^\xi | \bar{A} | f^{1-\xi} \rangle \\ &= \int dpdq f^\xi(q,p) A(q,p) f^{1-\xi}(q,p).\end{aligned} \tag{22.98}$$

Then, Eq. (22.83) is obtained when $\xi = \frac{1}{2}$. As is the case in TFD, however, there are other possibilities for ξ. For instance, if $\xi = 0$ and using the basis of states such that operators P and $\widehat{P}$ are diagonal, we obtain the formalism called dynamics of correlations. In fact, if P and $\widehat{P}$ are c-number operators, then $P|p,k\rangle = p|p,k\rangle$, $\widehat{P}|p,k\rangle = k|p,k\rangle$, so that $\langle p,k|f\rangle = f_k(p)$. As a consequence

$$\begin{aligned}f_k(p) &= \int dp'dq \langle p,k|p',q\rangle \langle f(p',q) \\ &= \int dq e^{ikp} f(q,p)\end{aligned} \tag{22.99}$$

The $f_k(p)$-functions are the correlation patterns in the dynamics of correlations [331]. As a particular case, the average, Eq. (22.98), for the thermal equilibrium,

$$\langle \bar{A} \rangle = \langle f^\xi | \bar{A} | f^{1-\xi} \rangle = \int dpdq \; e^{-\xi\frac{\beta}{2}H} \bar{A} \; e^{(1-\xi)\frac{\beta}{2}H},$$

is still a case similar to that in TFD. Another aspect to be noticed is that, when extended to many classical particles, the Schönberg-Liouville wave equation, given by Eq. (22.88), can be considered as a field equation defined in a Fock space. We study this representation of $\mathfrak{g}_T$ later. First, we discuss a simple example.

22.6 Liouville equation for the oscillator

Let us analyze here some similarities between TFD and the unitary representations of $\mathfrak{g}_T$, that we have studied. The dynamics of a system is generated by hat operators, which are in correspondence with the original dynamical variables via the Poisson brackets:

$$\begin{array}{ll} \text{Quantum TFD} & \text{Liouvillian Systems} \\ \widehat{A} = A - \widetilde{A}, & \widehat{A} = i\{A,\ \} = i\left(\dfrac{\partial A}{\partial q}\dfrac{\partial}{\partial_p} - \dfrac{\partial A}{\partial p}\dfrac{\partial}{\partial_q}\right). \end{array}$$

This relationship among classical operators and quantum operators is not transparent. We would like to see if there are additional connections. In order to do this, the p-variable is considered in its Fourier representation, such that

$$p \to i\partial_{\tilde{q}},\ \text{and}\ \partial_p \to i\tilde{q}.$$

$\widehat{p} = im\partial_q$ does not change. In particular, the generator of rotations is given by

$$\widehat{L} = i\epsilon_{ijk}(q_k\partial_{q_j} + p_k\partial_{p_j}) \to i\epsilon_{ijk}(q_k\partial_{q_j} - \tilde{q}_j\partial_{\tilde{q}_k}) = i\epsilon_{ijk}(q_k\partial_{q_j} + \tilde{q}_k\partial_{\tilde{q}_j}).$$

Assuming that $H = T + V$, we get

$$\widehat{H} = -i(p\partial_q - \partial_q V\partial_p) \to (\partial_q\partial_{\tilde{q}} - \partial_q V\tilde{q}).$$

For a harmonic oscillator, $\widehat{H} = -i(p\partial_q - q\partial_p)$ resembles the quantum angular momentum operator L_z, which can be considered as $L_z = a^\dagger a - \tilde{a}^\dagger\tilde{a}$, where a and $\tilde{a}$ are two independent annihilation operators. Indeed, consider a rotation of the form

$$\begin{pmatrix} q \\ \tilde{q} \end{pmatrix} = \begin{pmatrix} u & v \\ -v & u \end{pmatrix}\begin{pmatrix} X \\ \widetilde{X} \end{pmatrix},\ \begin{pmatrix} X \\ \widetilde{X} \end{pmatrix} = \begin{pmatrix} u & -v \\ v & u \end{pmatrix}\begin{pmatrix} q \\ \tilde{q} \end{pmatrix},$$

with $u^2 = v^2 = 1/2$, $\widehat{p} \longrightarrow imu(\partial_X + \partial_{\widetilde{X}})$. For a system of harmonic oscillators we have

$$\widehat{H} = \frac{1}{2}\sum_i \left[-\partial^2_{X_i} + X_i^2 + \partial^2_{\widetilde{X}_i} - \widetilde{X}_i^2\right] \tag{22.100}$$

$$= H(X) - \widetilde{H}(\widetilde{X}), \tag{22.101}$$

which is remarkably similar to the one in the TFD formalism. A more general system would then become

$$\widehat{H} = \sum_i \left[-\frac{1}{2}(\partial^2_{X_i} - \partial^2_{\widetilde{X}_i}) + \frac{1}{\sqrt{2}}(X_i - \widetilde{X}_i)V_i(X + \widetilde{X})\right],$$

where $V_i \equiv \partial_{q_i}V$. Even for such a general system the time generator for the distribution function is anti-tilde invariant in the TFD sense.

To see more connections with TFD, consider the following transformation

$$a = \frac{1}{\sqrt{2}}(X + \partial_X),\ a^\dagger = \frac{1}{\sqrt{2}}(X - \partial_X).$$

The original Hamiltonian becomes

$$H = \frac{1}{2}[p^2 + q^2] = \frac{1}{2}[q^2 - \partial_{\tilde{q}}^2] = \frac{1}{4}[(X + \widetilde{X})^2 - (\partial_X - \partial_{\widetilde{X}})^2] \qquad (22.102)$$

$$= g_1 + g_3, \qquad (22.103)$$

where g_1 and g_3 are two of the three generators defined in TFD as $g_1 = a\tilde{a} + a^\dagger\tilde{a}^\dagger$, $g_2 = i(a\tilde{a} - \tilde{a}^\dagger a^\dagger)$, and $g_3 = a^\dagger a + \tilde{a}^\dagger\tilde{a} + 1$. They commute with the time generator $\widehat{H}$. If a state $|0\rangle$ satisfies the static Schönberg-Liouville equation, so does $e^{\alpha H}|0\rangle$ where α is an arbitrary c-number, since $[H, \widehat{H}] = 0$. In fact, $f(H)|0\rangle$ is also a valid solution in the classical case, where $f(H)$ is an arbitrary function of H. Henceforth, we have the following correspondence between the Liouville system and TFD:

Liouvillian System	Thermofield Dynamics
$\widehat{H} = i\{H, .\}$	$\longrightarrow \widehat{H} = H - \widetilde{H}$,
H	$\longrightarrow G$ Transformation Generators,
$\|\theta\rangle$	$\|0\rangle$.

The last correspondence is the same for quantum systems as well.

The vacuum state of the quantum system is written as

$$\psi_0 = e^{-\frac{1}{2}(X^2 + \widetilde{X}^2)} = e^{-\frac{1}{2}(x^2 + y^2)} = \int dp e^{ipy} e^{-H(x,p)}$$

where $H(x,p) = \frac{1}{2}(x^2 + p^2)$. This solution corresponds to a classical system in thermal equilibrium at $\beta = 1$. The obvious solution of the classical Liouville equation is

$$e^{\alpha H}\psi_0 = \int dp e^{ipy} e^{-(1+\alpha)\frac{1}{2}(x^2 + p^2)}.$$

The following two generators

$$a\tilde{a} \pm a^\dagger\tilde{a}^\dagger \longrightarrow \begin{cases} q^2 + p^2 + \partial_q^2 + \partial_p^2 \\ q\partial_q + p\partial_p \end{cases},$$

however, do not generate any new class of solutions. The obvious solution is obtained by the use of polar coordinates $p = r\cos\theta$, $q = r\sin\theta$, $\widehat{L} \to \partial_\theta$. A time invariant solution must be of the form $f(r^2) = f(p^2 + x^2)$ which is independent of θ.

In TFD, the canonical transformations are, as a matter of fact, a restricted class of transformations. If we write

$$e^{-G}\begin{pmatrix} a \\ \tilde{a}^\dagger \end{pmatrix} e^G = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}\begin{pmatrix} a \\ \tilde{a}^\dagger \end{pmatrix},$$

then we have the constraint that $B_{12}B_{21} = \langle 0|a^\dagger a|0\rangle$ be positive. A closer examination reveals that the solution $e^{\alpha H}\psi_0$ with real α is actually forbidden in the quantum case. However there is no such constraint in the classical system. Therefore any solution $f(x^2 + p^2)$ is a valid solution in the classical case.

22.7 Non-relativistic symmetries in the Schönberg-Fock space

A unitary representation for $\mathfrak{g}_T$ is derived here using the Fock space ($\mathcal{F}$) defined by the tensor product of $\mathcal{H}(\Gamma)$; that is

$$\mathcal{F}(\Gamma) = \oplus_m \mathcal{H}(\Gamma)^{\otimes m}, \quad m = 0, 1, 2..., .$$

The elements of $\mathfrak{g}_T$ are assumed to be defined in the Schönberg-Fock space, $\mathcal{F}(\Gamma)$.

Let $\psi(q,p)$ and $\psi^\dagger(q,p)$ be the basic field operators satisfying the commutation relations at equal times

$$[\psi(q,p;t), \psi^\dagger(q',p';t)]_\pm = \delta(q-q')\delta(p-p'),$$
$$[\psi(q,p;t), \psi(q',p';t)]_\pm = [\psi^\dagger(q,p;t), \psi^\dagger(q',p';t)]_\pm = 0,$$

where $-$ $(+)$ in the brackets defines the classical bosons (fermions). For simplicity, we use in this section the notation: $\tau = (p,q)$, $\psi(\tau) = \psi(q,p)$ and $\delta(\tau - \tau') = \delta(q-q')\delta(p-p')$. We also assume that the particle spin is $S_i = 0$.

In the space $\mathcal{F}(\Gamma)$ there is a vacuum state, $|0\rangle$, such that $\psi(\tau)|0\rangle = 0$, $\langle 0|0\rangle = 1$, and $\psi^\dagger(\tau_i)|0\rangle = |\chi_i\rangle$. A general vector in $\mathcal{F}(\Gamma)$ is defined by

$$|\chi(t)\rangle = \theta(t)_0|0\rangle + \sum_{i=1}^{\infty} \frac{1}{\sqrt{n!}} \int \theta(\tau_1, \tau_2, \cdots \tau_n; t)|\chi_n\rangle d^n\tau, \tag{22.104}$$

where $d^n\tau = d\tau_1 d\tau_2 \cdots d\tau_n$,

$$|\chi_n\rangle = \psi^\dagger(\tau_1)\psi^\dagger(\tau_2)\cdots\psi^\dagger(\tau_n)|0\rangle,$$

and $\theta(\tau_1, \tau_2, \cdots \tau_n; t)$ are symmetric or anti-symmetric functions in the Hilbert space $\mathcal{H}(\Gamma)$, such that

$$\theta(\tau_1, \tau_2, \cdots \tau_n; t) = \frac{1}{\sqrt{n!}}\langle\chi_n|\chi\rangle = \frac{1}{\sqrt{n!}}\langle 0|\prod_{i=1}^{n}\psi(\tau_i)|\chi\rangle.$$

In addition

$$\langle\chi|\chi'\rangle = \theta_0^*\theta_0' + \sum_{i=1}^{\infty}\int \theta^*(\tau_1, \tau_2, \cdots \tau_n; t)\, \theta'(\tau_1, \tau_2, \cdots \tau_n; t) d^n\tau.$$

Therefore, for each operator $\bar{A}(\tau_1, \tau_2, \cdots \tau_n)$ defined on $\mathcal{H}$, and depending symmetrically on the variables $\tau_1, \tau_2, \cdots \tau_n$, we introduce a corresponding operator acting on $\mathcal{F}(\Gamma)$

$$\bar{\mathcal{A}} = \frac{1}{n!}\int \psi^\dagger(\tau_1)\cdots\psi^\dagger(\tau_n)\ \bar{A}(\tau_1, \tau_2, \cdots \tau_n)\ \psi(\tau_n)\cdots\psi(\tau_1) d^n\tau. \tag{22.105}$$

A representation for $\mathfrak{g}_T$ is obtained with this type of operator when $n = 1$. Using Eqs. (22.70)-(22.76) and $n = 1$ in Eq. (22.105), the non-null commutation relations for the thermal Galilei group are now written as

$$
\begin{aligned}
&[\widehat{\mathcal{J}}_i, \widehat{\mathcal{J}}_j] = i\varepsilon_{ijk}\widehat{\mathcal{J}}_k, \quad [\widehat{\mathcal{J}}_i, \mathcal{J}_j] = [\mathcal{J}_i, \widehat{\mathcal{J}}_j] = i\varepsilon_{ijk}\mathcal{J}_k,\\
&[\widehat{\mathcal{J}}_i, \widehat{\mathcal{P}}_j] = i\varepsilon_{ijk}\widehat{\mathcal{P}}_k, \quad [\widehat{\mathcal{J}}_i, \mathcal{P}_j] = [\mathcal{J}_i, \widehat{\mathcal{P}}_j] = i\varepsilon_{ijk}\mathcal{P}_k,\\
&[\widehat{\mathcal{J}}_i, \widehat{\mathcal{K}}_j] = i\varepsilon_{ijk}\widehat{\mathcal{K}}_k, \quad [\widehat{\mathcal{J}}_i, \mathcal{K}_j] = [\mathcal{J}_i, \widehat{\mathcal{K}}_j] = i\varepsilon_{ijk}\mathcal{K}_k,\\
&[\widehat{\mathcal{K}}_i, \widehat{\mathcal{H}}] = i\widehat{\mathcal{P}}_i, \qquad [\widehat{\mathcal{K}}_i, \mathcal{H}] = [\mathcal{K}_i, \widehat{\mathcal{H}}] = i\mathcal{P}_i,\\
&[\widehat{\mathcal{P}}_i, \mathcal{K}_j] = [\mathcal{P}_i, \widehat{\mathcal{K}}_j] = -i\mathcal{N}m\delta_{ij},
\end{aligned}
$$

where $\mathcal{N}$, the number operator, is defined by

$$\mathcal{N} = \int \mathcal{N}(\tau)d\tau = \int \psi^\dagger(\tau)\psi(\tau)d\tau, \tag{22.106}$$

such that

$$\mathcal{N}|\chi_n\rangle = n|\chi_n\rangle. \tag{22.107}$$

A dynamical variable $\bar{\mathcal{A}}$ has its average in a state $|\chi\rangle$ defined by

$$\langle\bar{\mathcal{A}}\rangle = \langle\chi|\bar{\mathcal{A}}|\chi\rangle. \tag{22.108}$$

On the other hand, the temporal evolution of $\bar{\mathcal{A}}$ is given by

$$\langle\chi_0|\exp(it\widehat{\mathcal{H}})\bar{\mathcal{A}}\exp(-it\widehat{\mathcal{H}})|\chi_0\rangle = \langle\chi_0|\bar{\mathcal{A}}(t)|\chi_0\rangle. \tag{22.109}$$

Thus, we have defined a Heisenberg picture for the temporal evolution of the dynamical variables, and from Eq. (22.109) we obtain

$$i\partial_t\bar{\mathcal{A}} = [\bar{\mathcal{A}}, \widehat{\mathcal{H}}]. \tag{22.110}$$

In the Schrödinger picture, the equation for the evolution of the state is

$$i\partial_t|\chi(t)\rangle = \widehat{\mathcal{H}}|\chi(t)\rangle, \tag{22.111}$$

which leads to

$$i\partial_t\theta(\tau_1, \tau_2, \cdots\tau_n; t) = L_\Gamma(\tau_1, \tau_2, \cdots\tau_n)\,\theta(\tau_1, \tau_2, \cdots\tau_n; t), \tag{22.112}$$

where

$$L_\Gamma(\tau_1, \tau_2, \cdots\tau_n) = \widehat{H}$$

is the Liouvillian for n particles. Therefore, Eq. (22.112) is the Schönberg-Liouville equation describing n classical bosons. To get a physically consistent interpretation of the theory, we define $f(\tau_1, \tau_2, \cdots\tau_n; t) = |\theta(\tau_1, \tau_2, \cdots\tau_n; t)|^2$ as the n-particle distribution function in Γ. The field operators $\psi(\tau; t)$, in the Heisenberg representation, satisfies the equation of motion

$$i\partial_t\psi(\tau; t) = L_\Gamma(\tau)\,\psi(\tau; t)(\tau; t).$$

We can define a general vector in $\mathcal{F}(\Gamma)$ by

$$|\chi^\xi(t)\rangle = \theta^\xi(t)_0|0\rangle + \sum_{i=1}^{\infty}\frac{1}{\sqrt{n!}}\int\theta^\xi(\tau_1, \tau_2, \cdots\tau_n; t)|\chi_n\rangle d^n\tau, \tag{22.113}$$

such that

$$\theta^{\xi}(\tau_1,\tau_2,\cdots\tau_n;t)=\frac{1}{\sqrt{n!}}\langle\chi_n|\chi^{\xi}\rangle=\frac{1}{\sqrt{n!}}\langle 0|\prod_{i=1}^{n}\psi(\tau_i)|\chi^{\xi}\rangle,$$

and

$$\langle\chi^{(1-\xi)}|\chi'^{\xi}\rangle=\theta_0^{(1-\xi)*}\theta_0'^{\xi}+\sum_{i=1}^{\infty}\int\theta^{(1-\xi)*}(\tau_1,\tau_2,\cdots\tau_n;t)\,\theta'^{\xi}(\tau_1,\tau_2,\cdots\tau_n;t)d^n\tau.$$

The average of an observable A is

$$\langle A\rangle_{\xi}=\langle\chi^{1-\xi}|A|\chi'^{\xi}\rangle.$$

For the case of $\xi=1$, we can take $\theta(\tau_1,\tau_2,\cdots\tau_n;t)$ as real, so that the substitution

$$\theta(\tau_1,\tau_2,\cdots\tau_n;t)\rightarrow f(\tau_1,\tau_2,\cdots\tau_n;t)$$

is allowed. In this case, we use the Schönberg-Fock space describing classical particles fulfilling the Boltzmann statistics. Then the state is described by a probability density, not an amplitude. This aspect opens the possibility to use quantum field theory tools to treat a broad class of stochastic problems. This was explored by Doi to deal with reaction-diffusion processes [341]. In this realm, the creation and annihilation field operators describe, for instance, the reagents in a chemical reaction. For this purpose, different methods have been developed, exploring functional methods [342–345], which have been extended and applied to different systems [346–354]. Some formal aspects about this method have been addressed by Grassberger and Scheunert [348] and Andersen [349]. One of the difficulties to improve this kind of theory is that, the Fock space and concepts such as indistinguishability of particles have been paradigmatical ingredients of quantum theories. However, as we have observed, the Fock space is taken as a representation vector space of kinematical groups describing classical systems. In this sense there is no $\hbar$ in the method, resulting in full consistency with classical and stochastic physics and no ambiguity with quantum theory. The basic result here is that this kind of theory can be studied with the support of symmetry.

