

Perturbative calculations in many-particle systems

by

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A Thesis submitted to the Faculty of Graduate Studies of

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Of

Doctor of Philosophy

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Final experimental achievement of Bose-Einstein condensation of trapped alkali atoms boosted a renewed interest in the properties of weakly interacting Bose gases. The low-temperature behavior of such systems has been established years ago and became a standard subject of numerous textbooks. However, attempts to consistently extend the treatment to finite-temperature domain are still rare. In order to bridge this gap, we developed an approach, which allows one to estimate the physical parameters of weakly interacting Bose gases from first principles. We show that our method captures all essential physics in the whole range of temperatures except of those close to the critical. The source of the latter drawback turns out to be common to all schemes which rely on perturbative expansions.

The issue can supposedly be dealt with by the use of the alternative framework, based on the n -particle irreducible effective action functional techniques. This approach attracts a lot of attention nowadays due to its unique resummation properties and its ability to deal with the non-equilibrium problems consistently. However, it is known to violate the gauge invariance when applied to high energy physics problems. We resolve the question by constructing a new modified effective theory, which not only preserves all the merits of the base formalism, but is also free from the gauge-dependence issues, thus making the entire approach internally consistent.

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Chapter 1

The weakly interacting Bose gas

Introduction

The Bose-Einstein condensation (BEC) phenomenon used to be a subject of purely theoretical studies for several decades, until it was experimentally realized by several independent groups in 1995 [1, 2, 3]. This achievement has also marked the beginning of a whole new area of research into the properties of atomic Bose condensates.

Although the experiments are carried out in magnetic and optical harmonic traps and deal with essentially non-homogenous gases, a much more elementary system, namely the homogeneous Bose gas, has also received renewed attention. First, because it is interesting in its own right. Second, because its simplicity allows one to gain some important insights, which carry over to the trapped case [4]. Thus, quite unexpectedly, the theory of the weakly interacting Bose-condensed gases has become a subject of intensive research efforts.

While the basics of the theory of BECs at ultralow temperatures have substantially been elaborated in the previous decades, very few studies, aimed to extend these developments to the finite-temperature domain, have been conducted.

A successful approach, intended to embrace such task, should possess several properties. It should be based on the most fundamental principles. It should be easily implementable, both analytically and computationally. It should be able to give consistent quantitative understanding of the thermodynamic properties of the weakly interacting Bose gases in a whole range of temperatures below critical.

Below we present an approach which, as we think, qualifies as the one.

Chapter 1 is organized as follows.

In sections 1.1 through 1.4 we introduce standard textbook results from quantum mechanics and statistical physics [5, 6, 7], which serve as elementary building blocks of further considerations. These include treatment of quantized motion of a particle in a box, computation of the corresponding number of quantum states, general properties of quantum distribution for an ideal gas consisting of particles, obeying Bose statistics, as well as the limiting case of this distribution, namely the Maxwell distribution, which describes a classical ideal gas.

In section 1.5 we discuss qualitative properties of Bose-Einstein statistics and its differences compared to the Maxwell-Boltzmann one.

In section 1.6 we review the thermodynamic properties of an ideal Bose gas at

temperatures below critical.

Section 1.7 presents the method of quantized fields, necessary for calculating the interaction corrections to the properties of ideal systems.

In section 1.8 the key concepts, underlying the BEC phenomenon, namely the order parameter, long-range order and spontaneous symmetry breaking are introduced and formulated in the field-theoretic language.

Thermodynamic properties and the nature of elementary excitations in the weakly-interacting Bose gas at zero temperature are developed in 1.9.

Section 1.10 is dedicated to the weakly interacting Bose gas at finite temperatures. We begin by introducing the basics of the thermo-field dynamics formalism (TFD) as a framework to treat the interacting quantum fields at nonzero temperatures. Then, with the use of this technique, we re-derive the famous Bogoliubov and the first order Popov approximations, as well as review other directions, which are being currently under active development.

In section 1.11 we formulate our approach to investigating the thermodynamic properties of dilute interacting Bose gases at finite temperatures below critical and discuss the results obtained.

1.1 Necessary results from classical and quantum mechanics

In the beginning of the 20th century it became obvious that classical concepts turn out to be inadequate for the study of the motion of atomic systems and that they must be replaced by the concepts of quantum theory. In order to analyze the changes which are introduced into statistical physics by the development, it is necessary to dwell on certain important results of quantum theory.

The following two propositions of quantum mechanics are of basic importance for statistical physics:

- (1) the existence of the discrete states of a system
- (2) the principle of identity of elementary particles

Let us now discuss both issues in more detail.

1.1.1 Quantized motion of a particle in a box

The problem of statistical physics is the investigation of the properties and behavior of macroscopic systems in a state of equilibrium on the basis of the known properties of the microparticles constituting them. It turns out that classical physics is unapplicable in the realm of atomic phenomena. Hence, the application of the laws of statistical physics to real systems is, in practice, impossible if one ties oneself to the classical concepts of the motion of atomic particles. In the following, we shall assume that atoms, molecules and other particles, forming macroscopic systems, move according to the laws of quantum mechanics.

The simplest quantum-mechanical system is a microparticle with mass m confined in a one-dimensional box with impenetrable walls. The motion of such a particle is restricted by the size of the box to the region $0 \leq x \leq a$, where the potential energy is equal to zero. At the limits of the region, at $x = 0$ and $x = a$, the potential energy of repulsion is infinitely large and the particle cannot go out of the box.

From the general propositions of quantum mechanics it follows that the energy and momentum of such a particle should have a discrete series of values. The allowed values of the energy and momentum are given by the formulae

$$p_n = \frac{nh}{2a}, \quad (1.1.1)$$

$$\varepsilon_n = \frac{p_n^2}{2m} = \frac{h^2 n^2}{8ma^2}. \quad (1.1.2)$$

Here h and n are the Planck constant and quantum number respectively.

Formula (1.1.1) shows that the energy levels of the particle form a discrete spectrum. The discreteness becomes apparent: 1) for small mass, 2) for motion of the particle in a small region, and 3) for small quantum numbers. On the contrary, for large masses, for motion in a large region, and for large quantum numbers the effects of quantization are relatively weak.

It turns out that the transition from quantum mechanics to classical mechanics can be made in two ways. First, simply by assuming $h = 0$. Thus, one disregards

all quantum effects – the existence of the wave properties of microparticles, the quantization of energy and other quantities, and so on. Second, by assuming, that h is small but nevertheless different from zero. It turns out that in this approximation the wave properties of particles are shown very weakly. Particles can be considered as moving along definite trajectories, as in classical mechanics. However, the quantization of states still arises in the fact that only some of the classical trajectories are possible. Such an approximation is called quasi-classical (as distinct from the classical approximation, in which the quantum properties of particles are not taken into account at all).

In order to see the nature of restrictions, we again turn to the example of a particle in one-dimensional box. We assume that use can be made of the concepts of classical mechanics and that the particle can be considered as a material point moving between reflecting walls. The phase diagram in Fig.1.1 shows the

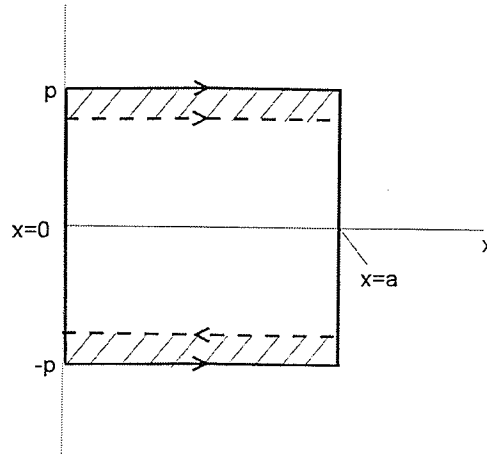


Figure 1.1: Quasiclassical phase space diagram. Shaded area corresponds to a single quantum state.

sequence of its states. We now take into account the quantization of states, and out of all possible states we choose only those, which satisfy the quantization condition (1.1.1). Not all states $p = \text{const}$ are possible, only those with separation, determined by the relation (1.1.1). Fig.1.1 shows the n th state (the solid line) and the $(n-1)$ th state (the dashed line). The number of possible quantum states with a momentum lying between $p_n = \frac{hn}{2a}$ and $p_n = \frac{h}{2a}$ is equal to n .

We now calculate the area S_n in the phase plane, corresponding to these n states. Obviously,

$$S_n = \oint p \, dx = 2p_n a = hn. \quad (1.1.3)$$

If the lines corresponding to other possible states are drawn, then the entire surface will be divided into cells. It is easily seen that the area of all the cells is the same and equal to h . Indeed, the distance between possible states along the p -axis is equal to

$$\frac{hn}{2a} - \frac{h(n-1)}{2a} = \frac{h}{2a}. \quad (1.1.4)$$

Then the area of a cell is $2(h/2a)a = h$.

Thus, in the quasi-classical approximation to each possible state there corresponds in phase space a cell of area h . The states, which are actually realized, are those, for which the condition

$$\oint p \, dx = nh \quad (1.1.5)$$

is fulfilled. This equality is called the Bohr condition.

The consideration demonstrated above is of general character. It can also be shown that the form of a cell is arbitrary.

It is illustrative to consider the motion of a free particle in a box with ideally reflecting walls, but now having three dimensions. For simplicity we assume that the box has a form of a cube with edge a . Since the motion in any of the three directions is independent and since all of the directions are in principle equivalent, we can write for each of the components of the momentum

$$p_x = \frac{hn_1}{2a}, \quad p_y = \frac{hn_2}{2a}, \quad p_z = \frac{hn_3}{2a}. \quad (1.1.6)$$

The motion of a particle in three dimensions is characterized by three quantum numbers n_1, n_2, n_3 , which can take on a number of integer values. The energy of the particle is equal to

$$\varepsilon = \frac{p_x^2 + p_y^2 + p_z^2}{2m} = \frac{h^2}{8ma^2}(n_1^2 + n_2^2 + n_3^2). \quad (1.1.7)$$

It is characterized by a number $n = \sqrt{n_1^2 + n_2^2 + n_3^2}$. However, given n , it does not depend on the values of the separate contributions n_1, n_2, n_3 , only on their overall sum. Because of this, several different quantum states can correspond to one and the same value of energy. For example, let $n_1 = 1, n_2 = 2, n_3 = 2$ and $n_1 = 2, n_2 = 1, n_3 = 2$. In both cases $n = 3$, so that both states have the same energy.

The number of states having the same energy is called the *degeneracy*, or *statistical weight*.

From now on, we define the following terminology to be used in subsequent development. We will say that the particle is in the quantum *state* (single-particle state, energy state), when its quantum numbers are explicitly specified. We will say that the particle is on an energy *level* ε , when it is in the state with energy ε , while the state itself (i.e. its quantum numbers) is not explicitly specified. By definition, the number of states, corresponding to an energy level, is the degeneracy of the level.

In the most general case of an arbitrary system having f degrees of freedom, it can be shown that in the transition to the quasi-classical approximation the motion of the system can be considered in the same way as in classical mechanics, but with a restriction imposed on the possible states: to each quantum state of a system with f degrees of freedom in the quasi-classical approximation there corresponds a cell in its phase space having a volume h^f .

1.1.2 Number of quantum states

It is an important task to calculate the number of quantum states corresponding to a given energy level. In quasi-classical approximation, this number could be obtained by dividing by h^3 the volume of phase space, which is given by

$$\omega = \int' \int' dx dp, \quad (1.1.8)$$

where primes indicate that integrations are restricted by the conditions that: 1) the particle is confined in physical space of volume V , and 2) the energy of the particle is constant and equal to ε . Obviously, ω is equal to zero, since the energy hypersurface is a set of measure zero in the phase space.

However, it is physically clear that a completely isolated system is an idealization. Weak interactions with surrounding and measurements inevitably lead to a small but finite widening of the energy level. Therefore, we will calculate the number of quantum states corresponding to the energy of a system, lying in a given interval between ε and $\varepsilon + \delta\varepsilon$. We shall denote it by $\Omega(\varepsilon)\delta\varepsilon$.

In calculating the phase space volume we will make use of the fact that in the quasi-classical approximation quantum jumps are small, and we will assume the momentum to vary almost continuously. The volume of the phase space, corresponding to an energy of the particle smaller than a given value ε , is

$$\Gamma = \int dx dy dz \int dp_x dp_y dp_z = 4\pi V \int_0^{\sqrt{2m\varepsilon}} p^2 dp = \frac{4\pi(2m)^{3/2}\varepsilon^{3/2}V}{3}. \quad (1.1.9)$$

Therefore, the volume of the phase space, corresponding to energies in the range between ε and $\varepsilon + \delta\varepsilon$, is

$$\Delta\Gamma = \frac{\partial\Gamma}{\partial\varepsilon}\delta\varepsilon = 4\pi mV\sqrt{2m\varepsilon} \delta\varepsilon. \quad (1.1.10)$$

Then the number of single-particle states with energies, which lie between ε and $\varepsilon + \delta\varepsilon$, is equal to

$$\Delta\Omega = \Omega(\varepsilon)\delta\varepsilon = \frac{1}{h^3} \frac{\partial\Gamma}{\partial\varepsilon} \delta\varepsilon = \frac{4\pi mV\sqrt{2m\varepsilon}}{h^3} \delta\varepsilon. \quad (1.1.11)$$

In what follows, we will call $\Omega(\varepsilon)$ the number of states with a given energy, or degeneracy.

1.2 The principle of identity of elementary particles

In the previous section we have taken into account the discreteness of quantum states and considered effects associated with it. However, up to now we have not treated the identity of microparticles properly.

In classical theory one considers two states, differing from each other only by a permutation of particles, as different ones. This way of calculating microstates, however, leads to incorrect values of thermodynamic parameters. In order to avoid

the problem, one divides the phase space by the number of possible permutations of particles. This division represents the simplest attempt of systematically taking into account the identity of underlying objects. It allows one to resolve the Gibbs' paradox and to obtain correct expressions for thermodynamic functions.

From another side, the inconsistency of this operation is obvious. Indeed, it still assumes that all particles are different from each other, so that one could, in principle, number them, ascribing a definite number or label to each.

Both experimental data and theory suggest, however, that the identity of quantum objects has a much more profound character. Their complete identity leads to the fact that the very attempt to number them loses any physical meaning. It makes no sense whatsoever to describe one of the particles as the first, another as the second, and so on. If one calls, for instance, the particle, which was initially in a definite state, the first particle, then at a subsequent moment it would already be impossible to assert that it is just that particle which is in this state, not a "different" one. Hence, it is necessary, from the very beginning, to renounce any attempt to distinguish between individual atomic objects.

We shall now explore, in which kind of physical restriction that results.

1.3 The Maxwell distribution

In order to make the differences between the classical and quantum considerations, introduced by the principle of identity, particularly striking, we will first consider the Maxwell distribution, which is the statistical distribution in a classical gas.

Assume that the molecules in a gas can be in the single-particle quantum *states* with the energies of translational motion $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_j, \dots$, listed in increasing order of the energy eigenvalue. For convenience of the treatment, we will assume that the latter form discrete spectrum. Also, each state above is listed separately, so that when degeneracy occurs, several successive ε_j 's will have the same value.