22.8 Classical relativistic representation

Considering a classical theory, the thermo-Poincaré-Lie algebra, $\mathfrak{p}_T$, is

$$\begin{aligned}
[\widehat{M}_{\mu\nu},\widehat{M}_{\sigma\rho}]&=i(g_{\mu\sigma}\widehat{M}_{\rho\nu}+g_{\rho\nu}\widehat{M}_{\sigma\mu}+g_{\mu\rho}\widehat{M}_{\nu\sigma}+g_{\sigma\nu}\widehat{M}_{\mu\rho}),\\
[\widehat{M}_{\mu\nu},\widehat{P}_{\rho}]&=i(g_{\mu\rho}\widehat{P}_{\nu}-g_{\nu\rho}\widehat{P}_{\mu}),\\
[\widehat{M}_{\mu\nu},M_{\sigma\rho}]&=i(g_{\mu\sigma}M_{\rho\nu}+g_{\rho\nu}M_{\sigma\mu}+g_{\mu\rho}M_{\nu\sigma}+g_{\sigma\nu}M_{\mu\rho}),\\
[\widehat{M}_{\mu\nu},P_{\sigma}]&=[M_{\mu\nu},\widehat{P}_{\sigma}]=i(g_{\mu\sigma}P_{\nu}-g_{\nu\sigma}P_{\mu}).
\end{aligned}$$

The commutations relations among non-hat operators are zero, since we have (classical) abelian observables. Three invariants are immediately identified as

$$I_1 = P^\mu P_\mu, \tag{22.114}$$
$$I_2 = \widehat{P}^\mu \widehat{P}_\mu \tag{22.115}$$
$$I_3 = P^\mu \widehat{P}_\mu. \tag{22.116}$$

Since the non-hat operators form an invariant abelian algebra, we can take such operators and the invariants I_1, I_2, I_3 to build a Hilbert space basis. In order to do so, first we notice that

$$e^{-\alpha_\mu \widehat{P}^\mu} P_\sigma e^{\alpha_\nu \widehat{P}^\nu} = P_\sigma, \tag{22.117}$$
$$e^{-\alpha_\mu \widehat{P}^\mu} M_{\sigma\rho} e^{\alpha_\nu \widehat{P}^\nu} = M_{\sigma\rho} + \alpha_\sigma P_\rho - \alpha_\rho P_\sigma, \tag{22.118}$$
$$e^{-\varepsilon_{\mu\nu} \widehat{M}^{\mu\nu}} P_\sigma e^{\varepsilon_{\mu\nu} \widehat{M}^{\mu\nu}} = P_\sigma + i(\varepsilon_{\sigma\nu} P^\nu - \varepsilon_{\nu\sigma} P^\nu). \tag{22.119}$$

Therefore, we find P_σ and $M_{\sigma\rho}$ as natural candidates for describing linear and angular momentum, respectively. On the other hand, $\widehat{P}^\mu$ and $\widehat{M}^{\mu\nu}$ can be taken as the generators of translations and rotations, respectively. That this interpretation is consistent can be verified, for instance, from Eq. (22.119) which establishes that under rotations the linear momentum transforms as a 4-vector. This interpretative aspect is a direct consequence of the fact that the algebra of non-hat operators is an invariant subalgebra of $\mathfrak{p}_T$. Now we assume the existence of a Hilbert space $\mathcal{H}(\Gamma)$ on which the elements of $\mathfrak{p}_T$ are defined and introduce a non-hat operator, say Q_μ , through the condition

$$e^{-\alpha_\mu \widehat{P}^\mu} Q_\sigma e^{\alpha_\nu \widehat{P}^\nu} = Q_\sigma + i\alpha,$$

where α is a constant. Then the operator Q_μ describes generalized coordinates. Therefore, a phase space frame for the Hilbert space $\mathcal{H}(\Gamma)$ can be introduced since $[P, Q] = 0$. Let us define $|q, p\rangle \in \mathcal{H}(\Gamma)$ such that

$$P|q,p\rangle = p|q,p\rangle, \quad Q|q,p\rangle = q|q,p\rangle,$$

with q and p being real 4-vectors, and $\langle q, p|\phi\rangle = \phi(q, p)$ being an L^2 (Lebesgue)-type function, that is $\int |\phi(q,p)|^2 dq\, dp < \infty$. This last condition is used to impose the normalization condition. In this way, we obtain a unitary representation for $\mathfrak{p}_T$ as

$$M_{\mu\nu} = P_\mu Q_\nu - P_\nu Q_\mu, \tag{22.120}$$
$$\widehat{M}_{\mu\nu} = P_\mu \widehat{Q}_\nu - P_\nu \widehat{Q}_\mu + Q_\nu \widehat{P}_\mu - Q_\mu \widehat{P}_\nu, \tag{22.121}$$

where

$$\widehat{P}_\mu = -i\frac{\partial}{\partial q_\mu}, \;\; \widehat{Q}_\mu = i\frac{\partial}{\partial p_\mu}, P_\mu = \mathbf{1}{\cdot}p_\mu, \quad \text{and } Q_\mu = \mathbf{1}{\cdot}q_\mu. \tag{22.122}$$

A general association between a hat and a non-hat operator, consistent with Eqs. (22.120)-(22.122), is thus introduced. Consider an arbitrary function of the

phase space, say $A(q,p)$, then we have two mappings, (i) c: $A(q,p) \to \mathsf{A} = \mathbf{1}\cdot A(q,p)$, giving rise to c-number operators, and (ii) $^\wedge : A(q,p) \to \widehat{A}$, such that, now we have,

$$\widehat{A} = (\widehat{p}\, A(q,p))\widehat{q} + \alpha(\widehat{q}A(q,p))\widehat{p} + \beta\widehat{q}(\widehat{p}A(q,p)),$$

where α and β are constants. Taking $\alpha = 1$ and $\beta = 0$, the association is such that $A \to \widehat{A} = i\{A(q,p),\ \cdot\}$, where $\{\ \cdot\,,\,\cdot\ \}$ is the Poisson bracket. In this case, we have

$$(\gamma A + B)^\wedge = \gamma(\widehat{A} + \widehat{B}),\quad (AB)^\wedge = A\widehat{B} + \widehat{B}A,\ (\gamma)^\wedge = 0, \tag{22.123}$$

where γ is a constant. This result is useful to derive another set of Casimir invariants of $\mathfrak{p}_T$. Defining $w_u = \frac{1}{2}\varepsilon_{\mu\nu\sigma\rho}M^{\nu\sigma}P^\rho$, the Pauli-Lubanski vector, we find the following invariants $W = w^\mu w_u$ and $\widehat{W} = 2w^\mu \widehat{w}_u$. Hence, we write Eq. (22.120) and (22.121) respectively as: $M_{\mu\nu} \to J_{\mu\nu} = M_{\mu\nu} + S_{\mu\nu}$ and $\widehat{M}_{\mu\nu} \to \widehat{J}_{\mu\nu} = \widehat{M}_{\mu\nu} + \widehat{S}_{\mu\nu}$, where the variable $S_{\mu\nu}$ and $\widehat{S}_{\mu\nu}$ are related to the spinor index of the representation, which is taken to be zero here (scalar representations).

We assume that the average of an one-body diagonal operator is given by

$$\begin{aligned}
\langle\overline{A}\rangle &= \langle\phi|\overline{A}|\phi\rangle \\
&= \int dqdpdq'dp'\langle\phi|q,p\rangle\langle q,p|\overline{A}|q',p'\rangle\langle q',p'|\phi\rangle \\
&= \int dqdpdq'dp'\phi^*(q,p)\overline{A}(q,p,q',p')\delta^4(q-q')\delta^4(p-p')\phi(q',p') \\
&= \int dqdp\phi^*(q,p)\overline{A}(q,p)\phi(q,p),
\end{aligned}$$

where the notation $\overline{A}$ stands for either a c-number operator, A, or a hat operator, $\widehat{A}$. If $\overline{A} = A$, then the average of A reduces to $\langle A\rangle = \int dqdpf(q,p)A(q,p)$ where $f(q,p) = |\phi(q,p)|^2$.

Let us now write down an equation of motion for $\phi(q,p)$. The invariant I_3, given in Eq. (22.116), has a fixed value in this phase space representation. Considering then $I_3 = 0$, from Eq. (22.122) we write

$$p^\mu \frac{\partial}{\partial q^\mu}\phi(q,p) = 0, \tag{22.124}$$

which is a collisionless transport equation, also furnished by the positive-defined real quantity $f(q,p)$. Then we can interpret $\phi(q,p)$ as a probability amplitude in phase space and $f(q,p)$ as a classical probability density.

For the completion of physical interpretation of this formalism, as well as for practical purposes, let us define the tensor

$$\overline{T}^{\mu\nu}(q) = \frac{1}{2(2\pi)^3}\int \frac{d^3p}{p^0}\phi^*(q,p)\overline{P}^\mu\overline{P}^\nu\phi(q,p).$$

Taking in particular $\overline{P} = P$, we get the usual definition of the energy-momentum tensor

$$\overline{T}^{\mu\nu} \to T^{\mu\nu}(q) = \frac{1}{2(2\pi)^3}\int \frac{d^3p}{p^0}p^\mu p^\nu f(q,p),$$

where $T^{00}(q)$ is the average value of the energy per particle, $T^{0i}(q)$ is the average value of the energy flow, $T^{i0}(q)$ is the macroscopic momentum flow and $T^{ij}(q)$ is the pressure tensor. This result shows the compatibility of our approach with the usual kinetic theory [360, 319].

22.9 Boltzmann equation and non-relativistic limit

In order to derive a collision term in Eq. (22.124), we use the notion of propagator in the Hilbert phase space $\mathcal{H}(\Gamma)$. Consider the (pointwise) collision between two particles (1) and (2) with initial (i) and final (f) momenta specified, respectively, by p^{μ}_{i1}, p^{μ}_{i2}, p^{μ}_{f1}, and p^{μ}_{f2}. Define now an amplitude of transition at a point q, say $W(q, p_{f1}, p_{f2}, p_{i1}p_{i2})$ is the propagator of the system, from a initial state $|q, p_{i1}; q, p_{i2}\rangle$ to a final state $|q, p_{f1}; q, p_{f2}\rangle$, that is

$$W(q, p_{f1}, p_{f2}|p_{i1}, p_{i2}) = \langle q, p_{f1}; q, p_{f2}|q, p_{i1}; q, p_{i2}\rangle.$$

Then the amplitude of transition for any point q of space-time is

$$W(p_{f1}, p_{f2}|p_{i1}, p_{i2}) = \int d^4q \, \langle q, p_{f1}; q, p_{f2}|q, p_{i1}; q, p_{i2}\rangle,$$

such that we can write

$$\langle q, p_{i1}; q, p_{i2}| = \int d^4p_{f1}d^4p_{f2} \, W(p_{i1}, p_{i2}|p_{f1}, p_{f2})\langle q, p_{f1}; q, p_{f2}|,$$

and so we have

$$\langle q, p_{i1}; q, p_{i2}|\phi_{12}\rangle = \int d^4p_{f1}d^4p_{f2} W(p_{i1}, p_{i2}|p_{f1}, p_{f2})\langle q, p_{f1}; q, p_{f2}|\phi_{12}\rangle.$$

Using the indistinguishability of particles, an intrinsic ingredient in our formalism since we are considering amplitudes, and the Hartree approximation $\langle q, p_{f1}; q, p_{f2}|\phi_{12}\rangle = \phi(q, p_{f1})\phi(q, p_{f2})$, we can compute the change in the probability amplitude, say $\Psi_+(q, p_{i1})$, due to particles leaving the collision at q with momentum p_{i1}, that is

$$\Psi_+(q, p_{i1}) = \frac{1}{2}\int d^4p_{i2}d^4p_{f1}d^4p_{f2}W(p_{f1}, p_{f2}|p_{i1}, p_{i2})\phi(q, p_{f1})\phi(q, p_{f2}).$$

The same reasoning is used to compute the effect of particles leaving the collision at q with momentum other than p_{i1}, that is

$$\Psi_-(q, p_{i1}) = \frac{1}{2}\int d^4p_{i2}d^4p_{f1}d^4p_{f2}W(p_{i1}, p_{i2}|p_{f1}, p_{f2})\phi(q, p_{f1})\phi(q, p_{f2}).$$

Therefore, we obtain the following transport equation

$$p^{\mu}\partial_{\mu}\phi(q, p) = \mathcal{C}(q, p), \tag{22.125}$$

where

$$\begin{aligned}\mathcal{C}(q, p) &= \Psi_+(q, p) - \Psi_-(q, p)\\ &= \frac{1}{2}\int d^4p_{i2}d^4p_{f1}d^4p_{f2}[W(p_{f1}, p_{f2}|p, p_{i2})\phi(q, p_{f1})\phi(q, p_{f2})\\ &\quad -W(p, p_{i2}|p_{f1}, p_{f2})\phi(q, p_{f1})\phi(q, p_{f2})].\end{aligned}$$

As a consequence, we have derived a relativistic Boltzmann equation, but for probability amplitudes in phase space [361]. An alternative way is to derive the Boltzmann equation for the density, $f(q,p)$. This is accomplished by the following substitutions in Eq. (22.125): $\phi(q,p) \to f(q,p)$ and $W(p_{f1},p_{f2}|p,p_{i2}) \to |W(p_{f1},p_{f2}|p,p_{i2})|^2$, such that now $\Psi_+(q,p_{i1})$ ($\Psi_-(q,p_{i1})$) is increasing (decreasing) in the probability density due to particles leaving a collision at q with momentum (other than) p_{i1}.

Let us analyze the non-relativistic limit of this approach. Considering Eqs. (22.120) and (22.121), we have that the components of the Lorentz boost generators are written as

$$\widehat{L}_{0m} = \frac{\widehat{K}_m}{c} = i(\frac{H}{c^2}\frac{\partial}{\partial p_m} - p_m\frac{\partial}{\partial H} + t\frac{\partial}{\partial q_m} - \frac{q_m}{c^2}\frac{\partial}{\partial t}),$$

Therefore, proceeding to the contraction, considering formally $c \to \infty$, we have

$$\widehat{K}_m = i(m\frac{\partial}{\partial p_m} + t\frac{\partial}{\partial q_m}),$$

where $\widehat{K}_m$ is the generator of usual Galilean boost transformation. On the other hand, for the energy we have

$$\lim_{c\to\infty}\frac{H}{c^2} = \lim_{c\to\infty}\frac{1}{c}\sqrt{m^2c^2 + p_jp^j} \tilde{=} m, \quad j = 1,2,3.$$

The remaining components of the total angular momentum operator reduce as well to the Galilean counterpart. Besides, with the above representation for the total energy operator, in the non-relativistic limit the generator of time translation $\widehat{P}_0$ becomes $\widehat{H} = i\partial_t$. Such operators are just the ones previously employed in this chapter. Observe also that we can introduce a Fock space representation via $\mathcal{H}(\Gamma)\otimes\mathcal{H}(\Gamma)\otimes\cdots\otimes\mathcal{H}(\Gamma)$ such that the amplitude $\phi(q,p)$ can be taken as field operators in phase space.

Chapter 23

Real-Time Method for Nonequilibrium Quantum Mechanics

Most natural phenomena, widely scoping from quark-gluon plasma in particle physics to biology and to cosmology, proceed via nonequilibrium (far from equilibrium) processes, though our understanding is still limited to physics of equilibrium. In spite of complicacy and model-dependence of nonequilibrium processes, most systems eventually settle down to equilibrium states that are characterized by a few variables. Statistical mechanics and thermodynamics describe the states of systems in equilibrium remarkably successfully. At a more sophisticated level, the processes not far from equilibrium belong to an area pretty well understood, where the linear-response theory and the dissipation-fluctuation theorem hold good and are useful tools to understand the processes towards equilibrium states.

Nonequilibrium phenomena are believed to involve two facets: kinematics and dynamics. Kinematics concerns about the states of a system and dynamics cares about how the system evolves from an initial state to a final one via various possible intermediate states. For instance, quark-gluon plasma, is a typical nonequilibrium physics, where the initial state of heavy ions with extremely high velocities and the final product of hadrons and mesons from quark pairs and gluons are pretty well understood. However, the intermediate states from the hadronic states to the quark-gluon plasma are not understood yet, except for some characteristic features.

Another arena where nonequilibrium physics would play an important role is the phase transition itself. Symmetry breaking has been a central concept in our understanding of phase transitions from condensed matter to particle physics. The electroweak (EW) phase transition and the QCD phase transition that would have occurred in the early universe relies on the spontaneous symmetry-breaking with the Higgs boson. The formation of topological defects also depends on phase transitions. Though we understand what would happen after the phase transition, that is, what the final state would look like, we do not have yet a complete comprehension of the transition process. In particular, the critical phenomena at the onset of phase transitions, in which the correlation length extends infinitely and thermal relaxation slows down infinitely, prevents one from directly applying the physics of equilibrium. Further, another puzzling issue is the last stage of thermalization toward the final state of equilibrium.

An aspect common to nonequilibrium phenomena is that they proceed dynamically in time. One conservative approach to nonequilibrium physics is to adopt the contemporary laws for the dynamics. Quantum theory has proved to be the most precise law of nature, at the subatomic particle scale and the atomic scale. From this view point, quantum field theory may be employed to describe nonequilibrium processes involving phase transitions unless an entirely new physics is required. This stratagem has been used in phase transitions in the past half a century. It is surprising that the progress in understanding phase transitions has been at a crawl in comparison to their universality and utmost importance.

In order to treat nonequilibrium problems like phase transitions, the closed-time path method [67] is one of the options. The development of TFD [67, 70, 51] as an operator formalism with real-time was motivated to consider such problems. In general it has not met with much success, since it is not easy to find a point providing an anchor to the physical development. Unlike the case of of systems in equilibrium, that have to be normalized to a distribution function, the nonequilibrium problems do not provide any such point.

In this chapter, we shall introduce another real-time formalism for quantum mechanical models for phase transitions. The quantum law is prescribed by the Schrödinger equation [363, 364, 63, 365, 366], but the density operator obeys the Liouville-von Neumann equation. Some time back, it was found that for an oscillator with time-dependent mass or frequency, the so-called invariant operator satisfying the Liouville-von Neumann equation may also be used to find the exact quantum states of the time-dependent Schrödinger equation [367]. This observation led us to the Liouville-von Neumann method for nonequilibrium quantum fields, where the Liouville-von Neumann equation is to be combined with the (functional) Schrödinger equation, so both the density operator and quantum states are found exactly from the knowledge of the invariant operators [368, 65, 66, 369].

23.1 Schrödinger, Heisenberg and Liouville pictures

A simple nonequilibrium process is prescribed by a time-dependent Hamiltonian, for which time enters explicitly through coupling constants or physical constants such as mass and frequency, etc. For a system interacting with a thermal bath, interactions may have both local and nonlocal effects on the system itself and may lead to a time-dependent Hamiltonian, when the system is separately handled and the nonlocal effects from the thermal bath are neglected. Let us denote the Hamiltonian by $H(t)$. Then, it describes a nonequilibrium process because it is not static and $e^{-\beta H(t)}$ is not truly a density operator from the LvN equation.