In the gas, there is a certain distribution of particles over states, such that in the first state there are n_1 particles, in the second state there are n_2 particles, and so on. Therefore, from the classical point of view, we have to describe the states of the system in the following way:

particles no. 1, 2, 3, ..., n_1 are in the state with energy ε_1 ,

particles no. $n_1 + 1$, ..., $n_1 + n_2$ are in the state with energy ε_2 ,

particles no. $n_1 + n_2 + 1$, ..., $n_1 + n_2 + n_3$ are in the state with energy ε_3 , and so on.

For further considerations, we need to choose a set of particles, which can be treated as a quasi-closed subsystem. It is convenient to regard as the one all the particles which are on a certain arbitrarily chosen quantum *level* with energy ε_k . Then the rest of the gas forms a reservoir.

This kind of choice is in complete agreement with those requirements, which must be satisfied by a quasi-closed subsystem. Indeed, in a result of collisions the particles possessing energy ε_k go over into other levels. Conversely, due to the same mechanism, other molecules, which earlier had an energy differing from ε_k and which belonged to the reservoir, can go into the level with energy ε_k . If the number of molecules, that are coming in or going out of the subsystem per unit time, is small compared to the number of particles in it, then it can be assumed that the

interaction between the subsystem and the reservoir is weak. This condition will be fulfilled, if the collisions between the particles occur sufficiently seldom, i.e. when the gas is substantially rarified.

In the process of interaction, the number of particles on the level with the given energy ε_k is changing. In this sense, the state of our subsystem varies. Its total energy is equal to

$$\varepsilon = \varepsilon_k n_{\varepsilon_k}, \quad (1.3.1)$$

where n_{ε_k} is the number of particles which are currently in the subsystem. Since ε_k is fixed, the quantity ε varies with n_{ε_k} and is completely determined by this number.

The great advantage of the subsystem thus constructed is that a complete characterization of its state is a relatively easy task. One has only to determine the mean number of particles, i.e. the mean number of particles on the energy level we have specified. For the calculation, use can be made of the general statistical mechanical formula

$$\bar{n}_{\varepsilon_k} = \frac{\sum_{n_{\varepsilon_k}} \sum_i n_{\varepsilon_k} \exp \left[\frac{\mu n_{\varepsilon_k} - \varepsilon_k n_{\varepsilon_k}}{kT} \right]}{\sum_{n_{\varepsilon_k}} \sum_i \exp \left[\frac{\mu n_{\varepsilon_k} - \varepsilon_k n_{\varepsilon_k}}{kT} \right]} = kT \frac{\partial}{\partial \mu} \ln \sum_{n_{\varepsilon_k}} \sum_i \exp \left[\frac{\mu n_{\varepsilon_k} - \varepsilon_k n_{\varepsilon_k}}{kT} \right] \quad (1.3.2)$$

which gives the mean number of particles in an open subsystem. Here k is the Boltzmann constant, T is the temperature of the subsystem, μ and ε_k are its chemical potential and energy, respectively. The first summation here is carried out over all possible values of the number of particles n_{ε_k} in the subsystem. The second summation is over all microstates i accessible to the subsystem with the given number of particles.

In order to actually perform the second summation, we have to seriously consider the way in which we take contributions from different microstates into account. In quasi-classical mechanics, where all particles can be numbered, the states of a system will always be degenerate, provided the system contains more than one particle of a given kind.

For example, let there be N molecules in the gas, n_1 of which are in a single-particle state with energy ε_1 , n_2 in state ε_2 , and so on. Then the microstate of the gas is determined by stating the single-particle states of each of them individually. Correspondingly, an interchange of two particles in different states leads to two distinct microstates of the entire gas. The total number of such permutations is, obviously,

$$\frac{N!}{n_1! n_2! \dots}$$

Of course, if an interchange takes place among the particles which are in the same single-particle state, then we do not regard the two resulting microstates as distinct. This is reflected by the denominator.

It turns out that considering states, differing only by a permutation of particles, as distinct ones, leads to incorrect expressions for the thermodynamic functions due to the overcounting of the microstates. The common recipe here, known as Gibbs' prescription, amounts to disregarding the details of the numbers n_i and

slashing the whole sequence of microstates by a common factor of $N!$. This is certainly correct in situations, in which all N particles happen to be in different energy states, but is certainly wrong in others.

Fortunately, actual gases under normal conditions satisfy such restrictions. For them, the expectation values of the single-particle occupation numbers n_i are much less than unity:

$$\langle n_i \rangle \ll 1. \quad (1.3.3)$$

In other words, the numbers n_i are generally 0, occasionally 1, and rarely greater than 1. This condition is also satisfied by the systems, which are at high enough temperatures (so that many more energy states become accessible) and have sufficiently low densities (so that there are not so many particles to accommodate).

Condition (1.3.3) in a way defines the classical limit and, simultaneously, the validity domain of the Gibbs prescription.

Let us now suppose that in our case the inequality (1.3.3) is well satisfied. Remembering that all particles of our subsystem have the same energy, we may rewrite expression (1.3.2) in the following form:

$$\begin{aligned} \bar{n}_{\varepsilon_k} = kT \frac{\partial}{\partial \mu} \ln \sum_{n_{\varepsilon_k}=0}^N \frac{1}{n_{\varepsilon_k}!} \\ \sum_{\{n_{\varepsilon_k i}\}} \frac{n_{\varepsilon_k}!}{n_{\varepsilon_k 1}! n_{\varepsilon_k 2}! \dots} \exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k 1}} \exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k 2}} \dots \end{aligned} \quad (1.3.4)$$

Here we have introduced the Gibbs' correction factor $1/n_{\varepsilon_k}!$ and grouped together all the terms which correspond to microstates differing only by particle positions exchange. Therefore, the second sum runs over the number of microstates $\{n_{\varepsilon_k i}\}$, which are different in this sense. Correspondingly, the value $n_{\varepsilon_k i}$ denotes the number of particles in a single-particle state i with energy ε_k .

This expression can be evaluated with the help of the multinomial theorem with the following result

$$\bar{n}_{\varepsilon_k} = kT \frac{\partial}{\partial \mu} \ln \sum_{n_{\varepsilon_k}=0}^N \frac{g_k^{n_{\varepsilon_k}}}{n_{\varepsilon_k}!} \exp \left[\frac{\mu n_{\varepsilon_k} - \varepsilon_k n_{\varepsilon_k}}{kT} \right], \quad (1.3.5)$$

where g_k represents the degeneracy of the energy level ε_k .

The number of particles n_{ε_k} , contained in our subsystem, can vary from zero to the total number of particles in the gas N . However, the probability of the latter is extremely low. Hence, for the n_{ε_k} , which are close to N , the terms of the sum (1.3.5) are so small, that the sum rapidly converges. Therefore, we will not commit an error, if we replace the upper limit N in the sum by infinity. After such a substitution the sum (1.3.5) goes over into a simple series:

$$\sum_{n_{\varepsilon_k}=0}^{\infty} \frac{g_k^{n_{\varepsilon_k}}}{n_{\varepsilon_k}!} \left(\exp \frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k}} = \sum_{n_{\varepsilon_k}=0}^{\infty} \frac{x^{n_{\varepsilon_k}}}{n_{\varepsilon_k}!} = e^x, \quad (1.3.6)$$

where we have provisionally denoted $g_k \exp(\mu - \varepsilon_k)/kT$ by x . Thus, the mean occupation of the specified energy level is

$$\bar{n}_{\varepsilon_k} = kT g_k \frac{\partial}{\partial \mu} \exp \frac{\mu - \varepsilon_k}{kT} = g_k \exp \frac{\mu - \varepsilon_k}{kT}. \quad (1.3.7)$$

At the same time, the mean occupation number of a single-particle state with energy ε_k turns out to be

$$\langle n_{\varepsilon_k} \rangle = \frac{\bar{n}_{\varepsilon_k}}{g_k} = \exp \frac{\mu - \varepsilon_k}{kT}. \quad (1.3.8)$$

In particular, if the states of the molecule and its energy vary continuously, which is always so in classical statistics, then the mean number of particles with an energy between ε and $\varepsilon + \delta\varepsilon$ is given by

$$dn = \bar{n} \frac{d\gamma}{h^3} = \left(\exp \frac{\mu - \varepsilon}{kT} \right) \frac{d\gamma}{h^3}, \quad (1.3.9)$$

where $d\gamma$ is the volume of the phase space corresponding to an energy between ε and $\varepsilon + \delta\varepsilon$, and $d\gamma/h^3$ is the number of states with this energy. Formula (1.3.9) is nothing else but a well known Maxwell distribution.