As far as the time-dependent Hamiltonian is concerned, all the information about the nonequilibrium evolution is carried by the evolution operator (in unit of

$\hbar = 1$)

$$i\frac{\partial}{\partial t}U(t) = H(t)U(t). \tag{23.1}$$

The evolution operator has a formal expression

$$U(t) = T\exp\Big(-i\int^t H(t')dt'\Big), \tag{23.2}$$

where T denotes the standard time-ordered integration, and in the static case, it takes the familiar form, $U(t) = e^{-iHt}$. In the Schrödinger picture, the time-dependent state is given by

$$|\Psi(t)\rangle = U(t)|\Psi\rangle_{\rm S}, \tag{23.3}$$

for any initial state $|\Psi\rangle_{\rm S}$.

On the other hand, in the Heisenberg picture, the time-dependent operator defined as

$$O_{\rm H}(t) = U^\dagger(t)O_{\rm S}U(t), \tag{23.4}$$

obeys the Heisenberg equation

$$i\frac{\partial}{\partial t}O_{\rm H}(t) + [H_{\rm H}(t), O_{\rm H}(t)] = 0. \tag{23.5}$$

Here, $H_{\rm H}(t) = U^\dagger(t)H(t)U(t)$ is the Heisenberg operator of the Hamiltonian. In the Heisenberg picture, the expectation value with respect to a pure or mixed state $\rho_{\rm S}$ takes the form

$$\langle O\rangle = {\rm Tr}(\rho_{\rm S}O_{\rm H}(t)) = {\rm Tr}(\rho(t)O_{\rm S}), \tag{23.6}$$

where $\rho(t)$ is the density operator

$$\rho(t) = U(t)\rho_{\rm S}U^\dagger(t). \tag{23.7}$$

However, as the task of evaluating the evolution operator Eq. (23.2) is not trivial, we have to rely on some analytical scheme such as the perturbation theory. Here, we shall follow the Liouville-von Neumann method, which is based on an invariant operator,

$$O_{\rm L}(t) = U(t)O_{\rm S}U^\dagger(t). \tag{23.8}$$

Note that the invariant operator evolves backward in the same way as the density operator Eq. (23.7) in contrast to the Heisenberg operator. Indeed, the invariant operator satisfies the Liouville-von Neumann equation

$$i\frac{\partial}{\partial t}O_{\rm L}(t) + [O_{\rm L}(t), H(t)] = 0. \tag{23.9}$$

Another reason to use the invariant operator is that any eigenstate of the invariant operator,

$$O_{\rm L}(t)|\lambda, t\rangle = \lambda|\lambda, t\rangle, \tag{23.10}$$

having a constant eigenvalue λ, yields an exact quantum state [367]

$$|\Psi_\lambda(t)\rangle = Ce^{i\int dt\langle\lambda,t|(i\frac{\partial}{\partial t}-H(t))|\lambda,t\rangle}|\lambda,t\rangle, \tag{23.11}$$

where C is a constant. From now on we shall work in the Liouville picture and omit the subscript L.

The most advantageous point of the Liouville picture [368] [66] is that the Liouville-von Neumann equation itself can provide all the quantum and statistical information of nonequilibrium systems. For a time-dependent system, the invariant operator $O_{\rm L}(t)$, whose eigenstates are exact states, may also be used for the density operator $\rho(t) = e^{-\beta O_{\rm L}(t)}$, thus unifying quantum statistical mechanics with quantum theory. The Liouville-von Neumann method treats the time-dependent, nonequilibrium system exactly in the same way as the time-independent, equilibrium one and is applied to nonequilibrium fermion systems [65].

23.2 Linear model for phase transition

Quantum mechanics is a (1+0)-dimensional field theory. As a quantum mechanical model for the second-order phase transition, let us consider the time-dependent harmonic oscillator [368]

$$H(t) = \frac{1}{2}p^2 + \frac{1}{2}m^2(t)q^2, \tag{23.12}$$

where $m^2(t)$ has the asymptotically positive value m_i^2 far before and the asymptotically negative value $-m_f^2$ far after the quench. The oscillator executes a stable motion about $q = 0$ before the quench but rolls down from $q = 0$ after the quench because it is an unstable equilibrium.

In the Liouville picture, we find a pair of time-dependent annihilation and creation operators defined as [66, 368, 370]

$$a(t) = i[\varphi^*(t)p - \dot{\varphi}^*(t)q], \quad a^\dagger(t) = -i[\varphi(t)p - \dot{\varphi}(t)q], \tag{23.13}$$

where p and q are Schrödinger operators. These operators satisfy the Liouville-von Neumann equation when φ satisfies the classical equation,

$$\ddot{\varphi}(t) + m^2(t)\varphi = 0. \tag{23.14}$$

Further, the Wronskian condition

$$\dot{\varphi}^*(t)\varphi(t) - \varphi^*(t)\dot{\varphi}(t) = i, \tag{23.15}$$

makes the equal-time commutator hold,

$$[a(t), a^\dagger(t)] = 1. \tag{23.16}$$

Far before the phase transition, the complex solution to Eq. (23.14) satisfying Eq. (23.15) is given by

$$\varphi_i(t) = \frac{e^{-im_i t}}{\sqrt{2m_i}}. \tag{23.17}$$

According to Eq. (23.13), the Fock space is now constructed from the annihilation and creation operators

$$a(t) = \frac{e^{im_i t}}{\sqrt{2m_i}}\Big(ip + m_i q\Big) = e^{im_i t} a_{\rm S},$$
$$a^{\dagger}(t) = \frac{e^{-im_i t}}{\sqrt{2m_i}}\Big(-ip + m_i q\Big) = e^{-im_i t} a_{\rm S}^{\dagger}. \tag{23.18}$$

Note that the Liouville-von Neumann operators $a(t)$ and $a^{\dagger}(t)$ have the opposite phase factors of the Heisenberg operators $a_{\rm H}(t) = e^{-im_i t} a_{\rm S}$ and $a_{\rm H}^{\dagger}(t) = e^{im_i t} a_{\rm S}^{\dagger}$. Though the Hamiltonian has the standard representation in all the three pictures

$$H_i = m_i\Big(a^{\dagger}(t)a(t) + \frac{1}{2}\Big) = m_i\Big(a_{\rm S}^{\dagger} a_{\rm S} + \frac{1}{2}\Big) = m_i\Big(a_{\rm H}^{\dagger}(t) a_{\rm H}(t) + \frac{1}{2}\Big), \tag{23.19}$$

the phase factors, which follow from Eq. (23.8), are necessary for $a(t)$ and $a^{\dagger}(t)$ to satisfy the Liouville-von Neumann equation (23.9) and, similarly, for $a_{\rm H}(t)$ and $a_{\rm H}^{\dagger}(t)$ to satisfy the Heisenberg equation (23.5). The vacuum minimizes both the uncertainty relation $\Delta q \Delta p = 1/2$ and the energy $\langle H \rangle = m_i/2$.

On the other hand, at later times far after the quench, the solution to Eq. (23.14) is given by

$$\varphi_f(t) = \frac{1}{2\sqrt{2}}\Big[\Big(C_1 - iC_2\Big)e^{m_f t} + \Big(C_1 + iC_2\Big)e^{-m_f t}\Big], \tag{23.20}$$

where $C_j, j = 1, 2$ depend on the intermediate process toward the final state. The kinetic and potential energies contribute equally to the vacuum and thermal expectation values so that $\langle H_f \rangle = 0$. The uncertainty

$$(\Delta q)(\Delta p) = \frac{1}{2}\Big[m_f C_1^2 \cosh^2(m_f t) + m_f C_1^2 \sinh^2(m_f t)\Big], \tag{23.21}$$

exponentially grows, suggesting the classicality of the phase transition out of equilibrium [364]. However, the phase transition depends on the whole process, how it evolves out of equilibrium from the initial equilibrium state.

To show the process dependence of the phase transition, we consider an exactly solvable model, describing a finite smooth quench [368],

$$m^2(t) = m_1^2 - m_0^2 \tanh\Big(\frac{t}{\tau}\Big). \tag{23.22}$$

The mass has $m_i^2 = m_0^2 + m_1^2$ at earlier times ($t = -\infty$) and has $-m_f^2 = -m_0^2 + m_1^2 < 0$ at later times ($t = \infty$). τ measures the quench rate, *i.e.* the rate of change of the mass. The instantaneous quench corresponds to the ($\tau = 0$)-limit. The solution to Eq. (23.14) is found to be

$$\varphi(t) = \frac{e^{-m_i t}}{\sqrt{2m_i}} F\Big(-\frac{\tau}{2}(im_i - m_f), -\frac{\tau}{2}(im_i + m_f); 1 - i\tau m_i; -e^{2t/\tau}\Big), \tag{23.23}$$

where F is the hypergeometric function. At earlier times this solution has the correct asymptotic form Eq. (23.17). On the other hand, at later times $\varphi(t)$ has the asymptotic form

$$\varphi_f(t) = \left[\frac{1}{\sqrt{2m_i}}\frac{(-1)\Gamma(1-im_i\tau)\Gamma(m_f\tau)}{\frac{\tau}{2}(im_i-m_f)\Gamma^2(-\frac{\tau}{2}(im_i-m_f)}\right]e^{m_f t} + \left[\frac{1}{\sqrt{2m_i}}\frac{(-1)\Gamma(1-im_i\tau)\Gamma(m_f\tau)}{\frac{\tau}{2}(im_i+m_f)\Gamma^2(-\frac{\tau}{2}(im_i+m_f)}\right]e^{-m_f t}. \tag{23.24}$$

Thus, the coefficients C_1, C_2 of Eq. (23.20) depend on the mass parameters m_i, m_f and the quench rate τ. In other words, the final asymptotic state of nonequilibrium evolution depends on the intermediate processes.

23.3 Nonlinear model for phase transition

We consider the nonlinear model for phase transition [368, 66]

$$H = \frac{1}{2}p^2 \pm \frac{m^2}{2}q^2 + \frac{\lambda}{4!}q^4. \tag{23.25}$$

The model with the upper (positive) sign has the global minimum at $q = 0$, while the model with the lower (negative) sign has the global minimum at $q = \pm\sqrt{6}m/\sqrt{\lambda}$, now with $q = 0$ being a local maximum, and exhibits a symmetry-breaking of the phase transition. Even for such a simple nonlinear model, there is no known method yet for exact quantum states except for perturbative methods. Further, the instability of a localized quantum state near $q = 0$ for the symmetry-breaking model causes another problem of the convergence of perturbation series.

As we do not know the Hilbert space for a nonlinear system, our stratagem here is first to find a suitable Fock space of all multiparticle or number states and then to represent an exact state of the nonlinear model (23.25) in the Fock space. Thus, this method is a time-dependent perturbation theory in the Fock space. To guarantee the stability of the perturbation method, we shall not truncate the Hamiltonian by the quadratic term only but include part of the nonlinear effects at the lowest order. As far as a nonlinear effect at the lowest order is concerned, the idea is similar to the Gaussian approximation method for static systems [371–374].

In the oscillator representation, the position and momentum operators are given by

$$\begin{aligned} q &= \varphi(t)a(t) + \varphi^*(t)a^\dagger(t), \\ p &= \dot{\varphi}(t)a(t) + \dot{\varphi}^*(t)a^\dagger(t). \end{aligned} \tag{23.26}$$

The normal-ordering of operators, where all annihilation operators stand to the right of all creation operators, is particularly useful for evaluating expectation values with respect to the vacuum. The normal-ordering of operators appearing in the Hamiltonian is such that $q^2 =: q^2 : +\langle q^2\rangle$ and $q^4 =: q^4 : +6 : q^2 : q^2 + 3\langle q^2\rangle^2$,

where : : denotes the normal ordering and $\langle\ \rangle$ is the expectation value with respect to the vacuum. The normal-ordered monomial of the position takes the form

$$: q^n : \ = \sum_{k=0}^{n} \frac{n!}{k!(n-k)!}\, \varphi^{*(n-k)} \varphi^k a^{\dagger(n-k)} a^k, \tag{23.27}$$

and a similar expression holds for the momentum. So the Hamiltonian H can be divided into two parts:

$$H = H_0 + \lambda H_{\rm P}, \tag{23.28}$$

where

$$H_0 = \frac{1}{2} : p^2 : \pm \frac{m^2}{2} : q^2 : + \frac{\lambda}{4} \langle q^2 \rangle : q^2 : + E_0, \tag{23.29}$$

$$H_{\rm P} = \frac{1}{4!} : q^4 : . \tag{23.30}$$

Here, the c-term from the normal ordering is the energy expectation E_0

$$\begin{aligned} E_0 &= \frac{1}{2}\langle p^2 \rangle \pm \frac{m^2}{2} \langle q^2 \rangle + \frac{\lambda}{8} \langle q^2 \rangle^2 \\ &= \frac{1}{2} \dot{\varphi}^* \dot{\varphi} \pm \frac{m^2}{2} \varphi^* \varphi + \frac{\lambda}{8} (\varphi^* \varphi)^2. \end{aligned} \tag{23.31}$$

Up to c-number terms, H_0 and $H_{\rm P}$ are equivalent to those of the Hartree method

$$\begin{aligned} H_0 &= \frac{1}{2} p^2 \pm \frac{m^2}{2} q^2 + \frac{\lambda}{4} \langle q^2 \rangle q^2, \\ H_{\rm P} &= \frac{1}{4!} q^4 - \frac{1}{4} \langle q^2 \rangle q^2. \end{aligned} \tag{23.32}$$

At this stage, the Gaussian vacuum is not necessarily the energy-minimizing state since φ is not fixed yet except for Eq. (23.15). The minimization of the energy with respect to φ or φ^* leads to

$$\ddot{\varphi}(t) + (\pm m^2 + \frac{\lambda}{2} \varphi^* \varphi) \varphi(t) = 0. \tag{23.33}$$

In fact, Eq. (23.33) makes $a(t)$ and $a^\dagger(t)$ the invariant operators for the Liouville-von Neumann equation. The coherent state, a state more general than the Gaussian vacuum, will be considered now.

23.3.1 *Correlation functions in coherent state*

The coherent state shifts the center of the vacuum to a classical trajectory. As the time-dependent annihilation and creation operators $a(t)$ and $a^\dagger(t)$ construct the Fock space of the system, they can be used to define the coherent state and other states. Following the definition of [375], the coherent state is an eigenstate of $a(t)$,

$$a(t)|\alpha, t\rangle = \alpha |\alpha, t\rangle, \tag{23.34}$$

with a complex eigenvalue α. It is a displaced state of the vacuum ,

$$|\alpha, t\rangle = D^\dagger(\alpha)|0, t\rangle = e^{-\alpha^*\alpha/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n, t\rangle, \tag{23.35}$$

for the displacement operator

$$D(\alpha) = e^{-\alpha a^\dagger(t)+\alpha^* a(t)}. \tag{23.36}$$

The position expectation value,

$$\bar{q} \equiv \langle\alpha, t|q|\alpha, t\rangle = \alpha\varphi(t) + \alpha^*\varphi^*(t), \tag{23.37}$$

is real and satisfies the same equation as φ, while the momentum expectation value,

$$\bar{p} \equiv \langle\alpha, t|p|\alpha, t\rangle = \alpha\dot{\varphi}(t) + \alpha^*\dot{\varphi}^*(t), \tag{23.38}$$

satisfies the classical relation $\bar{p} = \dot{\bar{q}}$. From the subtracted 2-point correlators

$$\begin{aligned}
g_{qq}(t) &= \langle\alpha, t|q^2|\alpha, t\rangle - \bar{q}^2 = \varphi^*(t)\varphi(t),\\
g_{pp}(t) &= \langle\alpha, t|p^2|\alpha, t\rangle - \bar{p}^2 = \dot{\varphi}^*(t)\dot{\varphi}(t),\\
g_{qp}(t) &= \langle\alpha, t|qp|\alpha, t\rangle - \bar{q}\bar{p} = \dot{\varphi}^*(t)\varphi(t),\\
g_{pq}(t) &= g^*_{qp}(t) = \varphi^*(t)\dot{\varphi}(t),
\end{aligned} \tag{23.39}$$

we obtain the evolution equations

$$\begin{aligned}
\dot{g}_{qq}(t) &= g_{qp}(t) + g_{pq}(t),\\
\dot{g}_{pp} &= -(\pm m^2 + \frac{\lambda}{2}g_{qq})(g_{qp} + g_{pq}),\\
\dot{g}_{qp} &= g_{pp} - (\pm m^2 + \frac{\lambda}{2}g_{qq})g_{qq}.
\end{aligned} \tag{23.40}$$

In contrast with the first order linear differential equations for a harmonic oscillator, the subtracted 2-point correlators for the nonlinear model satisfy nonlinear differential equations.

The wave function for the coherent state is the Gaussian vacuum whose center moves around $(\bar{q}, \bar{p})$. In fact, the coherent state expectation of the full Hamiltonian

$$H_{\rm eff} = \frac{1}{2}\bar{p}^2 \pm \frac{m^2}{2}\bar{q}^2 + \frac{\lambda}{4!}\bar{q}^4 + \frac{1}{2}g_{pp} + \frac{1}{2}g_{qq}(\pm m^2 + \frac{\lambda}{2}\bar{q}^2) + \frac{3\lambda}{4!}g_{qq}^2, \tag{23.41}$$

is a function of $(\bar{q}, \bar{p})$, $(\varphi, p_\varphi = \dot{\varphi}^*)$ and $(\varphi^*, p_{\varphi^*} = \dot{\varphi})$. The variation of the effective Hamiltonian with respect to φ leads to

$$\ddot{\varphi}(t) + (\pm m^2 + \frac{\lambda}{2}\bar{q}^2 + \frac{\lambda}{2}g_{qq})\varphi(t) = 0, \tag{23.42}$$

and, similarly,

$$\ddot{\bar{q}} + (\pm m^2 + \frac{\lambda}{6}\bar{q}^2 + \frac{\lambda}{2}g_{qq})\bar{q} = 0. \tag{23.43}$$

Note that when φ satisfies Eq. (23.42), $a(t)$ and $a^\dagger$ are the invariant operators for the Hamiltonian

$$\bar{H}_0 = \frac{1}{2}p^2 \pm \frac{m^2}{2}q^2 + \frac{\lambda}{4}(\bar{q}^2 + \langle q^2\rangle)q^2. \tag{23.44}$$

This Hamiltonian is nothing but that of the Hartree method, where the position and momentum are divided into classical part and quantum part, $q = \bar{q} + q_f$ and $p = \bar{p} + p_f$, and only quadratic terms of q_f and q_f are kept. The subtracted 2-point correlators now follow the evolution equations

$$\begin{aligned}
\dot{g}_{qq} &= g_{qp} + g_{pq}, \\
\dot{g}_{pp} &= -(\pm m^2 + \frac{\lambda}{2}\bar{q}^2 + \frac{\lambda}{2}g_{qq})(g_{qp} + g_{pq}), \\
\dot{g}_{qp} &= g_{pp} - (\pm m^2 + \frac{\lambda}{2}\bar{q}^2 + \frac{\lambda}{2}g_{qq})g_{qq}.
\end{aligned} \tag{23.45}$$

23.3.2 *Correlation functions in thermal state*

The nonlinear model with the unbroken symmetry in a thermal equilibrium may be described approximately by the coherent-thermal state

$$\rho_{\rm CT} = \frac{1}{Z_{\rm T}} \exp[-\beta(\Omega a^\dagger(t)a(t) + \delta a^\dagger(t) + \delta^* a(t) + \epsilon_0)], \tag{23.46}$$

where Ω is determined by the gap equation, $\Omega^2 = m^2 + \lambda/(4\Omega)$, and $\epsilon_0 = \Omega/2 + |\delta|^2/\Omega$. As $a(t)$ and $a^\dagger(t)$ satisfy the Liouville-von Neumann equation for H_0, this operator is the density operator for H_0. Using the unitary transformation by the displacement operator, we get

$$D(\alpha)a(t)D^\dagger(\alpha) = a(t) + \alpha, \quad D(\alpha)a^\dagger(t)D^\dagger(\alpha) = a^\dagger(t) + \alpha^*, \tag{23.47}$$

for $\alpha = -\delta/\Omega$, the coherent-thermal density transforms to a thermal one

$$D(\alpha)\rho_{\rm CT}D^\dagger(\alpha) = \frac{1}{Z_{\rm T}} \exp[-\beta\Omega(a^\dagger(t)a(t) + \frac{1}{2})] = \rho_{\rm T}. \tag{23.48}$$

The correlators are given by

$$\begin{aligned}
\langle q^2\rangle_{\rm CT} &\equiv {\rm Tr}(\rho_{\rm CT}q^2) = \bar{q}^2 + \coth\Big(\frac{\beta\Omega}{2}\Big)\varphi^*(t)\varphi(t), \\
\langle p^2\rangle_{\rm CT} &\equiv {\rm Tr}(\rho_{\rm CT}p^2) = \bar{p}^2 + \coth\Big(\frac{\beta\Omega}{2}\Big)\dot{\varphi}^*(t)\dot{\varphi}(t),
\end{aligned} \tag{23.49}$$

where $\bar{q}$ and $\bar{p}$ are given in Eqs. (23.37) and (23.38), and φ satisfies Eq. (23.42). The corresponding thermal 2-point correlators are then given by

$$\begin{aligned}
g_{{\rm T}qq}(t) &= \langle q^2\rangle_{\rm CT} - \bar{q}^2 = \coth(\frac{\beta\Omega}{2})\varphi^*(t)\varphi(t), \\
g_{{\rm T}pp}(t) &= \langle \hat{p}^2\rangle_{\rm CT} - \bar{p}^2 = \coth(\frac{\beta\Omega}{2})\dot{\varphi}^*(t)\dot{\varphi}(t), \\
g_{{\rm T}qp}(t) &= \langle qp\rangle_{\rm CT} - \bar{q}\bar{p} = \coth(\frac{\beta\Omega}{2})\dot{\varphi}^*(t)\varphi(t), \\
g_{{\rm T}pq}(t) &= g^*_{{\rm T}qp}(t) = \coth(\frac{\beta\Omega}{2})\varphi^*(t)\dot{\varphi}(t),
\end{aligned} \tag{23.50}$$

from which we obtain the evolution equations for the thermal 2-point correlators

$$\begin{aligned}
\dot{g}_{\mathrm{T}qq}(t) &= g_{\mathrm{T}qp}(t) + g_{\mathrm{T}pq}(t), \\
\dot{g}_{\mathrm{T}pp}(t) &= -(\pm m^2 + \frac{\lambda}{2}\varphi^*\varphi)(g_{\mathrm{T}qp} + g_{\mathrm{T}pq}), \\
\dot{g}_{\mathrm{T}qp}(t) &= g_{\mathrm{T}pp} - (\pm m^2 + \frac{\lambda}{2}\varphi^*\varphi)g_{\mathrm{T}qq}.
\end{aligned} \tag{23.51}$$

In the $T = 0$ limit, Eqs. (23.50) and (23.51) reduce to the evolution equations (23.42) and (23.45).

23.4 Beyond the Hartree approximation for nonlinear model

The most advantageous point of the Liouville-von Neumann method for the nonlinear model is that the Fock space for H_0 enables us to find the exact state by including the perturbation H_{P}. Thus, the Liouville-von Neumann method can go beyond the Gaussian approximation [66]. Since it includes $\lambda\langle q^2\rangle q^2$ in H_0, the Fock space itself is the Hartree approximation and, for a static system, is equivalent to the Gaussian effective potential method [371–374]. In this section, we follow Ref. [66].

The Fock space will be constructed by the time-dependent annihilation and creation operators, the invariant operators for H_0, such that

$$i\frac{\partial a}{\partial t} + [a, H_0] = 0, \quad i\frac{\partial a^\dagger}{\partial t} + [a^\dagger, H_0] = 0, \tag{23.52}$$

where φ in Eq. (23.13) satisfies the mean field equation

$$\ddot{\varphi}(t) + (\pm m^2 + \frac{\lambda}{2}\varphi^*\varphi)\varphi(t) = 0. \tag{23.53}$$

Note that the mean field equation above can also be obtained by minimizing E_0 in Eq. (23.31). The time-dependent Gaussian vacuum is annihilated by $a(t)$

$$a(t)|0,t\rangle_{(0)} = 0, \tag{23.54}$$

and the number states are obtained by applying $a^\dagger(t)$

$$|n,t\rangle_{(0)} = \frac{a^{\dagger n}(t)}{\sqrt{n!}}|0,t\rangle_{(0)}. \tag{23.55}$$

In fact, each number state is the solution of the time-dependent Schrödinger equation for H_0

$$i\frac{\partial}{\partial t}|n,t\rangle_{(0)} = H_0(t)|n,t\rangle_{(0)}. \tag{23.56}$$

Then, the number states constitute a Fock space of orthonormal basis

$${}_{(0)}\langle n,t|m,t\rangle_{(0)} = \delta_{nm}. \tag{23.57}$$

23.4.1 *Beyond the Hartree approximation*

To go beyond the Hartree approximation, the perturbation

$$H_{\rm P} = \frac{1}{4!}\Big(\varphi^{*4}a^{\dagger 4} + 4\varphi^{*3}\varphi a^{\dagger 3}a + 6\varphi^{*2}\varphi^2 a^{\dagger 2}a^2 + 4\varphi^{*}\varphi^3 a^{\dagger}a^3 + \varphi^4 a^4\Big) \tag{23.58}$$

has to be included in the solution. As the Fock space for H_0 is now known, we may follow the time-dependent perturbation theory by expanding the exact state as

$$|n,t\rangle = \sum_{l=0}^{\infty}\sum_{m=0}^{\infty} \lambda^l C^{(l)}_{n;m}(t)|m,t\rangle_{(0)}. \tag{23.59}$$

Here, the lowest order coefficient is

$$C^{(0)}_{n;m} = \delta_{n,m}. \tag{23.60}$$

The time-dependent Schrödinger equation for the full Hamiltonian in Eq. (23.25), is equivalent to the set of equations,

$$\sum_{l=0}^{\infty}\sum_{m=0}^{\infty} i\lambda^l \dot{C}^{(l)}_{n;m}(t)|m,t\rangle_0 = \sum_{l=0}^{\infty}\sum_{m=0}^{\infty} \lambda^{l+1} C^{(l)}_{n;m}(t)H_{\rm P}|m,t\rangle_{(0)}, \tag{23.61}$$

leading to a hierarchy of differential equations

$$\dot{C}^{(l)}_{n;m}(t) = -i\sum_{j=0}^{\infty} C^{(l-1)}_{n;j}(t)_{(0)}\langle m,t|H_{\rm P}(t)|j,t\rangle_{(0)}. \tag{23.62}$$

The hierarchy of coefficients may be found in a compact form in the representation of $a^{\dagger}(t)$ and $a(t)$. By summing over l

$$C_{n;m}(t) = \sum_{l=0}^{\infty} \lambda^l C^{(l)}_{n;m}(t), \tag{23.63}$$

Eq. (23.59) may be written by introducing an operator, $\hat{U}_1$ as

$$|n,t\rangle = \sum_{m=0}^{\infty} C_{n;m}(t)|m,t\rangle_{(0)} \equiv U_{\rm I}[a^{\dagger}(t), a(t); t, \lambda]|n,t\rangle_{(0)}. \tag{23.64}$$

Then, the Schrödinger equation for the full Hamiltonian Eq. (23.25) leads to

$$\Big(i\frac{\partial}{\partial t}U_{\rm I}(t,\lambda) + [U_{\rm I}(t,\lambda), H_0] - \lambda H_{\rm P}\Big)|n,t\rangle_{(0)} = 0. \tag{23.65}$$

Note that the operator $U_{\rm I}$ is a functional of $a(t)$, $a^{\dagger}(t)$ and depends on t explicitly. However, as $a(t)$, $a^{\dagger}(t)$ already satisfy Eq. (23.52), for which linearity holds, the time-dependence of $U_{\rm I}$ through $a(t)$, $a^{\dagger}(t)$ will be automatically satisfied. So Eq. (23.65) explicitly depends on time itself and becomes an interaction picture-like equation

$$i\frac{\partial}{\partial t}U_{\rm I}(t,\lambda) = \lambda H_{\rm P}U_{\rm I}(t,\lambda). \tag{23.66}$$

The formal solution is given by

$$U_{\rm I}(t,\lambda) = {\rm T}\exp\Big(-i\lambda\int H_{\rm P}dt\Big). \tag{23.67}$$

Here, T denotes a time-ordering for the integral and $a^\dagger(t)$ and $a(t)$ are fixed for each time.

The improved vacuum can be found up to any desired order either by solving Eq. (23.62) or by acting with the operator in Eq. (23.67) on the Gaussian vacuum. For instance, the improved vacuum to order λ^2 is given by

$$|0,t\rangle_{(2)} = |0,t\rangle_{(0)} + \lambda\sum_{m=0} C^{(1)}_{0;m}(t)|m,t\rangle_{(0)} + \lambda^2\sum_{m=0} C^{(2)}_{0;m}(t)|m,t\rangle_{(0)}, \tag{23.68}$$

where the only nonvanishing coefficients are

$$C^{(1)}_{0;4}(t) = -i\frac{1}{\sqrt{4!}}\int^t \varphi^{*4}(t'), \tag{23.69}$$

and

$$\begin{aligned}
C^{(2)}_{0;8}(t) &= (-i)^2\frac{\sqrt{70}}{4!}\int^t \varphi^{*4}(t')\int^{t'}\varphi^{*4}(t''),\\
C^{(2)}_{0;6}(t) &= (-i)^2\frac{\sqrt{5}}{3}\int^t \varphi^{*3}(t')\varphi(t')\int^{t'}\varphi^{*4}(t''),\\
C^{(2)}_{0;4}(t) &= (-i)^2\frac{3}{\sqrt{4!}}\int^t \varphi^{*2}(t')\varphi^2(t')\int^{t'}\varphi^{*4}(t''),\\
C^{(2)}_{0;2}(t) &= (-i)^2\frac{1}{3\sqrt{2}}\int^t \varphi^{*}(t')\varphi^3(t')\int^{t'}\varphi^{*4}(t''),\\
C^{(2)}_{0;0}(t) &= (-i)^2\frac{1}{4!}\int^t \varphi^{4}(t')\int^{t'}\varphi^{*4}(t'').
\end{aligned} \tag{23.70}$$

The non-Gaussian nature of the vacuum state (23.68) can be exploited by calculating the kurtosis (higher moments). The two-point and four-point correlators with respect to the Gaussian vacuum state are

$$\begin{aligned}
{}_{(0)}\langle 0,t|q^2|n,t\rangle_{(0)} &= \varphi^*\varphi,\\
{}_{(0)}\langle 0,t|q^4|0,t\rangle_{(0)} &= 3(\varphi^*\varphi)^2,
\end{aligned} \tag{23.71}$$

whereas those with respect to the improved vacuum state given by Eq. (23.68) are

$$\begin{aligned}
{}_{(2)}\langle 0,t|q^2|0,t\rangle_{(2)} &= \varphi^*\varphi + \lambda^2[\sqrt{2}(C^{(2)}_{0;2}\varphi^2 + C^{(2)*}_{0;2}\varphi^{*2})\\
&\quad +(C^{(2)*}_{0;0} + C^{(2)}_{0;0} + 9C^{(1)*}_{0;4}C^{(1)}_{0;4})\varphi^*\varphi] + \mathcal{O}(\lambda^3),
\end{aligned} \tag{23.72}$$

$$\begin{aligned}
{}_{(2)}\langle 0,t|q^4|0,t\rangle_{(2)} &= 3(\varphi^*\varphi)^2 + \sqrt{4!}\lambda(C^{(1)}_{0;4}\varphi^4 + C^{(1)*}_{0;4}\varphi^{*4})\\
&\quad +\lambda^2[\sqrt{4!}(C^{(2)}_{0;4}\varphi^4 + C^{(2)*}_{0;4}\varphi^{*4})\\
&\quad +6\sqrt{2}(C^{(2)}_{0;2}(\varphi^*\varphi)\varphi^2 + C^{(2)*}_{0;2}(\varphi^*\varphi)\varphi^{*2})\\
&\quad +(123C^{(1)*}_{0;4}C^{(1)}_{0;4} + 3C^{(2)*}_{0;0} + 3C^{(2)}_{0;0})(\varphi^*\varphi)^2] + \mathcal{O}(\lambda^3).
\end{aligned} \tag{23.73}$$

23.4.2 *Stability of the Liouville-von Neumann method*

The stability of a series solution is an important issue in the time-dependent perturbation theory, since there usually occur secular terms in coefficient that grow in time. These secular terms should be removed systematically to insure the physically meaningful solution.

To compare the Liouville-von Neumann method with the standard perturbation theory, let us first consider the well-known nonlinear model with unbroken symmetry (m^2 in Eq. (23.25)). In that case, the mean field equation (23.53) has the solution

$$\varphi(t) = \frac{1}{\sqrt{2\Omega}} e^{-i\Omega t}, \quad \Omega^2 = m^2 + \frac{\lambda}{4\Omega}. \tag{23.74}$$

The improved vacuum, corrected to $\mathcal{O}(\lambda^2)$,

$$\begin{aligned} |0,t\rangle_{(2)} = \exp\Big(-i(\frac{\Omega}{2} - \frac{\lambda}{32\Omega^2})t\Big) \\ \times\Big[(1 + i\frac{\lambda^2}{2^9\cdot 3\Omega^5}t)|0\rangle_{(0)} + \frac{\lambda^2}{2^7\cdot 3\sqrt{2}\Omega^6}|2\rangle_{(0)} - (\frac{\lambda}{2^5\sqrt{6}\Omega^3} - \frac{\sqrt{3}\lambda^2}{2^9\sqrt{2}\Omega^6})|4\rangle_{(0)} \\ + \frac{\lambda^2}{2^7\cdot 3^2\Omega^6}|6\rangle_{(0)} + \frac{\sqrt{70}\lambda^2}{2^{12}\cdot 3\Omega^6}|8\rangle_{(0)}\Big] + \mathcal{O}(\lambda^3), \end{aligned}$$

now has a secular term in the coefficient of $|0\rangle_{(0)}$. This term, $C^{(2)}_{0;0}$, originates from the four quanta creation and the subsequent annihilation. This is a consequence of the time-dependent perturbation theory in the time-dependent basis. In fact, the secular terms of $|0,t\rangle_{(0)}$, which are the first two terms of $\exp[i\lambda^2/(2^9\cdot 3\Omega^5)t]$, correct the energy up to $\mathcal{O}(\lambda^2)$,

$$E_{(2)} = \frac{\Omega}{2} - \frac{\lambda}{32\Omega^2} - \frac{\lambda^2}{2^9\cdot 3\Omega^5} + \mathcal{O}(\lambda^3). \tag{23.75}$$

The higher order terms arising from the creation of even number of quanta and its subsequent annihilation of equal quanta or vise versa also contain secular terms proportional to powers of t depending on the number of such processes. All these terms will provide the correct energy to the Schrödinger equation.

The origin of secular terms may be understood directly from the formal solution given by Eq. (23.67),

$$U_{\rm I}(t,\lambda) = \exp\Big(-i\lambda\int^t H_{\rm P}(t') + (-i\lambda)^2[\int^t dt' H(t'), \int^{t'} dt'' H_{\rm P}(t'')] + \mathcal{O}(\lambda^3)\Big). \tag{23.76}$$

The term for creation and annihilation of equal number of quanta arises from the commutator

$$\exp\Big(-\frac{\lambda^2}{(4!)^2}\int^t dt'\varphi^4(t')\int^{t'} dt''\varphi^{*4}(t'')[a^4, a^{\dagger 4}]\Big) \to \exp\Big(i\frac{\lambda^2}{2^9\cdot 3\Omega^5}t\Big). \tag{23.77}$$

Now the time-dependent vacuum state to $\mathcal{O}(\lambda^2)$ *does not* involve any secular term as shown

$$\begin{aligned} |0,t\rangle_{(2)} = e^{iE_{(2)}t}\Big[|0\rangle_{(0)} + e^{-i\frac{\lambda^2}{2^9\cdot 3\Omega^5}t}\Big(\frac{\lambda^2}{2^7\cdot 3\sqrt{2}\Omega^6}|2\rangle_{(0)} - (\frac{\lambda}{2^5\sqrt{6}\Omega^3} - \frac{\sqrt{3}\lambda^2}{2^9\sqrt{2}\Omega^6})|4\rangle_{(0)} \\ + \frac{\lambda^2}{2^7\cdot 3^2\Omega^6}|6\rangle_{(0)} + \frac{\sqrt{70}\lambda^2}{2^{12}\cdot 3\Omega^6}|8\rangle_{(0)}\Big)\Big] + \mathcal{O}(\lambda^3). \end{aligned} \tag{23.78}$$

The Liouville-von Neumann method not only perturbatively improves the state but also systematically removes the secular terms of time-dependent perturbation theory. The idea of removing the higher order secular terms by absorbing them into the improved energy is equivalent to removing the secular terms by renormalizing the energy in the multiple-scale perturbation theory [376]. The Liouville-von Neumann approach proves accurate since the lowest order vacuum state is a Gaussian state that extremizes the Hamiltonian and the corrected vacuum state is expanded in the Fock basis [377]. In Ref. [369], the secular terms are eliminated by using multiple-scale perturbation theory.

The Hartree approximation cannot be applied to phase transitions when the dynamical instability grows sufficiently after the quench. After the phase transition, the symmetry is broken, and thus the mean field equation for Eq. (23.25)

$$\ddot{\varphi} + (-m^2 + \frac{\lambda}{2}\varphi^*\varphi)\varphi = 0 \tag{23.79}$$

has the solution that exponentially grows as $\varphi \approx e^{mt}/\sqrt{2m}$ so that it does not take long for $(\lambda\varphi^*\varphi/2)$ to get larger than m^2. After this moment of time, the perturbation $H_{\rm P}$ that exponentially grows as powers of φ and φ^* should be treated on an equal footing as H_0 in finding the state for the phase transition.