1.4 Quantum distribution for an ideal gas

Let us now turn to the quantum case.

As we have just stressed, it follows from the principle of identity of particles that one cannot distinguish between individual microscopic objects.

Applying this point of view in a consequential way, one has to renounce the numbering of particles. Just like in the classical case, there is still a certain distribution of atoms over single-particle states, such that in the first state there are n_1 particles, in the second state there are n_2 particles, and so on. However, from the quantum point of view, we cannot say, which individual particle is in which energy state, but rather indicate only the number of particles in each of these states respectively as

n_1 particles in the single-particle state with energy ε_1 ,

n_2 particles in the single-particle state with energy ε_2 , and so on.

Thus, this kind of description turns out to be less detailed than the classical one.

The new way of calculating microstates modifies the expression for the mean number of particles in the open subsystem considerably. Indeed, since one cannot speak of a permutation of particles, the division by $n_{\varepsilon_k}!$ in (1.3.4) makes no sense. The mean number of particles on a level of energy ε_k is then still given by the formula (1.3.4)

$$\bar{n}_{\varepsilon_k} = kT \frac{\partial}{\partial \mu} \ln \sum_{n_{\varepsilon_k}} \sum_{\{n_{\varepsilon_{ki}}\}} \Omega(n_{\varepsilon_{ki}}) \exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k 1}} \exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k 2}} \dots \quad (1.4.1)$$

in which, however, the number of microstates $\Omega(n_{\varepsilon_{ki}})$, differing only by a permutation of particles, must be different from the classical one.

The principle of identity gives a clear prescription:

$$\Omega(n_{\varepsilon_{ki}}) = 1. \quad (1.4.2)$$

Substituting this value into (1.4.1), we find:

$$\bar{n}_{\varepsilon_k} = kT \frac{\partial}{\partial \mu} \ln \sum_{n_{\varepsilon_k}=0}^{\infty} \sum_{\{n_{\varepsilon_{ki}}\}} \exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k 1}} \exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k 2}} \dots \quad (1.4.3)$$

The first sum in this formula is over the number of particles n_{ε_k} in the open subsystem. The second sum is over the number of distinct subsystem configurations, when it contains n_{ε_k} particles. Therefore, this double summation is equivalent to a summation over all possible values of the single-particle occupation numbers $n_{\varepsilon_{ki}}$, independently of one another. Hence, we may write

$$\begin{aligned}\bar{n}_{\varepsilon_k} &= kT \frac{\partial}{\partial \mu} \ln \sum_{n_{\varepsilon_k 0}, n_{\varepsilon_k 1}, \dots} \left[\exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k 0}} \exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k 1}} \dots \right] \\ &= kT \frac{\partial}{\partial \mu} \ln \left[\sum_{n_{\varepsilon_k 0}} \exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k 0}} \right] \left[\sum_{n_{\varepsilon_k 1}} \exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k 1}} \right] \dots \\ &= kT \frac{\partial}{\partial \mu} \ln \left[\sum_{n_{\varepsilon_k}} \exp \left(\frac{\mu - \varepsilon_k}{kT} \right)^{n_{\varepsilon_k}} \right]^{g_k},\end{aligned}\quad (1.4.4)$$

where g_k is the degeneracy of the energy level ε_k .

If the following inequality holds

$$\exp \frac{\mu - \varepsilon_k}{kT} < 1, \quad (1.4.5)$$

then the sum in (1.4.4) represents an infinitely decreasing geometric progression and can be easily calculated. Namely,

$$\bar{n}_{\varepsilon_k} = kT g_k \frac{\partial}{\partial \mu} \ln \left(1 - \exp \frac{\mu - \varepsilon_k}{kT} \right)^{-1} = g_k \left(\exp \frac{\varepsilon_k - \mu}{kT} - 1 \right)^{-1}. \quad (1.4.6)$$

Formula (1.4.6) gives the mean number of particles with the energy ε_k . Then the mean number of particles, occupying a particular one-particle quantum state with energy ε_k , is, obviously,

$$\frac{\bar{n}_{\varepsilon_k}}{g_k} = \left(\exp \frac{\varepsilon_k - \mu}{kT} - 1 \right)^{-1}. \quad (1.4.7)$$

This is nothing else but the Bose-Einstein distribution.

It should be noted that, since the sum (1.4.4) must always converge for any value of the energy, in particular for $\varepsilon_k = 0$, in addition to the inequality (1.4.5), the following restriction

$$e^{\mu/kT} < 1 \quad (1.4.8)$$

must also hold. This suggests that the chemical potential of a system of particles, obeying the Bose-Einstein statistics, must be an essentially negative quantity:

$$\mu < 0. \quad (1.4.9)$$

In all cases encountered in practice, the spacing between the energy levels of the translational motion is so small in comparison with the thermal energy kT that the energy spectrum can be assumed to be continuous. Then, instead of the mean number of particles at the k th energy level, it is necessary to introduce the mean number dn of particles with an energy lying between ε and $\varepsilon + \delta\varepsilon$. It is

obvious that $dn = \bar{n}h^{-3}d\gamma$, where $h^{-3}d\gamma$ is the number of states corresponding to an energy in the interval $\varepsilon, \varepsilon + \delta\varepsilon$. Substituting the value of $\bar{n}$ from (1.4.6), we find:

$$dn = \left(\exp \frac{\varepsilon - \mu}{kT} - 1 \right)^{-1} \frac{d\gamma}{h^3}. \quad (1.4.10)$$

The chemical potential, figuring in the Bose distribution, is determined from the obvious normalization condition

$$\int dn = N, \quad (1.4.11)$$

which expresses the constancy of the number of particles in a given volume.

The expressions, derived above, are of general character and do not depend on the way one defines an open subsystem. Therefore, in the future we will drop all the subscripts, distinguishing any particular choice of the one.

Comparing the derivation of the Bose distribution with that of the Maxwell-Boltzmann distribution, we see, first of all, that the first distribution represents a realization of the Gibbs distribution for the case of an ideal gas whose particles obey the laws of quantum mechanics. As one may observe, there is a profound difference in the statistical distributions for particles obeying the laws of classical mechanics and for particles obeying the laws of quantum mechanics. This difference is not associated with any change in the statistical laws and not even with taking account of the discrete character of the energy spectrum, but with a radical change in the method of calculating the statistical weights of the microstates due to the identity of microparticles.

Gases, which obey Bose-Einstein statistics, are called *degenerate*. Otherwise, if a gas follows the Maxwell-Boltzmann distribution, it is called to be *non-degenerate*.

The following question naturally arises. The laws of quantum mechanics are known to include the laws of classical motion as a first approximation. Under certain conditions, the laws of classical mechanics are sufficiently good approximation for describing dynamics of microparticles. Consequently, there must exist also such limiting cases, where the Bose-Einstein distribution smoothly transforms into the Maxwell-Boltzmann one.

In solving this problem we will proceed from the fact that the Bose-Einstein distribution is a more accurate law. Comparing distributions (1.4.7) and (1.3.8), we see that they have, in general case, an essentially different character (see Fig.1.2). However, this difference vanishes if the following inequality is satisfied:

$$\exp \frac{\varepsilon - \mu}{kT} \gg 1. \quad (1.4.12)$$

Both distributions have the same functional form when the inequality (1.4.12) is fulfilled. In this case, the unit in the denominator in (1.4.6) can be neglected, and the Bose distribution automatically changes to the Maxwell-Boltzmann one. Thus, the inequality (1.4.12) is the condition of applicability of classical statistics.

For the fulfilment of (1.4.12) at energies $\varepsilon \approx kT$ (for $\varepsilon > kT$ the exponential rapidly increases), it is necessary to require that $e^{-\mu/kT} \gg 1$. Assume, that this inequality is satisfied, so that for all energies

$$\left(\exp \frac{\varepsilon - \mu}{kT} - 1 \right)^{-1} \approx \exp \frac{\mu - \varepsilon}{kT}. \quad (1.4.13)$$

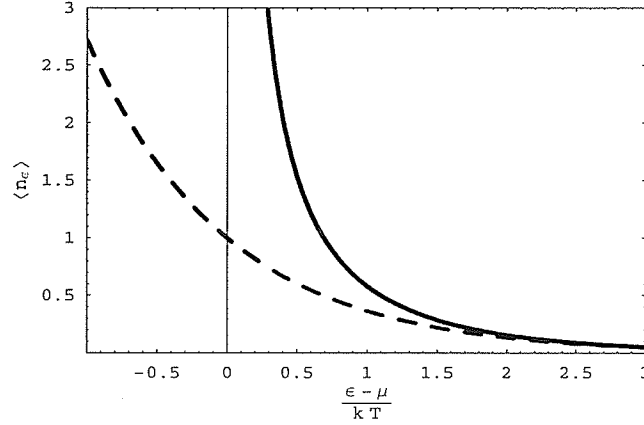


Figure 1.2: The mean occupation number $\langle n_\epsilon \rangle$ of a single-particle state ϵ in a system of non-interacting particles. Dashed curve represents the Maxwell-Boltzmann particles, solid curve the Bose ones.

Then, from the normalization condition (1.4.11), we find:

$$\begin{aligned} N &= \int \exp \frac{\mu - \epsilon}{kT} \frac{dp_x dp_y dp_z dV}{h^3} = \frac{2\pi(2m)^{3/2}V}{h^3} e^{\mu/kT} \int_0^\infty e^{\epsilon/kT} \epsilon^{1/2} d\epsilon \\ &= V \left(\frac{2\pi mkT}{h^2} \right)^{3/2} e^{\mu/kT}. \end{aligned} \quad (1.4.14)$$

Therefore,

$$e^{-\mu/kT} = \frac{V}{N} \left(\frac{2\pi mkT}{h^2} \right)^{3/2}. \quad (1.4.15)$$

Thus, the criterion of the validity of the application of classical statistics is

$$\frac{V}{N} \left(\frac{2\pi mkT}{h^2} \right)^{3/2} \gg 1. \quad (1.4.16)$$

If the inverse inequality is fulfilled, then the quantum effects become significant and one cannot use the Maxwell-Boltzmann distribution.

As one may observe, the criterion (1.4.16) contains several parameters. First of all, it contains the mass m of the particles: the larger the mass, the larger the left-hand side of the inequality. Further, (1.4.16) contains the density of the gas and its temperature T . As it could be expected, the inequality (1.4.16) is satisfied for high temperatures and is violated for low temperatures, so that at low temperatures quantum effects must appear. The fulfillment of the inequality (1.4.16) is also favored by a small gas density.

In the inverse limiting case, when

$$\frac{V}{N} \left(\frac{2\pi mkT}{h^2} \right)^{3/2} \ll 1, \quad (1.4.17)$$

degeneracy of the gas arises. Thus, the degeneracy can be due to the following causes: (1) a small particle mass, (2) a large gas density, (3) a low temperature.

For all ordinary gases the difference between quantum statistics and classical statistics for not particularly low values of the temperature and large values of the density turns out to be negligibly small. Thus, the quantum Bose distribution can, with a high degree of accuracy, be replaced by the Maxwell one.

Despite that, the creation of quantum statistics made it possible to solve a number of important physical problems. To one of them, known as Bose condensation, we will dedicate a lot of attention in what follows.

1.5 Qualitative properties of Bose-Einstein distribution

Having established the form of the Bose-Einstein and Maxwell-Boltzmann distributions as well as their domains of applicability, we may turn to a more detailed exploration. It is surprising that a purely qualitative treatment of the quantum law reveals a curious phenomenon, which is absent in the classical case.

To start with, let us evaluate the quantity $p_\varepsilon(n)$, which is the probability of finding exactly n particles in the single-particle state with energy ε . To indicate the difference with the classical case, we begin with the Maxwell-Boltzmann distribution.

From the general considerations of the previous chapters we infer that

$$p_\varepsilon(n)|_{M.B} \approx \frac{(e^{-\beta(\varepsilon-\mu)})^n}{n!}. \quad (1.5.1)$$

Normalizing (1.5.1) to unit, we get

$$p_\varepsilon(n)|_{M.B} = \frac{(e^{-\beta(\varepsilon-\mu)})^n / n!}{\sum_{n=0}^{\infty} (e^{-\beta(\varepsilon-\mu)})^n / n!} = \frac{(e^{-\beta(\varepsilon-\mu)})^n / n!}{\exp(e^{-\beta(\varepsilon-\mu)})}, \quad (1.5.2)$$

which, expressed in terms of the mean occupation number $\langle n_\varepsilon \rangle$ of the state, gives:

$$p_\varepsilon(n)|_{M.B} = \frac{(\langle n_\varepsilon \rangle)^n}{n!} e^{-\langle n_\varepsilon \rangle}. \quad (1.5.3)$$

Distribution (1.5.3) is clearly a Poisson distribution, which arises in statistics when one tries to describe the probability of observing a certain number of *independent* events, when the average number of such events per unit time is known. The common property of this kind of models is that the ratio $p_\varepsilon(n)/p_\varepsilon(n-1)$ varies inversely with n , which means that the probability of observing a greater number of uncorrelated outcomes varies inversely with n .

Let us now do the same for the Bose-Einstein statistics. Due to the indistinguishability of quantum particles, the corresponding Gibbs factor $1/n!$ drops out and we get

$$p_\varepsilon(n)|_{B.E} = \frac{(e^{-\beta(\varepsilon-\mu)})^n}{\sum_{n=0}^{\infty} (e^{-\beta(\varepsilon-\mu)})^n} = (e^{-\beta(\varepsilon-\mu)})^n [1 - e^{-\beta(\varepsilon-\mu)}], \quad (1.5.4)$$

or, expressed in terms of the mean occupation number,

$$p_\varepsilon(n)|_{B.E} = \frac{(\langle n_\varepsilon \rangle)^n}{(\langle n_\varepsilon \rangle + 1)^{n+1}}. \quad (1.5.5)$$

We observe that the Bose-Einstein distribution is radically different from the Maxwell-Boltzmann one. It is geometric, i.e. it has a constant common ratio $\langle n_\epsilon \rangle / (\langle n_\epsilon \rangle + 1)$. This means that the probability of a single-particle state ϵ to acquire one more particle is independent of the number of particles already occupying that state. Thus, in comparison with the classical statistical behavior, bosons exhibit a special tendency of “bunching” together, which indicates a presence of a positive statistical correlation between them. The latter is responsible for the *long-range order*, which will be discussed in later sections.