23.5 TFD for time-dependent boson system

We close this chapter by discussing briefly a possibility to construct a time-dependent TFD from the Liouville-von Neumann approach. We start once again with the Hamiltonian

$$H(t) = \hbar\Big[\omega_0(t)a^\dagger a + \frac{1}{2}\omega_+(t)a^{\dagger 2} + \frac{1}{2}\omega_+^* a^2\Big], \tag{23.80}$$

where a and $a^\dagger$ are the Schrödinger (time-independent) annihilation and creation operators, and ω_0 is real and ω_+ is complex. We may find the time-dependent annihilation operator, an invariant operator, of the form

$$a(t) = f^{(-)}(t)a + f^{(+)}(t)a^\dagger \tag{23.81}$$

and its Hermitian conjugate $a^\dagger(t)$, and impose the Liouville-von Neumann equations

$$\begin{aligned} i\hbar\frac{\partial a(t)}{\partial t} + [a(t), H(t)]_- &= 0, \\ i\hbar\frac{\partial a^\dagger(t)}{\partial t} + [a^\dagger(t), H(t)]_- &= 0. \end{aligned} \tag{23.82}$$

The time-dependent creation operator $a^\dagger(t)$ is another invariant operator. The pair $\{a(t), a^\dagger(t)\}$ form a complete set. Therefore any invariant operator can be constructed out of them. Observe that this provides equations for $f^{(-)}$ and $f^{(+)}$.

Using the tilde conjugation rules, the tilde Hamiltonian reads

$$\tilde{H}(t) = \hbar\Big[\omega_0(t)\tilde{a}^\dagger\tilde{a} + \frac{1}{2}\omega_+^*(t)\tilde{a}^{\dagger 2} + \frac{1}{2}\omega_+\tilde{a}^2\Big]. \tag{23.83}$$

Let us introduce the time-dependent annihilation operator for the tilde operators as

$$\tilde{a}(t) = f^{(-)*}(t)\tilde{a} + f^{(+)*}(t)\tilde{a}^\dagger. \tag{23.84}$$

The operators $\tilde{a}(t)$ and its Hermitian conjugate $\tilde{a}^\dagger(t)$ satisfy the equations

$$\begin{aligned} i\hbar\frac{\partial\tilde{a}(t)}{\partial t} + [\tilde{a}(t), -\tilde{H}(t)]_- = 0, \\ i\hbar\frac{\partial\tilde{a}^\dagger(t)}{\partial t} + [\tilde{a}^\dagger(t), -\tilde{H}(t)]_- = 0. \end{aligned} \tag{23.85}$$

The equal-time commutator also holds

$$[\tilde{a}(t), \tilde{a}^\dagger(t)]_- = 1. \tag{23.86}$$

The number states

$$\tilde{N}(t)|\tilde{n}, t\rangle = \tilde{a}^\dagger(t)\tilde{a}(t)|\tilde{n}, t\rangle = \tilde{n}|\tilde{n}, t\rangle \tag{23.87}$$

are the exact quantum states for the Hamiltonian, Eq. (23.83).

The generator of time translations is

$$\hat{H}(t) = H(t) - \tilde{H}(t), \tag{23.88}$$

where the operators of the boson and their tilde operators commute with each other, that is,

$$[\tilde{a}, a]_- = [\tilde{a}, a^\dagger]_- = [\tilde{a}^\dagger, a]_- = [\tilde{a}^\dagger, a]_- = 0, \tag{23.89}$$

and

$$[\tilde{a}(t), a(t)]_- = [\tilde{a}(t), a^\dagger(t)]_- = [\tilde{a}^\dagger(t), a(t)]_- = [\tilde{a}^\dagger(t), a(t)]_- = 0. \tag{23.90}$$

The boson operators $a(t)$, $a^\dagger(t)$, $\tilde{a}(t)$ and $\tilde{a}^\dagger(t)$ are the invariant operators satisfying the Liouville-von Neumann equations for the hat Hamiltonian, Eq. (23.88). A basis element in the doubled Hilbert space is

$$|n, \tilde{m}, t\rangle = |n, t\rangle \otimes |\tilde{m}, t\rangle = \frac{a^{\dagger n}(t)}{\sqrt{n!}}\frac{\tilde{a}^{\dagger m}(t)}{\sqrt{m!}}|0, \tilde{0}, t\rangle. \tag{23.91}$$

The density operators are

$$\rho(t) = \frac{1}{Z}e^{-\beta\hbar\omega a^\dagger(t)a(t)}, \tag{23.92}$$

$$\tilde{\rho}(t) = \frac{1}{Z}e^{+\beta\hbar\omega\tilde{a}^\dagger(t)\tilde{a}(t)}, \tag{23.93}$$

which obviously satisfy the Liouville-von Neumann equation. Here β and ω are constants that may be fixed by the initial temperature and frequency. The density operator in the doubled Hilbert space is given by

$$\hat{\rho}(t) = \rho(t) \otimes \tilde{\rho}(t) = \frac{1}{Z^2}e^{-\beta\hbar\omega(a^\dagger(t)a(t) - \tilde{a}^\dagger(t)\tilde{a}(t))}. \tag{23.94}$$

The thermal expectation value of an observable A takes the form

$$\langle A\rangle = \mathrm{Tr}[\rho(t)A] = \langle 0(\beta),t|A|0(\beta),t\rangle, \tag{23.95}$$

where the thermal vacuum state is given by

$$\begin{aligned}|0(\beta),t\rangle &= \frac{1}{Z^{1/2}}\sum_n e^{-\beta\hbar\omega n/2}\frac{1}{n!}a^{\dagger n}(t)\tilde{a}^{\dagger\tilde{n}}(t)|0,\tilde{0},t\rangle \\ &= \sqrt{1-e^{-\beta\hbar\omega}}e^{e^{-\beta\hbar\omega/2}a^\dagger(t)\tilde{a}^\dagger(t)}|0,t\rangle,\end{aligned} \tag{23.96}$$

with $|0,t\rangle = |0,\tilde{0},t\rangle$. The thermal state is an exact eigenstate of the Schrödinger equation for the total system, Eq. (23.88). The thermal state is also written as a time-dependent two-mode squeezed state of the vacuum state

$$|0(\beta),t\rangle = e^{-iG(t)}|0,t\rangle, \tag{23.97}$$

where

$$G(t) = -i\theta(\beta)[\tilde{a}(t)a(t) - a^\dagger(t)\tilde{a}^\dagger(t)]. \tag{23.98}$$

As the density operator involves a constant β, we find the time- and temperature-dependent annihilation and creation operators through the Bogoliubov transformation

$$\begin{aligned}a(\beta,t) &= \cosh\theta(\beta)a(t) - \sinh\theta(\beta)\tilde{a}^\dagger(t), \\ \tilde{a}(\beta,t) &= \cosh\theta(\beta)\tilde{a}(t) - \sinh\theta(\beta)a^\dagger(t).\end{aligned} \tag{23.99}$$

The inverse transformation of these relations are

$$\begin{aligned}a(t) &= \cosh\theta(\beta)a(\beta,t) + \sinh\theta(\beta)\tilde{a}^\dagger(\beta,t), \\ \tilde{a}(t) &= \cosh\theta(\beta)\tilde{a}(\beta,t) + \sinh\theta(\beta)a^\dagger(\beta,t).\end{aligned} \tag{23.100}$$

We obtain similar equations for $a^\dagger(\beta,t)$, $\tilde{a}^\dagger(\beta,t)$, $a^\dagger(t)$ and $\tilde{a}^\dagger(t)$ by using the Hermitian conjugate of these equations. As $\theta(\beta)$ is a constant, $a(\beta,t)$, $\tilde{a}(\beta,t)$ are also invariant operators. Then the thermal state is the time- and temperature-dependent vacuum

$$a(\beta,t)|0(\beta),t\rangle = \tilde{a}(\beta,t)|0(\beta),t\rangle = 0. \tag{23.101}$$

The thermal state $|0(\beta),t\rangle$, as an eigenstate of the invariant operators $a(\beta,t)$ and $\tilde{a}(\beta,t)$, is an exact eigenstate of the total system. At each moment, the boson still keeps the same boson distribution since the expectation value of the time-dependent number operator yields

$$\langle 0(\beta),t|a^\dagger(t)a(t)|0(\beta),t\rangle = \sinh^2\theta(\beta) = \frac{1}{e^{\beta\hbar\omega}-1}. \tag{23.102}$$

Using the Bogoliubov transformations from $\{a(t),a^\dagger(t)\}$ to $\{a(\beta,t),a^\dagger(\beta,t)\}$, we find

$$\begin{aligned}\langle F(a(t),a^\dagger(t))\rangle_{\mathrm{T}} = \langle 0(\beta),t|F(&\cosh\theta(\beta)a(\beta,t) + \sinh\theta(\beta)\tilde{a}^\dagger(\beta,t), \\ &\cosh\theta(\beta)a^\dagger(\beta,t) + \sinh\theta(\beta)\tilde{a}(\beta,t))|0(\beta),t\rangle.\end{aligned} \tag{23.103}$$

This provides the basic rule for calculating matrix element of any operator in TFD. For instance, using the position representation

$$q = \sqrt{\hbar}\cosh\theta(\beta)[v(t)a(\beta,t) + v^*(t)a^\dagger(\beta,t)] + \sqrt{\hbar}\sinh\theta(\beta)[v^*(t)\tilde{a}(\beta,t) + v(t)\tilde{a}^\dagger(\beta,t)], \tag{23.104}$$

we obtain

$$\langle 0(\beta),t|q^{2n}|0(\beta),t\rangle = \hbar^n \sum_{k=0}^{n} \binom{2n}{2k} \langle 0,t|\cosh^{2k}\theta(\beta)[v(t)a(\beta,t) + v^*(t)a^\dagger(\beta,t)]^{2k} \times \sinh^{2n-2k}\theta(\beta)[v^*(t)\tilde{a}(\beta,t) + v(t)\tilde{a}^\dagger(\beta,t)]^{2n-2k}|0,t\rangle. \tag{23.105}$$

After normal ordering, it results in

$$\langle q^{2n}\rangle_{\mathrm{T}} = \langle 0(\beta),t|q^{2n}|0(\beta),t\rangle = \frac{(2n)!}{2^n n!}[\hbar v^*(t)v(t)]^n(1+2\sinh^2\theta(\beta))^n. \tag{23.106}$$

Consider a time-dependent interaction from initial ω_i's at $t = t_i$ to final ones, ω_f's at t_f. That is, all ω's change from ω_i's to ω_f's. From the constants ω_f's, we find a Bogoliubov transformation of the form

$$a_i = \mu a_f + \nu a_f^\dagger, \qquad a_i^\dagger = \mu^* a_f^\dagger + \nu^* a_f, \tag{23.107}$$

where $\{a_i, a_i^\dagger\}$ for ω_i's and $\{a_f, a_f^\dagger\}$ for ω_f's. Here μ and ν, which should be determined by $f^{(\pm)}$, carry all the information about the history of interaction and may take the form

$$\mu = \mu(t_i,t_f;\omega_i,\omega_f), \quad \nu = \nu(t_i,t_f;\omega_i,\omega_f), \tag{23.108}$$

and satisfy

$$\mu^*\mu - \nu^*\nu = 1. \tag{23.109}$$

If the boson is initially in thermal equilibrium with the inverse temperature β and has the boson distribution $\bar{n}_i = 1/(e^{\beta\hbar\omega} - 1)$, then the final state is such that

$$\langle 0(\beta),t_f|a_i^\dagger a_i|0(\beta),t_f\rangle = \nu^*\nu + \frac{1+2\nu^*\nu}{e^{\beta\hbar\omega}-1}. \tag{23.110}$$

The first term originates from the particle production by vacuum fluctuations [378], $\langle 0,t_f|a_i^\dagger a_i|0,t_f\rangle = \nu^*\nu$, and the second term is a purely thermal result, having an overall amplification factor, $(1+2\nu^*\nu)$, to the boson distribution. Thus the evolution of the time-dependent system leads to a distribution quite different from the boson distribution function. The extension to fermion can be performed accordingly [64].

Chapter 24

Dressed and Bare State Approaches to the Thermalization Process

A thermalization process occurs in some cases for a system of material particles coupled to an environment, in the sense that as it evolves after an infinitely long time, the matter particles loose the memory of their initial states. This study is, in general, not easy from a theoretical point of view, due to the complex nonlinear character of the interactions between the matter particles and the environment. To get over these difficulties, linearized models have been adopted. An account on the subject of the evolution of quantum systems on general grounds can be found in [379–384]. Besides, the main analytical method used to treat these systems at zero or finite temperature is, except for a few special cases, perturbation theory. In this framework, the perturbative approach is carried out by means of the introduction of *bare*, non-interacting objects (fields, to which are associated bare quanta), the interaction being introduced order by order in powers of the coupling constant.

In spite of remarkable achievements of perturbative methods, there are situations where they cannot be employed, or are of little use. These cases have led to attempts to improve non-perturbative *analytical* methods, in particular, where strong effective couplings are involved. Among these trials there are methods that perform resummations of perturbative series, even if they are divergent, which amounts in some cases to extending the weak-coupling regime to a strong-coupling domain [145–149, 144]. In chapter 10 we have described one of these methods, the Borel resummation of perturbative series.

In this chapter we follow a different non-perturbative approach: we investigate a simplified linear version of a particle–field or particle–environment system, where the particle, taken in the harmonic approximation, is coupled to the reservoir, modelled by independent harmonic oscillators. We will employ, in particular, *dressed* states and *renormalized* coordinates. Using this method non-perturbative treatments can be considered for both weak and strong couplings. A linear model permits a better understanding of the need for non-perturbative analytical treatments of coupled systems, which is the basic problem underlying the idea of a *dressed* quantum mechanical system. Of course, the use of such an approach to a realistic nonlinear system is an extremely hard task, while the linear model provides a good compromise between physical reality and mathematical reliability. The

whole system is supposed to reside inside a spherical cavity of radius R in thermal equilibrium at temperature $T = \beta^{-1}$. In other words, we consider the spatially regularized theory (finite R) at finite temperature. The free space case is obtained by suppressing the regulator, $(R \to \infty)$. For a detailed comparison between this procedure and the one considering an *a priori* unbounded space, see [387].

24.1 The model

Let us start by considering a particle approximated by a harmonic oscillator, having *bare* frequency ω_0, linearly coupled to a set of N other harmonic oscillators, with frequencies ω_k, $k = 1, 2, \ldots, N$. The Hamiltonian for such a system is written in the form,

$$H = \frac{1}{2}\left[p_0^2 + \omega_0^2 q_0^2 + \sum_{k=1}^{N}\left(p_k^2 + \omega_k^2 q_k^2\right)\right] - q_0 \sum_{k=1}^{N} c_k q_k, \tag{24.1}$$

leading to the following equations of motion,

$$\ddot{q}_0 + \omega_0^2 q_0 = \sum_{i=1}^{N} c_i q_i(t) \tag{24.2}$$

$$\ddot{q}_i + \omega_i^2 q_i = c_i q_0(t). \tag{24.3}$$

In the limit $N \to \infty$, we recover our case of the particle coupled to the environment, after redefining divergent quantities, in a manner analogous to mass renormalization in field theories. A Hamiltonian of the type Eq. (24.1) has been largely used in the literature, in particular to study the quantum Brownian motion with the path-integral formalism [379, 380]. It has also been employed to investigate the linear coupling of a particle to the scalar potential [387–391].

The Hamiltonian is transformed to principal axis by means of a point transformation,

$$\begin{aligned} q_\mu = \sum_{r=0}^{N} t_\mu^r Q_r\,, \quad p_\mu = \sum_{r=0}^{N} t_\mu^r P_r; \\ \mu = (0, \{k\}), \qquad k = 1, 2, ..., N; \quad r = 0, ...N, \end{aligned} \tag{24.4}$$

performed by an orthonormal matrix $T = (t_\mu^r)$. The subscripts $\mu = 0$ and $\mu = k$ refer respectively to the particle and the harmonic modes of the reservoir and r refers to the normal modes. In terms of normal momenta and coordinates, the transformed Hamiltonian reads

$$H = \frac{1}{2}\sum_{r=0}^{N}(P_r^2 + \Omega_r^2 Q_r^2), \tag{24.5}$$

where the Ω_r's are the normal frequencies corresponding to the collective *stable* oscillation modes of the coupled system. Using the coordinate transformation in

the equations of motion and explicitly making use of the normalization

$$\sum_{\mu=0}^{N}(t_{\mu}^{r})^{2}=1,$$

we get

$$t_{k}^{r}=\frac{c_{k}}{\omega_{k}^{2}-\Omega_{r}^{2}}t_{0}^{r}\ ,\ \ t_{0}^{r}=\left[1+\sum_{k=1}^{N}\frac{c_{k}^{2}}{(\omega_{k}^{2}-\Omega_{r}^{2})^{2}}\right]^{-\frac{1}{2}}, \tag{24.6}$$

with the condition

$$\omega_{0}^{2}-\Omega_{r}^{2}=\sum_{k=1}^{N}\frac{c_{k}^{2}}{\omega_{k}^{2}-\Omega_{r}^{2}}. \tag{24.7}$$

We take $c_k = \eta(\omega_k)^u$, where η is a constant independent of k. In this case the environment is classified according to $u > 1$, $u = 1$, or $u < 1$, respectively as *supraohmic*, *ohmic* or *subohmic*. This terminology has been used in studies of the quantum Brownian motion and of dissipative systems [380–384]. For a subohmic environment the sum in Eq. (24.7) is convergent in the limit $N \to \infty$ and the frequency ω_0 is well defined. For ohmic and supraohmic environments, this sum diverges for $N \to \infty$. This makes the equation meaningless, unless a renormalization procedure is implemented. From now on we restrict ourselves to an *ohmic* system. In this case, Eq. (24.7) is written in the form

$$\omega_{0}^{2}-\delta\omega^{2}-\Omega_{r}^{2}=\eta^{2}\Omega_{r}^{2}\sum_{k=1}^{N}\frac{1}{\omega_{k}^{2}-\Omega_{r}^{2}}, \tag{24.8}$$

where we have defined the counterterm

$$\delta\omega^{2}=N\eta^{2}. \tag{24.9}$$

There are $N+1$ solutions of Ω_r, corresponding to the $N+1$ normal collective modes. Let us for a moment suppress the index r of Ω_r^2. If $\omega_0^2 > \delta\omega^2$, all possible solutions for Ω^2 are positive, physically meaning that the system oscillates harmonically in all its modes. If $\omega_0^2 < \delta\omega^2$, then a single negative solution exists. In order to prove this let us define the function

$$I(\Omega^{2})=\omega_{0}^{2}-\delta\omega^{2}-\Omega^{2}-\eta^{2}\Omega^{2}\sum_{k=1}^{N}\frac{1}{\omega_{k}^{2}-\Omega^{2}}, \tag{24.10}$$

so that Eq. (24.8) becomes $I\left(\Omega^2\right) = 0$. We find that

$$I(\Omega^{2})\to\infty\ \text{ as }\ \Omega^{2}\to-\infty\ \text{ and }\ I(0)=\omega_{0}^{2}-\delta\omega^{2}<0,$$

in the interval $(-\infty, 0]$. As $I\left(\Omega^2\right)$ is a monotonically decreasing function in this interval, we conclude that $I\left(\Omega^2\right) = 0$ has a single negative solution in this case. This means that there is a mode whose amplitude grows or decays exponentially, so that no stationary configuration is allowed. Nevertheless, it should be remarked

that in a different context, it is precisely this runaway solution that is related to the existence of a bound state in the Lee–Friedrichs model [392]. This solution is considered in the framework of a model to describe qualitatively the existence of bound states in particle physics.