Next consideration turns out to be even more surprising.

Consider a collection of N non-interacting particles, which can each be in one of two states, $|0\rangle$ or $|1\rangle$. Once again, we will treat the classical and quantum cases separately, in order to stress the difference between the two. Let us start with the classical one.

If states $|0\rangle$ and $|1\rangle$ are of equal energy, then each single particle is equally likely to occupy any of these states. The system, composed of N such particles, n_0 of which are in state $|0\rangle$ and n_1 in state $|1\rangle$, has a statistical weight equal to

$$W_{M.B.}\{n_0, n_1\} = \frac{N!}{n_0!n_1!}. \quad (1.5.6)$$

As we have seen before, this is just a number of permutations between the particles in different states. One may easily check that $W|_{M.B.}$ reaches maximum, when $n_0 = n_1$, i.e. the maximal statistical weight belongs to a configuration in which particles are distributed evenly among the states, half in $|0\rangle$ and half in $|1\rangle$. As $N \rightarrow \infty$, $W|_{M.B.}$ quickly acquires a form of a delta-function.

Suppose now, that the energy E_0 of the state $|0\rangle$ is equal to zero, while the energy of the state $|1\rangle$ has a small but finite value E_1 . In this case, the average fraction of particles in state $|0\rangle$ is

$$\frac{\langle n_0 \rangle}{N} = \frac{\sum_{n_i} \frac{n_0}{N} \frac{N!}{n_0!n_1!} e^{-\beta E_1 n_1}}{\sum_{n_i} \frac{N!}{n_0!n_1!} e^{-\beta E_1 n_1}} = \frac{\sum_{n_i} \frac{(N-1)!}{(n_0-1)!n_1!} e^{-\beta E_1 n_1}}{\sum_{n_i} \frac{N!}{n_0!n_1!} e^{-\beta E_1 n_1}}, \quad (1.5.7)$$

where summations goes over all possible system configurations. Performing them, we obtain:

$$\frac{\langle n_0 \rangle}{N} = \frac{(1 + e^{-\beta E_1})^{N-1}}{(1 + e^{-\beta E_1})^N} = \frac{1}{1 + e^{-\beta E_1}}. \quad (1.5.8)$$

As one may readily observe, the resulting function is a smooth function of energy E_1 and is equal to $1/2$ when $E_1 = 0$. (see Fig.1.3).

We may conclude that the actual physics of the system of classical particles is the result of the outcome of the competition between energy and entropy. While the energy's role is to put as many particles as possible into a ground state, the entropy's role, conversely, is to spread the particles evenly among the states. As we may observe from Fig.1.3, statistical spreading in the case of distinguishable particles is huge and determines the outcome. Only substantial distance between the energy levels allows the energy to win this competition.

Now consider the system of indistinguishable particles. Compared to the previous case, the total number of different configurations of the system, consisting of N such particles, is now only $N + 1$. If there are K particles in state $|1\rangle$, there

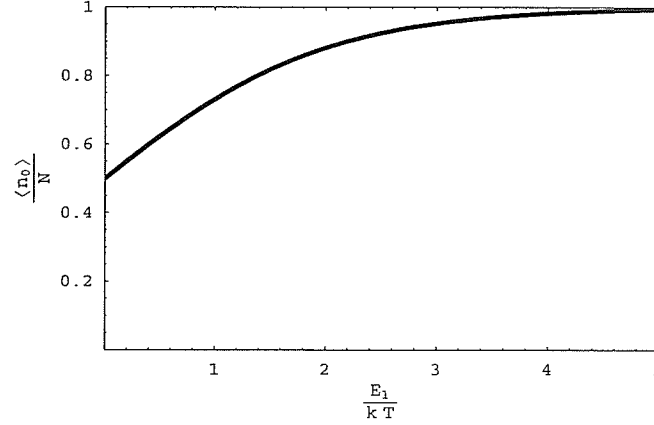


Figure 1.3: Average fraction of the number n_0 of distinguishable particles in the ground state as a function of the energy E_1 of the nearest excited state.

are $N - K$ particles in state $|0\rangle$. Whether any particular particle is in state $|0\rangle$ or in state $|1\rangle$ cannot be specified, so each value of K determines a unique quantum state for the whole system. When the energies of the states are the same, there is no statistical spreading – it is just as likely for all the particles to be found in the state $|0\rangle$, as for the particles to be split half and half.

Now suppose, as earlier, that the state $|0\rangle$ is the ground state and $|1\rangle$ is the lowest-lying excited state with energy E_1 . As before, each value of K determines a single state, which has its own separate Boltzmann probability. Furthermore, each state has a statistical weight equal to unit. Therefore, the probability to find a system in a state with K particles, occupying the single-particle state $|1\rangle$, is

$$p(K) = \frac{(e^{-\beta E_1})^K}{\sum_{K=0}^{\infty} (e^{-\beta E_1})^K} = e^{-\beta K E_1} [1 - e^{-\beta E_1}]. \quad (1.5.9)$$

Then the average fraction of the number of particles which are in the excited state is

$$\frac{\langle n_1 \rangle}{N} = \frac{\sum_{K=0}^{\infty} \frac{K}{N} e^{-\beta K E_1}}{\sum_{K=0}^{\infty} (e^{-\beta E_1})^K} = \frac{1}{N} \frac{e^{-\beta E_1}}{1 - e^{-\beta E_1}}. \quad (1.5.10)$$

The most striking observation from (1.5.10) is that the ratio goes down as the number of particles N goes up and gradually approaches zero in the thermodynamic limit $N \rightarrow \infty$. This is in complete disagreement with the classical case, where the number of particles in the excited state grows infinitely as N becomes large. It says that in the indistinguishable case the capacity of the non-ground state is limited, so in the thermodynamic equilibrium most of the particles will be in a vacuum, no matter how small is the energy gap.

In this case, the energy takes completely over the entropy due to the lack of statistical pressure, which plays an important role in classical systems. An infinitesimally small energy gap between the states is enough for most of the particles to collapse into the vacuum.

One may readily generalize the above conclusions to the case of a continuous spectrum. For example, consider a gas of particles, each of which can be in different momentum states, labeled $|\mathbf{k}\rangle$. If the number of particles is less than the number of thermally accessible states, which is always so for the high temperatures and low densities, then the particles can be found in distinct energy states. In this limit the gas is classical. However, as the density increases or the temperature decreases, the number of accessible states per particle becomes smaller, and at some point more particles will have to occupy the same state than the maximum allowed for that state by statistical weighting. From this point on, any extra particle, added to the system, will inevitably fall into the ground state. This is the essence of the *spontaneous symmetry breaking* phenomenon, which will be discussed in some detail in later sections.

1.6 Thermodynamic properties of an ideal Bose gas

Now, that we have qualitatively outlined the general properties of an ideal Bose gas, it is time to turn to more specific quantitative considerations.

As it is well known, the equation of state of an ideal Bose gas has the following form:

$$\frac{PV}{kT} = - \sum_{\epsilon} \ln(1 - ze^{-\beta\epsilon}). \quad (1.6.1)$$

Here P is the pressure and summation is carried over all single-particle quantum states accessible to a system. Parameter z is the activity of the gas, related to the chemical potential μ as

$$z = \exp(\mu/kT). \quad (1.6.2)$$

As we have mentioned earlier, the latter can be defined with the help of the normalization condition

$$N = \sum_{\epsilon} \langle n_{\epsilon} \rangle = \sum_{\epsilon} \frac{1}{z^{-1}e^{\beta\epsilon} - 1}. \quad (1.6.3)$$

It is always less than zero and decreases in an absolute value with decrease of temperature.

In the thermodynamic limit, when the volume V of the system goes to infinity, the spectrum of single particle states becomes almost continuous and summations on the right-hand sides of (1.6.1) and (1.6.3) may be replaced by integrations. In doing so, we make use of the asymptotic expression (1.1.11) for the density of states $\Omega(\epsilon)$ in a neighborhood of a given energy ϵ , namely

$$\Omega(\epsilon)d\epsilon = (2\pi V/h^3)(2m)^{3/2}\epsilon^{1/2}d\epsilon. \quad (1.6.4)$$

We note, however, that by substituting this expression into our integrals, we are unintentionally giving a weight zero to the energy state $\epsilon = 0$. This is wrong, because in a quantum-mechanical treatment we must give a statistical weight

unity to each nondegenerate single-particle state in the system. Therefore, it is common practice to take this particular term out of the sum before carrying out an integration. We thus obtain:

$$\frac{P}{kT} = -\frac{2\pi}{h^3}(2m)^{3/2} \int_0^\infty \varepsilon^{1/2} \ln(1 - ze^{\beta\varepsilon}) d\varepsilon - \frac{1}{V} \ln(1 - z) \quad (1.6.5)$$

and

$$\frac{N}{V} = \frac{2\pi}{h^3}(2m)^{3/2} \int_0^\infty \frac{\varepsilon^{1/2} d\varepsilon}{z^{-1}e^{\beta\varepsilon} - 1} + \frac{1}{V} \frac{z}{1 - z}. \quad (1.6.6)$$

Of course, the lower limit of the integrals can still be taken as equal to 0, because the state $\varepsilon = 0$ is not going to contribute towards the integrals anyway.

One may estimate the relative importance of the last terms in (1.6.5) and (1.6.6) right away. For $z \ll 1$, which corresponds to situations which are not far removed from the classical limit, each of these terms is of order $1/N$, i.e. negligible. However, as z increases, its values come close to unity. Then the term $z/(1 - z)V$ in (1.6.6), which is identically equal to the density of the particles in the ground state N_0/V , can well become a significant fraction of the quantity N/V . This phenomenon, when a macroscopic number of particles crashes simultaneously into the vacuum, is called the *Bose-Einstein condensation*.

Nevertheless, since $z/(1 - z) = N_0$ and hence $z = N_0/(N_0 + 1)$, the term $-V^{-1} \ln(1 - z)$ in (1.6.5) is equal to $V^{-1} \ln(N_0 + 1)$, which is at most $O(N^{-1} \ln N)$. This term is, therefore, negligible for all values of z and hence may be dropped.

We now obtain from (1.6.5) and (1.6.6), on substituting $\beta\varepsilon = p^2/(2mkT) = x$,

$$\frac{P}{kT} = -\frac{2\pi(2mkT)^{3/2}}{h^3} \int_0^\infty x^{1/2} \ln(1 - ze^{-x}) dx = \frac{1}{\lambda^3} g_{5/2}(z) \quad (1.6.7)$$

and

$$\frac{N - N_0}{V} = \frac{2\pi(2mkT)^{3/2}}{h^3} \int_0^\infty \frac{x^{1/2} dx}{z^{-1}e^x - 1} = \frac{1}{\lambda^3} g_{3/2}(z). \quad (1.6.8)$$

Here

$$\lambda = \frac{h}{(2\pi mkT)^{1/2}} \quad (1.6.9)$$

is the mean thermal wavelength, while $g_\nu(z)$ are the Bose-Einstein functions, defined by

$$g_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1} dx}{z^{-1}e^x - 1} = z + \frac{z^2}{2^\nu} + \frac{z^3}{3^\nu} + \dots \quad (1.6.10)$$

Equations (1.6.7) and (1.6.8) are our basic results. Upon elimination of z , they would give us the equation of state of an ideal Bose gas.

We see that the precise value of z is now obtained from (1.6.8), which may be written as

$$N_e = V \frac{(2\pi mkT)^{3/2}}{h^3} g_{3/2}(z), \quad (1.6.11)$$

where N_e is the number of particles in the excited states ($\varepsilon \neq 0$). Of course, unless z gets extremely close to unity, $N_e \sim N$. It is obvious, that, for $0 < z < 1$, the function $g_{3/2}(z)$ increases monotonically with z and is bounded from above. Its largest value is given by the Riemann zeta function:

$$g_{3/2}(1) = \zeta\left(\frac{3}{2}\right) \equiv 2.612. \quad (1.6.12)$$

Hence, for all z of interest,

$$g_{3/2}(z) \leq \zeta\left(\frac{3}{2}\right). \quad (1.6.13)$$

Consequently, for given V and T , the total equilibrium number of particles in all excited states, taken together, is also bounded, i.e.

$$N_e \leq V \frac{(2\pi mkT)^{3/2}}{h^3} \zeta\left(\frac{3}{2}\right). \quad (1.6.14)$$

As long as the actual number of particles in the system is less than this limiting value, everything is well. Practically all of them are distributed over the excited states and the precise value of z is determined by (1.6.11) with $N_e \sim N$. However, at one point, the actual number of particles may exceed this limiting value. Then it is natural to assume that the excited states will receive as many particles as they can hold, namely

$$N_e = V \frac{(2\pi mkT)^{3/2}}{h^3} \zeta\left(\frac{3}{2}\right), \quad (1.6.15)$$

while the rest will be pushed into the ground state $\varepsilon = 0$, whose capacity under all circumstances is practically unlimited:

$$N_0 = N - V \frac{(2\pi mkT)^{3/2}}{h^3} \zeta\left(\frac{3}{2}\right). \quad (1.6.16)$$

The precise value of z would then be determined by the formula

$$z = \frac{N_0}{N_0 + 1} = 1 - \frac{1}{N_0} \quad (1.6.17)$$

which shows that this parameter is unity for all reasonable purposes.

In some sense, the phenomenon of Bose condensation is similar to the familiar process of a vapor condensing into the liquid state, which takes place in the ordinary physical space. Conceptually, however, the two processes are very different. First, because the phenomenon of Bose-Einstein condensation is purely of quantum origin, occurring even in the absence of intermolecular forces. Second, because it takes place in the momentum space and not in the coordinate space.

The condition for the onset of Bose-Einstein condensation is

$$N > VT^{3/2} \frac{(2\pi mk)^{3/2}}{h^3} \zeta\left(\frac{3}{2}\right) \quad (1.6.18)$$

or, if we hold N and V constant and vary T ,

$$T < T_c = \frac{h^2}{2\pi m k} \left[\frac{N}{V \zeta(\frac{3}{2})} \right]^{2/3}. \quad (1.6.19)$$

Here T_c denotes a characteristic temperature, that depends on the particle mass m and the particle density N/V in the system. Accordingly, for $T < T_c$, the system may be looked upon as a mixture of two "phases":

- (i) a normal phase, consisting of $N_e = N(T/T_c)^{3/2}$ particles, distributed over the excited states ($\varepsilon \neq 0$), and
- (ii) a condensed phase, consisting of $N_0 = N - N_e$ particles, accumulated in the ground state ($\varepsilon = 0$).