Considering the situation where all normal modes are harmonic, which corresponds to the first case above, $\omega_0^2 > \delta\omega^2$, we define the *renormalized* frequency

$$\bar{\omega}^2 = \omega_0^2 - \delta\omega^2 = \lim_{N\to\infty}(\omega_0^2 - N\eta^2), \tag{24.11}$$

Then Eq. (24.8) in the limit $N \to \infty$ becomes,

$$\bar{\omega}^2 - \Omega^2 = \eta^2 \sum_{k=1}^{\infty} \frac{\Omega^2}{\omega_k^2 - \Omega^2}. \tag{24.12}$$

In this limit, the above procedure is exactly the analog of the mass renormalization in quantum field theory: the addition of a counterterm $-\delta\omega^2 q_0^2$ allows one to compensate the infinite component in ω_0^2 in such a way as to leave a finite, physically meaningful renormalized frequency $\bar{\omega}$. This simple renormalization scheme has been introduced earlier [394]. Unless explicitly stated, the limit $N \to \infty$ is understood in the following.

Let us define a constant g, with dimension of frequency, by

$$g = \frac{\eta^2}{2\Delta\omega}, \tag{24.13}$$

where $\Delta\omega = \pi c/R$. The environment frequencies ω_k are given by,

$$\omega_k = k\frac{\pi c}{R}, \quad k = 1, 2, \dots, \tag{24.14}$$

where R is the radius of the cavity that contains the whole system. Then, using the identity

$$\sum_{k=1}^{\infty} \frac{1}{k^2 - u^2} = \frac{1}{2}\left[\frac{1}{u^2} - \frac{\pi}{u}\cot(\pi u)\right], \tag{24.15}$$

Eq. (24.12) is written in a closed form,

$$\cot\left(\frac{R\Omega}{c}\right) = \frac{\Omega}{\pi g} + \frac{c}{R\Omega}\left(1 - \frac{R\bar{\omega}^2}{\pi g c}\right). \tag{24.16}$$

The solutions of the above equation with respect to Ω give the spectrum of eigenfrequencies Ω_r corresponding to the collective normal modes.

In terms of the physically meaningful quantities Ω_r and $\bar{\omega}$, the transformation matrix elements turning the particle-field system to the principal axis are obtained. They are

$$\begin{aligned} t_0^r &= \frac{\eta\Omega_r}{\sqrt{(\Omega_r^2 - \bar{\omega}^2)^2 + \frac{\eta^2}{2}(3\Omega_r^2 - \bar{\omega}^2) + \pi^2 g^2 \Omega_r^2}}, \\ t_k^r &= \frac{\eta\omega_k}{\omega_k^2 - \Omega_r^2} t_0^r. \end{aligned} \tag{24.17}$$

These matrix elements play a central role in quantities describing the system.

24.2 The thermalization process in bare coordinates

We now consider the thermalization problem using bare coordinates . For the model described by Eq. (24.1), this problem was addressed in an alternative way in [393] with the canonical Liouville-von Neumann formalism. We consider the initial state described by the density operator,

$$\rho(t=0) = \rho_0 \otimes \rho_\beta \ , \tag{24.18}$$

where ρ_0 is the density operator of the particle, that in principle can be in a pure or in a mixed state and ρ_β is the density operator of the thermal bath, at a temperature β^{-1}, that is,

$$\rho_\beta = Z_\beta^{-1} \exp\left[-\beta \sum_{k=1}^{\infty} \omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right)\right] \ , \tag{24.19}$$

with $Z_\beta = \prod_{k=1}^{N} z_\beta^k$ being the partition function of the reservoir, and

$$z_\beta^k = \mathrm{Tr}_k \left[e^{-\beta\omega_k\left(a_k^\dagger a_k + 1/2\right)}\right] = \frac{1}{2\sinh\left(\frac{\beta_k\omega_k}{2}\right)} \, . \tag{24.20}$$

Creation and annihilation operators are given by

$$a_\mu = \sqrt{\frac{\bar{\omega}_\mu}{2}} q_\mu + \frac{i}{\sqrt{2\bar{\omega}_\mu}} p_\mu \tag{24.21}$$

$$a_\mu^\dagger = \sqrt{\frac{\bar{\omega}_\mu}{2}} q_\mu - \frac{i}{\sqrt{2\bar{\omega}_\mu}} p_\mu \ , \tag{24.22}$$

where $\bar{\omega}_\mu = (\bar{\omega}, \omega_k)$. The thermalization problem is addressed by investigating the time evolution of the state $\rho(t)$.

The thermalization problem concerns the time evolution of the initial state to thermal equilibrium. The subsystem corresponding to the particle oscillator is described by an arbitrary density operator ρ_0. As we will show, the expectation value of the number operator corresponding to particles will evolve in time to a value that is independent of the initial density operator ρ_0, the dependence will be exclusively on the mixed density operator corresponding to the thermal bath.

Our aim is to obtain expressions for the time evolution of the expectation values for the occupation number and in particular for the one corresponding to particles. We will solve the problem in the framework of the Heisenberg picture. It is to be understood that when a quantity appears without the time argument it means that such quantity is evaluated at $t = 0$. The Heisenberg equation of motion for the annihilation operator $a_\mu(t)$ is given by

$$\frac{\partial}{\partial t} a_\mu(t) = i\left[\hat{H}, a_\mu(t)\right] \ . \tag{24.23}$$

Due to the linear character of our problem, this equation is solved by writing $a_\mu(t)$ as

$$a_\mu(t) = \sum_{\nu=0}^{\infty} \left(\dot{B}_{\mu\nu}(t)\hat{q}_\nu + B_{\mu\nu}(t)\hat{p}_\nu \right) , \tag{24.24}$$

where all the time dependence is in the *c-number* functions $B_{\mu\nu}(t)$. Then, Eq. (24.23) reduces to the following coupled equations for $B_{\mu\nu}(t)$:

$$\ddot{B}_{\mu 0}(t) + \bar{\omega}^2 B_{\mu 0}(t) - \sum_{k=1}^{\infty} \eta\omega_k B_{\mu k}(t) = 0, \tag{24.25}$$

$$\ddot{B}_{\mu k}(t) + \omega_k^2 B_{\mu k}(t) - B_{\mu 0}(t) \sum_{k=1}^{\infty} \eta\omega_k = 0. \tag{24.26}$$

These equations are formally identical to the classical equations of motion, Eqs. (24.2) and (24.3), for bare coordinates q_μ. Then we decouple Eqs. (24.25) and (24.26) with the same matrix, $\{t_\mu^r\}$, that diagonalizes the Hamiltonian Eq. (24.1). In an analogous manner, we write $B_{\mu\nu}(t)$ as

$$B_{\mu\nu}(t) = \sum_{r=0}^{\infty} t_\nu^r C_\mu^r(t), \tag{24.27}$$

such that from Eqs. (24.25) and (24.26), we obtain the following equations for the normal-axis functions $C_\mu^r(t)$,

$$\ddot{C}_\mu^r(t) + \Omega_r^2 C_\mu^r(t) = 0, \tag{24.28}$$

which gives the solution

$$C_\mu^r(t) = a_\mu^r e^{i\Omega_r t} + b_\mu^r e^{-i\Omega_r t}.$$

Then substituting this expression into Eq. (24.27) we find

$$B_{\mu\nu}(t) = \sum_{r=0}^{\infty} t_\nu^r \left(a_\mu^r e^{i\Omega_r t} + b_\mu^r e^{-i\Omega_r t} \right) . \tag{24.29}$$

The time independent coefficients a_μ^r, b_μ^r are determined by the initial conditions at $t = 0$ for $B_{\mu\nu}(t)$ and $\dot{B}_{\mu\nu}(t)$. From Eqs. (24.21) and (24.24) we find that these initial conditions are given by

$$\begin{aligned} B_{\mu\nu} &= \frac{i\delta_{\mu\nu}}{\sqrt{2\bar{\omega}_\mu}}, \\ \dot{B}_{\mu\nu} &= \sqrt{\frac{\bar{\omega}_\mu}{2}}\delta_{\mu\nu} . \end{aligned} \tag{24.30}$$

Using these equations, we obtain for a_μ^r and b_μ^r,

$$a_\mu^r = \frac{it_\mu^r}{\sqrt{8\bar{\omega}_\mu}} \left(1 - \frac{\bar{\omega}_\mu}{\Omega_r} \right) , \tag{24.31}$$

$$b_\mu^r = \frac{it_\mu^r}{\sqrt{8\bar{\omega}_\mu}} \left(1 + \frac{\omega_\mu}{\Omega_r} \right) . \tag{24.32}$$

We write $a_\mu(t)$ and $a_\mu^\dagger(t)$ in terms of a_μ and $a_\mu^\dagger$ using Eqs. (24.21), (24.22) and (24.24),

$$a_\mu(t) = \sum_{\nu=0}^{\infty} \left(\alpha_{\mu\nu}(t)\hat{a}_\nu + \beta_{\mu\nu}(t)\hat{a}_\nu^\dagger\right) , \tag{24.33}$$

$$a_\mu^\dagger(t) = \sum_{\nu=0}^{\infty} \left(\beta_{\mu\nu}^*(t)\hat{a}_\nu + \alpha_{\mu\nu}^*(t)\hat{a}_\nu^\dagger\right) , \tag{24.34}$$

where $\alpha_{\mu\nu}(t)$ and $\beta_{\mu\nu}(t)$ are the Bogoliubov coefficients given by,

$$\alpha_{\mu\nu}(t) = \frac{1}{\sqrt{2\omega_\nu}}\dot{B}_{\mu\nu}(t) - i\sqrt{\frac{\omega_\nu}{2}}B_{\mu\nu}(t) \tag{24.35}$$

and

$$\beta_{\mu\nu}(t) = \frac{1}{\sqrt{2\omega_\nu}}\dot{B}_{\mu\nu}(t) + i\sqrt{\frac{\omega_\nu}{2}}B_{\mu\nu}(t) . \tag{24.36}$$

Using the definition of $B_{\mu\nu}(t)$ we get

$$\begin{aligned}\alpha_{\mu\nu}(t) = \sum_{r=0}^{\infty}\sqrt{\frac{\omega_\nu}{\omega_\mu}}\frac{t_\mu^r t_\nu^r}{4\Omega_r}\Big\{\frac{\Omega_r}{\omega_\nu}\left[(\omega_\mu-\Omega_r)e^{i\Omega_r t}+(\omega_\mu+\Omega_r)e^{-i\Omega_r t}\right] \\ +\left[(\Omega_r-\omega_\mu)e^{i\Omega_r t}+(\Omega_r+\omega_\mu)e^{-i\Omega_r t}\right]\Big\} ,\end{aligned} \tag{24.37}$$

and

$$\begin{aligned}\beta_{\mu\nu}(t) = \sum_{r=0}^{\infty}\sqrt{\frac{\omega_\nu}{\omega_\mu}}\frac{t_\mu^r t_\nu^r}{4\Omega_r}\Big\{\frac{\Omega_r}{\omega_\nu}\left[(\omega_\mu-\Omega_r)e^{i\Omega_r t}+(\omega_\mu+\Omega_r)e^{-i\Omega_r t}\right] \\ -\left[(\Omega_r-\omega_\mu)e^{i\Omega_r t}+(\Omega_r+\omega_\mu)e^{-i\Omega_r t}\right]\Big\} .\end{aligned} \tag{24.38}$$

Now we study the time evolution of $n_\mu(t)$, the expectation value of the number operator $N_\mu(t) = a_\mu^\dagger(t)a_\mu(t)$, that is,

$$n_\mu(t) = \mathrm{Tr}\left[a_\mu^\dagger(t)a_\mu(t)\rho_0\otimes\rho_\beta\right] . \tag{24.39}$$

Using the basis $|n_0, n_1, n_2, \cdots, n_N\rangle$ we obtain,

$$n_\mu(t) = \sum_{\nu=0}^{\infty}\left[|\alpha_{\mu\nu}(t)|^2 + |\beta_{\mu\nu}(t)|^2\right]n_\nu + \sum_{\nu=0}^{\infty}|\beta_{\mu\nu}(t)|^2 , \tag{24.40}$$

where

$$n_0 = \sum_{n=0}^{\infty} n\langle n|\rho_0|n\rangle \tag{24.41}$$

is the expectation value of the number operator corresponding to the particle and the set $\{n_k\}$ stands for the thermal expectation values corresponding to thermal bath oscillators, given by the Bose-Einstein distribution,

$$n_k = \frac{1}{e^{\beta\omega_k}-1} . \tag{24.42}$$

In Eq. (24.40) there appears a term that does not depend on the temperature of the thermal bath . This term has its origin in the instability of the initial bare vacuum state, $|0,0,\cdots,0\rangle$. To see this, we compute the expectation value of the time dependent number operator $N_\mu(t) = a^\dagger_\mu(t)a_\mu(t)$ in this vacuum state. Thus all the terms containing operators different from the identity give a zero contribution. The only term, that gives a non-zero contribution, arises from the normal ordering and is just the last one in Eq. (24.40). This term leads to the creation of excited states (particles, in a field theoretical language) from the initial unstable bare vacuum state.

We are interested in evaluating the expectation value of the number operator corresponding to particles. Thus taking $\mu = 0$ in Eq. (24.40) and using Eq. (24.42), we obtain

$$n_0(t) = \left[|\alpha_{00}(t)|^2 + |\beta_{00}(t)|^2\right] n_0 + \sum_{k=1}^{\infty} \left[|\alpha_{0k}(t)|^2 + |\beta_{0k}(t)|^2\right] \frac{1}{e^{\beta\omega_k} - 1}$$
$$+|\beta_{00}(t)|^2 + \sum_{k=1}^{\infty} |\beta_{0k}(t)|^2 \,, \tag{24.43}$$

where the coefficients of this expression are [393],

$$\alpha_{00}(t) = \frac{e^{-\pi g t/2}}{16\bar{\omega}\kappa}\left[(2\bar{\omega} + 2\kappa - i\pi g)^2\, e^{-i\kappa t} - (2\bar{\omega} - 2\kappa - i\pi g)^2\, e^{i\kappa t}\right] \,, \tag{24.44}$$

$$\beta_{00}(t) = \frac{\pi g e^{-\pi g t/2}}{8\bar{\omega}\kappa}\left[(\pi g + 2i\kappa)\, e^{-i\kappa t} - (\pi g - 2i\kappa)\, e^{i\kappa t}\right] \,, \tag{24.45}$$

$$\alpha_{0k}(t) = \sqrt{\frac{\omega_k}{2\bar{\omega}}}\frac{(\bar{\omega} + \omega_k)\sqrt{g\Delta\omega}\, e^{-i\omega_k t}}{(\omega_k^2 - \bar{\omega}^2 + i\pi g\omega_k)} + \sqrt{\frac{\omega_k}{\bar{\omega}}}\frac{\sqrt{2g\Delta\omega}}{4\kappa}$$
$$\times e^{-\pi g t/2}\left[\frac{(2\kappa + 2\bar{\omega} - i\pi g)}{(2\kappa - 2\omega_k - i\pi g)} e^{-i\kappa t} + \frac{(2\bar{\omega} - 2\kappa - i\pi g)}{(2\kappa + 2\omega_k + i\pi g)} e^{i\kappa t}\right] \tag{24.46}$$

and

$$\beta_{0k}(t) = \sqrt{\frac{\omega_k}{2\bar{\omega}}}\frac{(\omega_k - \bar{\omega})\sqrt{g\Delta\omega}\, e^{i\omega_k t}}{(\omega_k^2 - \bar{\omega}^2 - i\pi g\omega_k)} - \sqrt{\frac{\omega_k}{\bar{\omega}}}\frac{\sqrt{2g\Delta\omega}}{4\kappa}$$
$$\times e^{-\pi g t/2}\left[\frac{(2\bar{\omega} + 2\kappa - i\pi g)}{(2\kappa + 2\omega_k - i\pi g)} e^{-i\kappa t} + \frac{(2\bar{\omega} - 2\kappa - i\pi g)}{(2\kappa - 2\omega_k + i\pi g)} e^{i\kappa t}\right] \,, \tag{24.47}$$

such that

$$\kappa = \sqrt{\bar{\omega}^2 - \pi^2 g^2/4}. \tag{24.48}$$

The parameter κ measures the strenght of the interaction: if $\kappa^2 >> 0$, *i.e* $g << 2\bar{\omega}/\pi$, we are in the *weak* coupling regime. On the contrary if $\kappa^2 << 0$, i.e. $g >> 2\bar{\omega}/\pi$, the system is in the *strong* coupling regime. Here we will restrict ourselves to the weak coupling regime. This case includes the important class of electromagnetic interactions, $g = \alpha\bar{\omega}$, with α being the fine structure constant $\alpha = 1/137$ [388].

In the continuum limit $\Delta\omega \to 0$, sums over k become integrations over a continuous variable ω and we obtain for $n_0(t)$,

$$\begin{aligned} n_0(t) = & \frac{e^{-\pi g t}}{\bar{\omega}^2\kappa^2}\left[\bar{\omega}^4 + \frac{\pi^2 g^2}{8}\left(2\bar{\omega}^2 - \pi^2 g^2\right)\cos(2\kappa t) - \frac{\pi^3 g^3 \kappa}{4}\sin(2\kappa t)\right] n_0 \\ & + \frac{\pi^2 g^2 e^{-\pi g t}}{16\bar{\omega}^2\kappa^2}\left[2\bar{\omega}^2 + \left(2\bar{\omega}^2 - \pi^2 g^2\right)\cos(2\kappa t) - 2\pi g\kappa \sin(2\kappa t)\right] \\ & + \frac{g}{\bar{\omega}}\int_0^\infty d\omega \left[\frac{F(\omega,\bar{\omega},g,t)}{(e^{\beta\omega}-1)} + G(\omega,\bar{\omega},g,t)\right], \end{aligned} \tag{24.49}$$

where

$$\begin{aligned} F(\omega,\bar{\omega},g,t) = & \frac{\omega(\omega^2+\bar{\omega}^2)}{[(\omega^2-\bar{\omega}^2)^2+\pi^2 g^2\omega^2]}\left\{1 + \frac{e^{-\pi g t}}{4\kappa^2}[4\bar{\omega}^2 - \pi^2 g^2\cos(2\kappa t)\right. \\ & -2\pi g\kappa\frac{(\omega^2-\bar{\omega}^2)}{(\omega^2+\bar{\omega}^2)}\sin(2\kappa t)] - \frac{e^{-\pi g t/2}}{\kappa}[2\kappa\cos(\omega t)\cos(\kappa t) \\ & \left. + \frac{4\omega\bar{\omega}^2}{(\omega^2+\bar{\omega}^2)}\sin(\omega t)\sin(\kappa t) - \pi g\frac{(\omega^2-\bar{\omega}^2)}{(\omega^2+\bar{\omega}^2)}\cos(\omega t)\sin(\kappa t)]\right\} \end{aligned} \tag{24.50}$$

and

$$\begin{aligned} G(\omega,\bar{\omega},g,t) = & \frac{\omega(\omega-\bar{\omega})^2}{[(\omega^2-\bar{\omega}^2)^2+\pi^2 g^2\omega^2]}\left\{1 + \frac{e^{-\pi g t}}{4\kappa^2}\left[4\bar{\omega}^2 + \frac{2\pi^2 g^2\bar{\omega}\omega}{(\omega-\bar{\omega})^2}\right.\right. \\ & \left. -\pi^2 g^2\frac{(\omega^2+\bar{\omega}^2)}{(\omega-\bar{\omega})^2}\cos(2\kappa t) - 2\pi g\kappa\frac{(\omega+\bar{\omega})}{(\omega-\bar{\omega})}\sin(2\kappa t)\right] \\ & - \frac{e^{-\pi g t/2}}{\kappa}[2\kappa\cos(\omega t)\cos(\kappa t) - 2\bar{\omega}\sin(\omega t)\sin(\kappa t) \\ & \left. -\pi g\frac{(\omega+\bar{\omega})}{(\omega-\bar{\omega})}\cos(\omega t)\sin(\kappa t)]\right\}. \end{aligned} \tag{24.51}$$

It is to be noted that the second and the third lines in Eq. (24.49) are independent of the initial distributions. Also the integral on $G(\omega,\bar{\omega},g,t)$ in the third line of Eq. (24.49) is logarithmically divergent. We can understand the origin of this divergence in the following way: suppose that initially, in the absence of the linear interaction, we prepare the system in its ground state, that is, at $t = 0$ we have $|0,0,\cdots,0\rangle$. Then, we can compute, in the Heisenberg picture, the time evolution for the expectation value of the number operator corresponding to the particle, that is $\langle 0,0,\cdots,0|\hat{a}_0^\dagger(t)\hat{a}_0(t)|0,0,\cdots,0\rangle$, takes the value,

$$\langle 0,0,\cdots,0|\hat{a}_0^\dagger(t)\hat{a}_0(t)|0,0,\cdots,0\rangle = |\beta_{00}(t)|^2 + \sum_{k=1}^{\infty}|\beta_{0k}(t)|^2\,, \tag{24.52}$$

which in the continuum limit gives the second line of Eq. (24.49). Then, the origin of the divergence appearing in Eq. (24.49) is interpreted as the excitations produced from the unstable bare (vacuum) ground state, as a response to the linear interaction.

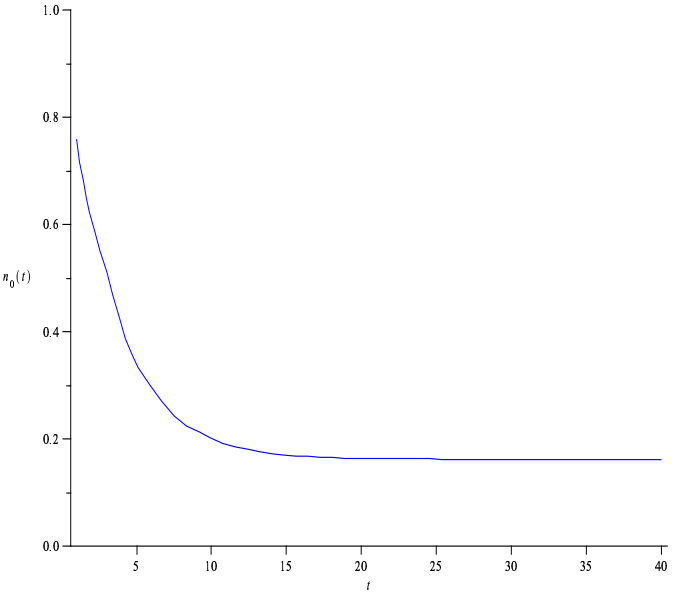


Fig. 24.1 Time behavior for $\bar{n}_0(t)$ given by Eq. (24.53) for $(t > 1)$, $n_0 = 1$, $\bar{\omega} = 1$, $\beta = 2$ and $g = 0.1$.

As we are interested in the thermal behavior of $n_0(t)$ only, the second line and the term $G(\omega, \bar{\omega}, g, t)$ in the third line of Eq. (24.49) can be neglected. This is a renormalization procedure. Thus we write the following *renormalized* expectation value for the particle number operator,

$$\bar{n}_0(t) = K(\bar{\omega}, g, t) n_0 + \frac{g}{\bar{\omega}} \int_0^\infty d\omega \frac{F(\omega, \bar{\omega}, g, t)}{(e^{\beta\omega} - 1)} \tag{24.53}$$

where

$$K(\bar{\omega}, g, t) = \frac{e^{-\pi g t}}{\bar{\omega}^2 \kappa^2} \left[\bar{\omega}^4 + \frac{\pi^2 g^2}{8} \left(2\bar{\omega}^2 - \pi^2 g^2 \right) \cos(2\kappa t) - \frac{\pi^3 g^3 \kappa}{4} \sin(2\kappa t) \right] . \tag{24.54}$$

In the limit $t \to \infty$, $\bar{n}_0(t)$ has a well-defined value, that is, the system reaches a final equilibrium state. Also, since $K(\bar{\omega}, g, t \to \infty) \to 0$, this final equilibrium state is independent of n_0. The equilibrium expectation value of the number operator corresponding to the particle is independent of its initial value, and the only dependence is on the initial distribution of the thermal bath, that is, the particle thermalizes with the environment. Before the interaction enters into play for $t < 0$, $n(t < 0) = n_0$, then we have that $K(\omega, \bar{\omega}, g, t < 0) = 1$. Taking $t = 0$ in Eq. (24.54) we obtain $K(\omega, \bar{\omega}, g, t = 0) = \bar{\omega}^2/\kappa^2 + \pi^2 g^2 (2\bar{\omega}^2 - \pi^2 g^2)/(8\bar{\omega}^2 \kappa^2)$. Thus $K(\omega, \bar{\omega}, g, t)$ is a discontinuous function of t; the discontinuity appearing just at $t = 0$. From the physical standpoint this discontinuity can be viewed as a response to the sudden onset of the interaction between particles and the environment.

Although the integral in Eq. (24.53) cannot be computed analytically, we can perform numerical calculations. We display in Fig. 1.1 the time behavior for $n_0 = 1$, $\bar{\omega} = 1$, $\beta = 2$ and $g = 0.1$; $(t > 1)$. In the next section we develop an alternative approach based on the notion of dressed particles. We will find that, in this new realm, no renormalization is needed.

24.3 Dressed coordinates and dressed states

Let us start with the eigenstates of our system, $|n_0, n_1, n_2...\rangle$, represented by the normalized eigenfunctions in terms of the normal coordinates $\{Q_r\}$,

$$\phi_{n_0 n_1 n_2 ...}(Q,t) = \prod_s \left[\sqrt{\frac{2^{n_s}}{n_s!}} H_{n_s}\left(\sqrt{\frac{\Omega_s}{\hbar}} Q_s \right) \right] \Gamma_0 e^{-i\sum_s n_s \Omega_s t}, \tag{24.55}$$

where H_{n_s} stands for the n_s-th Hermite polynomial and Γ_0 is the normalized vacuum eigenfunction,

$$\Gamma_0 = \mathcal{N} e^{-\frac{1}{2}\sum_{r=0}^{\infty} \Omega_r^2 Q_r^2}. \tag{24.56}$$

We introduce *dressed* or *renormalized* coordinates q_0' and $\{q_i'\}$ for, respectively, the *dressed* particle and the *dressed* field, defined by,

$$\sqrt{\bar{\omega}_\mu} q'_\mu = \sum_r t_\mu^r \sqrt{\Omega_r} Q_r, \tag{24.57}$$

valid for arbitrary R and $\bar{\omega}_\mu = \{\bar{\omega},\ \omega_i\}$. In terms of dressed coordinates, we define for a fixed instant, $t = 0$, *dressed* states , $|\kappa_0, \kappa_1, \kappa_2...\rangle$ by means of the complete orthonormal set of functions

$$\psi_{\kappa_0 \kappa_1 ...}(q') = \prod_\mu \left[\sqrt{\frac{2^{\kappa_\mu}}{\kappa_\mu!}} H_{\kappa_\mu}\left(\sqrt{\frac{\bar{\omega}_\mu}{\hbar}} q'_\mu \right) \right] \Gamma_0, \tag{24.58}$$

where $q'_\mu = \{q_0', q_i'\}$, $\bar{\omega}_\mu = \{\bar{\omega}, \omega_i\}$. Notice that the ground state Γ_0 in the above equation is the same as in Eq.(24.55). The invariance of the ground state is due to our definition of dressed coordinates given by Eq. (24.57). Each function $\psi_{\kappa_0 \kappa_1 ...}(q')$ describes a state in which the dressed oscillator q'_μ is in its κ_μ-th excited state.

It is worthwhile to note that our renormalized coordinates are new objects, different from both the bare coordinates, q, and the normal coordinates Q. In particular, the renormalized coordinates and dressed states, although both are collective objects, should not be confused with the normal coordinates Q, and the eigenstates Eq. (24.55). While the eigenstates ϕ are stable, the dressed states ψ are all unstable, except for the ground state obtained by setting $\{\kappa_\mu = 0\}$ in Eq. (24.58). The idea is that dressed states are physically meaningful states. This can be seen as an analog of the wave function renormalization in quantum field theory, which justifies the denomination of *renormalized* to the new coordinates q'. Thus, the dressed state given by Eq. (24.58) describes the particle in its κ_0-th excited level and each mode

k of the cavity in the $\kappa_k - th$ excited level. It should be noticed that the introduction of the renormalized coordinates guarantees the stability of the dressed vacuum state , since by definition it is identical to the ground state of the system. The fact that the definition given by Eq. (24.57) assures this requirement can be easily seen by replacing Eq. (24.57) in Eq. (24.58). We obtain $\Gamma_0(q') \propto \Gamma_0(Q)$, which shows that the dressed vacuum state given by Eq. (24.58) is the same ground state of the interacting Hamiltonian given by Eq. (24.5).

The necessity of introducing renormalized coordinates can be understood by considering what would happen if we write Eq. (24.58) in terms of the bare coordinates q_μ. In the absence of interaction, the bare states are stable since they are eigenfuntions of the free Hamiltonian. But when we consider the interaction they all become unstable. The excited states are unstable, since we know this from experiment. On the other hand, we also know from experiment that the particle in its ground state is stable, in contradiction with what our simplified model for the system describes in terms of the bare coordinates. So, if we wish to have a nonperturbative approach in terms of our simplified model something should be modified in order to remedy this problem. The solution is just the introduction of the renormalized coordinates q'_μ as the physically meaningful ones.

In terms of bare coordinates, the dressed coordinates are expressed as

$$q'_\mu = \sum_\nu \alpha_{\mu\nu} q_\nu, \tag{24.59}$$

where

$$\alpha_{\mu\nu} = \frac{1}{\sqrt{\bar{\omega}_\mu}} \sum_r t^r_\mu t^r_\nu \sqrt{\Omega_r}. \tag{24.60}$$

If we consider an arbitrarily large cavity ($R \to \infty$), the dressed coordinates reduce to

$$q'_0 = A_{00}(\bar{\omega}, g) q_0, \tag{24.61}$$

$$q'_i = q_i, \tag{24.62}$$

with $A_{00}(\bar{\omega}, g)$ given by,

$$A_{00}(\bar{\omega}, g) = \frac{1}{\sqrt{\bar{\omega}}} \int_0^\infty \frac{2g\Omega^2\sqrt{\Omega} d\Omega}{(\Omega^2 - \bar{\omega}^2)^2 + \pi^2 g^2 \Omega^2}. \tag{24.63}$$

In other words, in the limit $R \to \infty$, the particle is still dressed by the field, while for the field there remain bare modes.

Let us consider a particular dressed state $|\Gamma^\mu_1(0)\rangle$, represented by the wavefunction $\psi_{00\cdots 1(\mu)0\cdots}(q')$. It describes the configuration in which only the dressed oscillator q'_μ is in the *first* excited level. Then the following expression for its time evolution is valid [387]:

$$|\Gamma^\mu_1(t)\rangle = \sum_\nu f^{\mu\nu}(t) \, |\Gamma^\nu_1(0)\rangle$$

$$f^{\mu\nu}(t) = \sum_s t^s_\mu t^s_\nu e^{-i\Omega_s t}. \tag{24.64}$$

Moreover we find that

$$\sum_{\nu} |f^{\mu\nu}(t)|^2 = 1\,. \tag{24.65}$$

Then the coefficients $f^{\mu\nu}(t)$ are simply interpreted as probability amplitudes.

In approaching the thermalization process in this framework, we have to write the initial physical state in terms of dressed coordinates, or equivalently in terms of dressed annihilation and creation operators a'_μ and $a'^{\dagger}_\mu$ instead of a_μ and $a^{\dagger}_\mu$. This means that the initial dressed density operator corresponding to the thermal bath is given by

$$\rho_\beta = Z_\beta^{-1} \exp\left[-\beta \sum_{k=1}^{\infty} \omega_k \left(a'^{\dagger}_k a'_k + \frac{1}{2}\right)\right], \tag{24.66}$$

where we define

$$a'_\mu = \sqrt{\frac{\bar{\omega}_\mu}{2}} q'_\mu + \frac{i}{\sqrt{2\bar{\omega}_\mu}} p'_\mu \tag{24.67}$$

$$a'^{\dagger}_\mu = \sqrt{\frac{\bar{\omega}_\mu}{2}} q'_\mu - \frac{i}{\sqrt{2\bar{\omega}_\mu}} p'_\mu\,. \tag{24.68}$$

Now we analyze the time evolution of dressed coordinates.

24.4 Thermal behavior for a cavity of arbitrary size with dressed coordinates

The solution for the time-dependent annihilation and creation dressed operators follows similar steps as for bare operators. The time evolution of the annihilation operator is given by,

$$\frac{d}{dt} a'_\mu(t) = i\left[\hat{H}, a'_\mu(t)\right] \tag{24.69}$$

and a similar equation for $a'^{\dagger}_\mu(t)$. We solve this equation with the initial condition at $t = 0$,

$$a'_\mu(0) = \sqrt{\frac{\omega_\mu}{2}} q'_\mu + \frac{i}{\sqrt{2\omega_\mu}} p'_\mu\,, \tag{24.70}$$

which, in terms of bare coordinates, becomes

$$a'_\mu(0) = \sum_{r,\nu=0}^{N} \left(\sqrt{\frac{\Omega_r}{2}} t^r_\mu t^r_\nu \hat{q}_\nu + \frac{i t^r_\mu t^r_\nu}{\sqrt{2\Omega_r}} \hat{p}_\nu\right)\,. \tag{24.71}$$

We assume a solution for $a'_\mu(t)$ of the type

$$a'_\mu(t) = \sum_{\nu=0}^{\infty} \left(\dot{B}'_{\mu\nu}(t)\hat{q}_\nu + B'_{\mu\nu}(t)\hat{p}_\nu\right)\,. \tag{24.72}$$

Using Eq.(24.1) we find

$$B'_{\mu\nu}(t) = \sum_{r=0}^{\infty} t_\nu^r \left(a_\mu'^r e^{i\Omega_r t} + b_\mu'^r e^{-i\Omega_r t} \right) \ . \tag{24.73}$$

In the present case the time independent coefficients are different from those in the bare coordinate approach, Eq. (24.29). The initial conditions for $B'_{\mu\nu}(t)$ and $\dot{B}'_{\mu\nu}(t)$ are obtained by setting $t = 0$ in Eq. (24.72) and comparing with Eq. (24.71); Then

$$B'_{\mu\nu}(0) = i \sum_{r=0}^{\infty} \frac{t_\mu^r t_\nu^r}{\sqrt{2\Omega_r}} \ , \tag{24.74}$$

$$\dot{B}'_{\mu\nu}(0) = \sum_{r=0}^{\infty} \sqrt{\frac{\Omega_r}{2}} t_\mu^r t_\nu^r \ . \tag{24.75}$$

Using these initial conditions and the orthonormality of the matrix $\{t_\mu^r\}$ we obtain $a_\mu'^r = 0$, $b_\mu'^r = i t_\mu^r / \sqrt{2\Omega_r}$. Replacing these values for $a_\mu'^r$ and $b_\mu'^r$ in Eq. (24.73) we get

$$B'_{\mu\nu}(t) = i \sum_{r=0}^{\infty} \frac{t_\mu^r t_\nu^r}{\sqrt{2\Omega_r}} e^{-i\Omega_r t} \ . \tag{24.76}$$

We have

$$\begin{aligned} a'_\mu(t) &= \sum_{r,\nu=0}^{N} t_\mu^r t_\nu^r \left(\sqrt{\frac{\Omega_r}{2}} \hat{q}_\nu + \frac{i}{\sqrt{2\Omega_r}} \hat{p}_\nu \right) e^{-i\Omega_r t} \\ &= \sum_{r,\nu=0}^{N} t_\mu^r t_\nu^r \left(\sqrt{\frac{\omega_\nu}{2}} \hat{q}'_\nu + \frac{i}{\sqrt{2\omega_\nu}} \hat{p}'_\nu \right) e^{-i\Omega_r t} = \sum_{\nu=0}^{\infty} f_{\mu\nu}(t) \hat{a}'_\nu \ , \end{aligned} \tag{24.77}$$

where

$$f_{\mu\nu}(t) = \sum_{r=0}^{\infty} t_\mu^r t_\nu^r e^{-i\Omega_r t} \ . \tag{24.78}$$

For the occupation number $n'_\mu(t) = \langle a_\mu'^\dagger(t) a'_\mu(t) \rangle$ we get

$$n'_\mu(t) = \mathrm{Tr} \left(a_\mu'^\dagger(t) a'_\mu(t) \rho'_0 \otimes \rho'_\beta \right) \ . \tag{24.79}$$

where ρ'_0 is the density operator for the dressed particle and ρ'_β is the density operator for the thermal bath, which coincides with the corresponding operator for the bare thermal bath if the system is in free space (in the sense of an arbitrarily large cavity)[387, 388].

To evaluate $n'_\mu(t)$ we choose the basis $|n_0, n_1, \cdots, n_N\rangle = \prod_{\mu=0}^{\infty} |n_\mu\rangle$, where $|n_\mu\rangle$ are eigenvectors of the number operators $a_\mu'^\dagger a'_\mu$. From Eq. (24.77) we get

$$\begin{aligned} a_\mu'^\dagger(t) a'_\mu(t) &= \sum_{\nu,\rho=0}^{\infty} f^*_{\mu\rho}(t) f_{\mu\nu}(t) \hat{a}_\rho'^\dagger \hat{a}'_\nu \\ &= \sum_{\nu=0}^{\infty} |f_{\mu\nu}(t)|^2 \hat{a}_\nu'^\dagger \hat{a}'_\nu + \sum_{\nu \neq \rho} f^*_{\mu\rho}(t) f_{\mu\nu}(t) \hat{a}_\nu'^\dagger \hat{a}'_\rho \ . \end{aligned} \tag{24.80}$$

Then we obtain

$$n'_\mu(t) = |f_{\mu 0}(t)|^2 n'_0 + \sum_{k=1}^{\infty} |f_{\mu k}(t)|^2 n'_k \ , \tag{24.81}$$

where n'_0 and n'_k are the expectation values of the initial number operators, respectively, for the dressed particle and dressed bath modes. We assume that, dressed field modes obey a Bose-Einstein distribution. This can be justified by remembering that in the free space limit, $R \to \infty$, dressed field modes are identical to the bare ones, according to Eqs. (24.61) and (24.62). Now, no term independent of the temperature appears in the thermal bath. This should be expected since the dressed vacuum is stable, particle production from the vacuum is not possible. Setting $\mu = 0$ in Eq. (24.81) we obtain the time evolution for the occupation number of the particle,

$$n'_0(t) = |f_{00}(t)|^2 n'_0 + \sum_{k=1}^{\infty} |f_{0k}(t)|^2 n'_k \ . \tag{24.82}$$

24.5 The limit of arbitrarily large cavity: unbounded space

In a large cavity (free space) we must compute the quantities $f_{00}(t)$ and $f_{0k}(t)$ in the continuum limit to study the time evolution of the occupation number for the particle.Remember that in Eqs. (24.17), $\omega_k = k\pi c/R$, $k = 1, 2, ...$ and $\eta = \sqrt{2g\Delta\omega}$, with $\Delta\omega = (\omega_{i+1} - \omega_i) = \pi c/R$. When $R \to \infty$, we have $\Delta\omega \to 0$ and $\Delta\Omega \to 0$ and then, the sum in Eq. (24.78) becomes an integral. To calculate quantities $f_{\mu\nu}(t)$ we first note that, in the continuum limit, Eq. (24.17) becomes

$$t_0^r \to t_0^\Omega \sqrt{\Delta\Omega} \equiv \lim_{\Delta\Omega \to 0} \frac{\Omega\sqrt{2g\Delta\Omega}}{\sqrt{(\Omega^2 - \bar{\omega}^2)^2 + \pi^2 g^2 \Omega^2}}, \tag{24.83}$$

$$t_k^r \to \frac{\omega\sqrt{2g\Delta\omega}}{\omega^2 - \Omega^2} t_0^\Omega \sqrt{\Delta\Omega}. \tag{24.84}$$

In the following, we suppress the labels in the frequencies, since they are continuous quantities.

We start by defining a function $W(z)$,

$$W(z) = z^2 - \bar{\omega}^2 + \sum_{k=1}^{\infty} \frac{\eta^2 z^2}{\omega_k^2 - z^2} \ . \tag{24.85}$$

We find that the Ω's are the roots of $W(z)$. Using $\eta^2 = 2g\Delta\omega$, we have in the continuum limit,

$$W(z) = z^2 - \bar{\omega}^2 + 2gz^2 \int_0^\infty \frac{d\omega}{\omega^2 - z^2} \ . \tag{24.86}$$

For complex values of z the above integral is well defined and is evaluated by using Cauchy theorem, to be

$$W(z) = \begin{cases} z^2 + ig\pi z - \bar{\omega}^2, \ \mathrm{Im}(z) > 0 \\ z^2 - ig\pi z - \bar{\omega}^2, \ \mathrm{Im} < 0 \ . \end{cases} \tag{24.87}$$

We now compute $f_{00}(t) = \sum_{r=0}^{\infty}(t_0^r)^2 e^{-i\Omega_r t}$ which, in the continuum limit, is given by

$$f_{00}(t) = \int_0^\infty (t_0^\Omega)^2 e^{-i\Omega t}\, d\Omega\ . \tag{24.88}$$

We find that,

$$(t_0^\Omega)^2 = \frac{1}{W(\Omega)}\ , \tag{24.89}$$

and since the Ω's are the roots of $W(z)$, we write Eq. (24.88) as

$$f_{00}(t) = \frac{1}{i\pi}\oint_C \frac{dz e^{-izt}}{W(z)}\ , \tag{24.90}$$

where C is a counterclockwise contour in the z-plane that encircles the real positive roots of $W(z)$. Choosing a contour infinitesimally close to the positive real axis, that is $z = \alpha - i\epsilon$ below it and $z = \alpha + i\epsilon$ above it with $\alpha > 0$ and $\epsilon \to 0^+$, we obtain

$$f_{00}(t) = \frac{1}{i\pi}\int_0^\infty d\alpha\alpha e^{-i\alpha t}\left[\frac{1}{W(\alpha - i\epsilon)} - \frac{1}{W(\alpha + i\epsilon)}\right]\ . \tag{24.91}$$

In the limit $\epsilon \to 0^+$, Eq. (24.87) gives $W(\alpha \pm i\epsilon) = \alpha^2 - \bar{\omega}^2 \pm ig\pi\alpha$ which leads to

$$f_{00}(t) = C_1(t;\bar{\omega},g) + iS_1(t;\bar{\omega},g), \tag{24.92}$$

where

$$C_1(t;\bar{\omega},g) = 2g\int_0^\infty d\alpha \frac{\alpha^2\cos(\alpha t)}{(\alpha^2-\bar{\omega}^2)^2 + \pi^2 g^2\alpha^2}, \tag{24.93}$$

$$S_1(t;\bar{\omega},g) = -2g\int_0^\infty d\alpha \frac{\alpha^2\sin(\alpha t)}{(\alpha^2-\bar{\omega}^2)^2 + \pi^2 g^2\alpha^2}. \tag{24.94}$$

Notice that $C_1(t=0;\bar{\omega},g) = 1$ and $S_1(t=0;\bar{\omega},g) = 0$, so that $f_{00}(t=0) = 1$ as expected from the orthonormality of the matrix (t_μ^r). The real part of $f_{00}(t)$ is calculated using the residue theorem. For $\kappa^2 = \bar{\omega}^2 - \pi^2 g^2/4 > 0$, which includes the weak coupling regime, one finds

$$C_1(t;\bar{\omega},g) = e^{-\pi g t/2}\left[\cos(\kappa t) - \frac{\pi g}{2\kappa}\sin(\kappa t)\right] \quad (\kappa^2 > 0). \tag{24.95}$$

Although $S_1(t;\bar{\omega},g)$ cannot be analytically evaluated for all t, however for long times, i.e. $t \gg 1/\bar{\omega}$, we have

$$S_1(t;\bar{\omega},g) \approx \frac{4g}{\bar{\omega}^4 t^3} \quad (t \gg \frac{1}{\bar{\omega}}). \tag{24.96}$$

Thus, we get for large t

$$|f_{00}(t)|^2 \approx e^{-\pi g t}\left[\cos(\kappa t) - \frac{\pi g}{2\kappa}\sin(\kappa t)\right]^2 + \frac{16g^2}{\bar{\omega}^8 t^6}. \tag{24.97}$$

Next we compute the quantity $f_{0k}(t) = \sum_{r=0}^{\infty} t_0^r t_k^r e^{-i\Omega_r t}$ in the continuum limit. It is

$$f_{0\omega}(t) = \eta\omega\int_0^\infty \frac{(t_0^\Omega)^2 e^{-i\Omega t}d\Omega}{(\omega^2-\Omega^2)} = \frac{\eta\omega}{i\pi}\oint_C \frac{z e^{-izt}}{(\omega^2 - z^2)W(z)}\ , \tag{24.98}$$

where $\eta = \sqrt{2g\Delta\omega}$. Taking the same contour as that used to calculate $f_{00}(t)$, we obtain

$$f_{0\omega}(t) = -\frac{\eta\omega}{i\pi}\int_0^\infty d\alpha \left[\frac{\alpha e^{-i\alpha t}}{W(\alpha - i\epsilon)[(\alpha - i\epsilon)^2 - \omega^2]} - \frac{\alpha e^{-i\alpha t}}{W(\alpha + i\epsilon)[(\alpha + i\epsilon)^2 - \omega^2]}\right]. \tag{24.99}$$

Thus, taking $\epsilon \to 0^+$, $f_{0\omega}(t)$ is written as

$$f_{0\omega}(t) = \omega\sqrt{\Delta\omega}\left[C_2(\omega, t; \bar{\omega}, g) + iS_2(\omega, t; \bar{\omega}, g)\right], \tag{24.100}$$

where

$$C_2(\omega, t; \bar{\omega}, g) = (2g)^{\frac{3}{2}}\int_0^\infty d\alpha \frac{\alpha^2\cos(\alpha t)}{(\omega^2 - \alpha^2)\left[(\alpha^2 - \bar{\omega}^2)^2 + \pi^2 g^2\alpha^2\right]}, \tag{24.101}$$

$$S_2(\omega, t; \bar{\omega}, g) = -(2g)^{\frac{3}{2}}\int_0^\infty d\alpha \frac{\alpha^2\sin(\alpha t)}{(\omega^2 - \alpha^2)\left[(\alpha^2 - \bar{\omega}^2)^2 + \pi^2 g^2\alpha^2\right]}. \tag{24.102}$$

Notice that the integrals defining the functions C_2 and S_2 are actually Cauchy principal values.

The function C_2 is calculated analytically using Cauchy theorem; we find

$$\begin{aligned} C_2(\omega, t; \bar{\omega}, g) = \sqrt{2g}\Bigg[e^{-\pi g t/2}\Bigg\{&\frac{\omega^2 - \bar{\omega}^2}{(\omega^2 - \bar{\omega}^2)^2 + \pi^2 g^2\omega^2}\cos\kappa t \\ &- \frac{\pi g}{2\kappa}\frac{\omega^2 + \bar{\omega}^2}{(\omega^2 - \bar{\omega}^2)^2 + \pi^2 g^2\omega^2}\sin\kappa t\Bigg\} \\ &+ \frac{\pi g\omega}{(\omega^2 - \bar{\omega}^2)^2 + \pi^2 g^2\omega^2}\sin\omega t\Bigg]. \end{aligned} \tag{24.103}$$

The function S_2 cannot be evaluated analytically for all t, it has to be calculated numerically. For long times, we have

$$S_2(t; \bar{\omega}, g) \approx \frac{4\sqrt{2}g\sqrt{g}}{\omega^2\bar{\omega}^4 t^3} \quad (t \gg \frac{1}{\bar{\omega}}). \tag{24.104}$$

In the continuum limit, we get the average of the particle occupation number,

$$\begin{aligned} n_0'(t) = &\left[C_1^2(t; \bar{\omega}, g) + S_1^2(t; \bar{\omega}, g)\right] N_0' \\ &+ \int_0^\infty d\omega\, \omega^2\left[C_2^2(\omega, t; \bar{\omega}, g) + S_2^2(\omega, t; \bar{\omega}, g)\right] N'(\omega), \end{aligned} \tag{24.105}$$

where $n'(\omega) = 1/(e^{\beta\omega} - 1)$ is the density of occupation of the environment modes, the functions C_1 and C_2 are given by Eqs. (24.95) and (24.103) while the functions S_1 and S_2 are given by the integrals Eqs. (24.94) and (24.102), respectively. In Fig. 24.2 we display the behavior of $n_0'(t)$ in time for $n_0 = 1$, $\bar{\omega} = 1$, $\beta = 2$ and $g = 0.1$.

In summary, we have considered a linearized version of a particle-environment system and we have carried out a nonperturbative treatment of the thermalization process [395]. We have adopted a physicist's point of view, in the sense that we have renounced an approach very close to the real behavior of a nonlinear system,

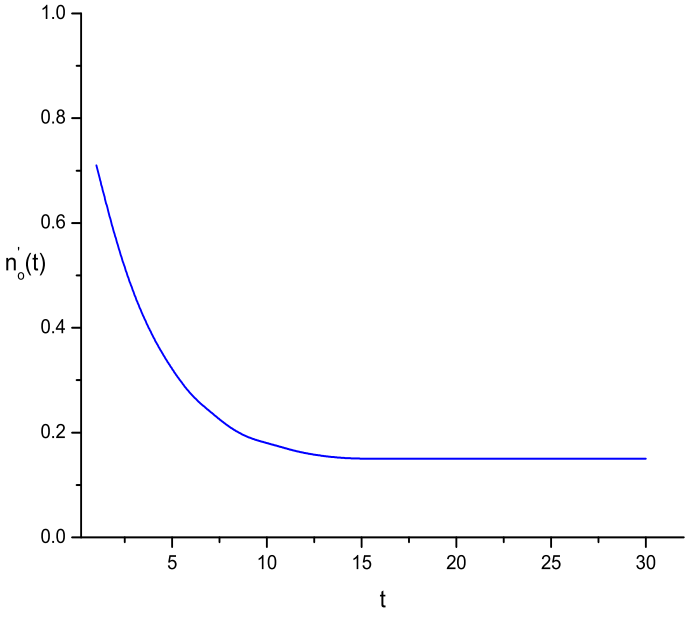


Fig. 24.2 Time behavior for $n_0'(t)$ given by Eq. (24.105), for $(t > 1)$, $n_0 = 1$, $\bar{\omega} = 1$, $\beta = 2$ and $g = 0.1$.

to study instead a linear model. As a counterpart, an exact solution has been possible. We have presented an ohmic quantum system consisting of a particle, in the larger sense of a material body, an atom or a Brownian particle coupled to an environment modelled by non-interacting oscillators. We have used the formalism of dressed states to perform a non-perturbative study of the time evolution of the system, contained in a cavity or in free space. Distinctly to what happens in the bare coordinate approach, in the dressed coordinate approach no renormalization procedure is needed. Our renormalized coordinates contain in them the renormalization aspects.

For weak (electromagnetic-type) coupling, this formalism could be used to study situations in plasma physics; in this case we would take the cavity radius R, as the average dimension of a tokomak device. The precise formulation of this problem could be the subject of further research work. For microscopic values of R, since the model also applies for strong coupling, the system can be seen as a simplified linear model for confined quarks and gluons inside a hadron. In this case all coordinates would be effectively dressed, in the sense that they are all collective, both field modes and the particle could not be separated in this language. Of course the normal coordinates are also collective, but they correspond to stable eigenstates, no change in time exists for them. If we ascribe physical meaning to our dressed coordinates and states, matter and gauge quanta inside hadrons, could not be individualized as quarks and gluons, instead we would have a kind of quarkgluon magma. Since

quarks and gluons are permanently confined, we could think that, in the context of our model, quarks and gluons should not really exist, they would be actually an artifact of perturbation theory. As far as the thermalization process is concerned from a formal viewpoint, both bare and dressed approaches are in agreement with what we expect for this process. Both curves in Fig. 24.1 and Fig. 24.2 approach steadily to an asymptotic value of the bare and dressed ocupation numbers of the particle. For long times, all the information about the particle occupation numbers depends only on the environment.

Epilogue

This book was planned to be a monograph that would bring the central ideas of symmetry in connection with thermal field theories and its applications to physical systems. We have accomplished this goal by putting forward the notion of thermo-algebra, that has its origin in the representations of Lie groups associated with kinematical symmetry based on a physical distinction among observables and generators of symmetry describing thermal systems. This procedure provides a clear idea about the connection among theories, such as the imaginary time approach of Matsubara, the analytical formalism in the complex plane of Schwinger and Keldysh, and the real time finite temperature (TFD) method due to Takahashi and Umezawa. The latter two methods require a duplication of the Hilbert space, either through a specific contour in the complex plane or as a fundamental *ansatz*. However, the representations of the Lie groups provide the proper connection between the three diverse approaches to the finite temperature quantum field theory.

An analysis of the Green function by Kubo, Martin and Schwinger had established a periodicity (anti-periodicity) condition for the case of bosons (fermions). This may be viewed as a statement on the compactified status for the time variable that is considered as the temperature in the Matsubara method. The notion of thermo-algebra suggested a generalization of this idea to space coordinates, thus leading to a description of quantum fields in compactified space and time. The representations of Lie groups lead directly to the Liouville-von Neumann equation for different fields and to the duplication of the Hilbert space. Since the temperature effects are introduced by a Bogoliubov transformation, this leads us immediately to generalize the Bogoliubov transformation to compactifying both time and space coordinates. Such an extension of these notions have physical implications. We have shown applications of the generalized Bogoliubov transformation to the Casimir effect, that is often considered for some compactified geometry since the effect decreases rapidly for large separations between the boundaries. This generalized notion is used to treat systems in a $(\mathbb{S}^1)^d \times \mathbb{R}^{D-d}$ topology. Further applications are in superconductivity in confined space regions.

There are domains not covered due to lack of space. After all we cannot pretend to cover completely such a large and growing field. In particular, several of these subjects are treated extensively in excellent books by Umezawa [72], Umezawa, Matsumoto and Tachiki [73], Kapusta [50], Le Bellac [51] and Das [52], among others. Only a brief space is devoted to considering problems in open systems, i.e. systems in nonequilibrium state. It is suggested that a combination of the Schrödinger approach and TFD may provide a viable alternative to studying open systems. Details of this need to be pursued. Other topics have not found a great deal of attention by us. Let us comment on some of these.

Phase transitions. Approaches to phase transition and beyond are not fully covered. Instead, we choose to examine the subject of phase transitions in confined systems, since it is a theme not yet very well explored. There are dynamical aspects that remain elusive to detailed analysis. This is true for systems in the laboratory as well as to the early evolution of the universe which cooled down very rapidly, such that the quark-gluon plasma reached a point to make a transition to hadrons. The quark-gluon plasma is believed to be formed in heavy ion collisions. However, the whole question of its formation and the hadronization is not yet really understood. This requires a full theory that will allow a microscopic understanding of the dynamical processes that are responsible for their behavior.

Galilean physics. The role of temperature in Galilean theories is not fully understood if dynamical processes have to be taken into account. For instance, how do condensed systems become liquid and vice versa? No doubt there are many books that deal with this topic, but no consistent dynamical theory for these transitions exists. Nuclear physics, as another example, is likely a system with Galilean symmetry. The presence and behavior of collective states, a consequence of spontaneous symmetry breaking as a function of temperature, would be an important feature in trying to understand the properties of excited nuclei and reaction processes. Can we find the answers within representations of the Galilei group? If so, a theory based on Galilean covariance [396, 397] at finite temperature might be needed to study these properties in detail. In classical contexts, as in stochastic lattices, there have been in the literature numerous methods enunciated in this book. In many cases, however, some developments have been carried in an *ad hoc* fashion. Hopefully, the present approach, addressing these problems from a symmetry point of view, would stimulate more coordinated activity in various different fields, providing a unifying feature that would give a sound basis for many of them.

Quantum optics. We have touched on the various possible states that may be useful to developments in quantum optics. However, the use in, for example, cryptography, encryption and teleportation have not been considered. Developments along these directions may provide further impetus to new ideas and notions in this fertile area of research, to treat the temperature effect, a central aspect in the experimental context.

Symmetry restoration at high temperature. It is believed that spontaneous symmetry breaking at low temperatures is restored as the temperature is raised to a critical point and beyond. At present, it is not known in detail how this happens and what is the behavior of systems as this is occurring, mainly in nonequilibrium situations. We have considered the problem, in part, by choosing to examine systems in compactified spaces that are not currently analyzed carefully.

We are rather hopeful that the ideas based on symmetry presented in this book would find a wider class of applications. We could envisage considering confined systems, where other type of topological confinement, other than the ones studied here, would be described by Bogoliubov transformations.

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