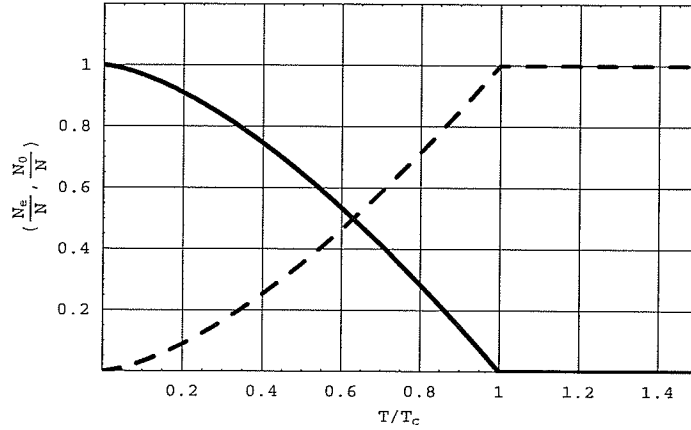


Figure 1.4: Fractions of the normal phase (dashed line) and the condensed phase (solid line) as functions of the temperature parameter T/T_c .

Figure 1.4 shows the manner in which the complementary functions N_e/N and N_0/N vary with T . For $T > T_c$, we have the normal phase alone. The number of particles in the ground state, $z/(1 - z)$, is $O(1)$, which is completely negligible in comparison with the total number N . Clearly, the situation is singular as $T = T_c$.

For the later reference we note that, at $T < T_c$, the condensate fraction vanishes as follows:

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c} \right)^{3/2}. \quad (1.6.20)$$

A knowledge of the variation of z with T is also of interest here. It is, however, simpler to consider the variation of z with (v/λ^3) , which is the ratio between the free volume per particle $v = V/N$ and the "thermal volume" of the atom. As one may observe from (1.6.9), this ratio is proportional to $T^{3/2}$. For $0 \leq (v/\lambda^3) \leq (2.612)^{-1}$, which corresponds to $0 \leq T \leq T_c$, the parameter $z \sim 1$ (see (1.6.17)). For $(v/\lambda^3) > (2.612)^{-1}$, $z < 1$ and is determined by the relationship

$$g_{3/2}(z) = (v/\lambda^3) < 2.612 \quad (1.6.21)$$

(see (1.6.8)). For $(v/\lambda^3) \gg 1$ we have $g_{3/2}(z) \ll 1$ and, hence, $z \ll 1$. Under these circumstances, $g_{3/2}(z) \sim z$ (see (1.6.10)). Therefore, in this region $z \sim (v/\lambda^3)^{-1}$, which is in complete agreement with the classical case.

Thus, the chemical potential of an ideal Bose gas has constant maximum value of zero in the whole range of temperatures below critical and slowly goes down above T_c as temperature increases, asymptotically approaching the classical values. Figure 1.5 shows these specifics.

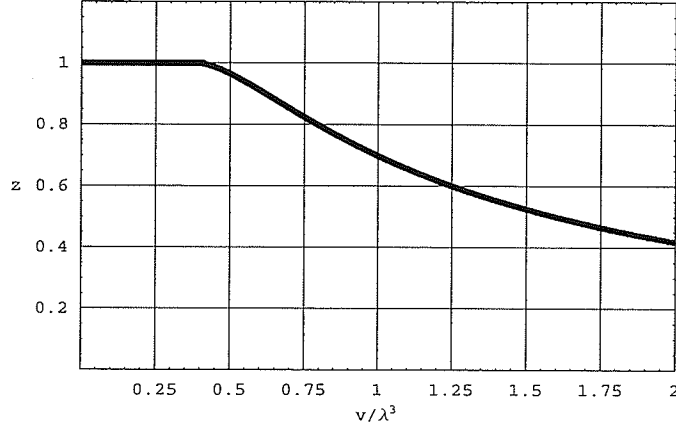


Figure 1.5: The activity z of an ideal Bose gas as a function of v/λ^3 . Condensed phase of the gas disappears at the breaking point.

Next, we examine the (P, T) -diagram of the system, i.e. the variation of P with T , keeping v fixed. For $T < T_c$, the pressure is given by (1.6.7), with z replaced by unity, i.e.

$$P(T) = \frac{kT}{\lambda^3} \zeta\left(\frac{5}{2}\right), \quad (1.6.22)$$

which is proportional to $T^{5/2}$ and is independent of v , implying *infinite compressibility*. At the transition point, the value of the pressure is

$$P(T_c) = \left(\frac{2\pi m}{h^2}\right)^{3/2} (kT_c)^{5/2} \zeta\left(\frac{5}{2}\right). \quad (1.6.23)$$

In order to estimate its order of magnitude, we use (1.6.19) and rewrite (1.6.23) as

$$P(T_c) = \frac{\zeta\left(\frac{5}{2}\right)}{\zeta\left(\frac{3}{2}\right)} \left(\frac{N}{V} kT_c\right) \sim 0.5134 \left(\frac{N}{V} kT_c\right). \quad (1.6.24)$$

Thus, the pressure, exerted by the particles of an ideal Bose gas at the transition temperature T_c , is about one-half of that of an equivalent Boltzmann gas.

For $T > T_c$, the pressure is given by

$$P = \frac{N}{V} kT \frac{g_{5/2}(z)}{g_{3/2}(z)}, \quad (1.6.25)$$

where $z(T)$ is determined by the implicit relationship

$$g_{3/2}(z) = \frac{\lambda^3}{v} = \frac{N}{V} \frac{h^3}{(2\pi mkT)^{3/2}}. \quad (1.6.26)$$

Unless T is very high, the expression for P cannot be represented with simpler terms. As $T \rightarrow \infty$, the pressure approaches the classical value NkT/V .

All these features are shown in Fig.1.6. The transition line in the figure por-

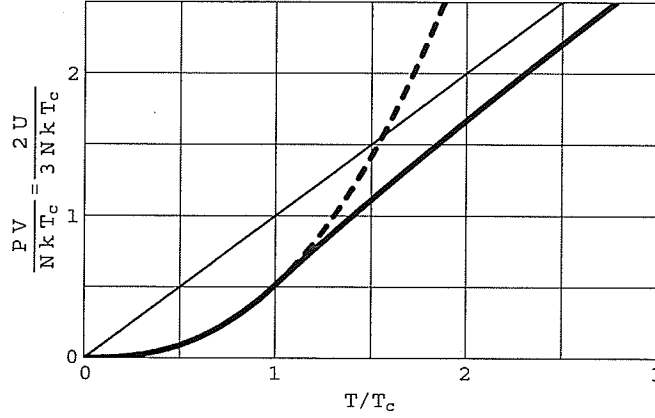


Figure 1.6: The pressure and the internal energy per particle of an ideal Bose gas as a function of a temperature parameter T/T_c . Thick solid line represents the ideal Bose gas, dashed line the classical Boltzmann gas and the thin solid one is the transition line described in text.

trays (1.6.22). The actual (P, T) -curve follows this line from $T = 0$ up to $T = T_c$ and thereafter departs, tending asymptotically to the classical limit. It may be pointed out that the region on the right of the transition line belongs to the normal phase alone, the line itself belongs to the mixed phase, while the region to the left is inaccessible to the system.

There is a direct relationship between the internal energy of a Bose gas and its pressure. Indeed, the internal energy of the system is given by

$$\begin{aligned} U &= \left(\frac{\partial}{\partial \beta} \sum_{\epsilon} \ln(1 - ze^{-\beta \epsilon}) \right)_{z, V} = kT^2 \left[\frac{\partial}{\partial T} \left(\frac{PV}{kT} \right) \right]_{z, V} \\ &= \frac{3}{2} kT \frac{V}{\lambda^3} g_{5/2}(z). \end{aligned} \quad (1.6.27)$$

Thus, quite generally, our system satisfies the relationship

$$P = \frac{2}{3} (U/V). \quad (1.6.28)$$

Therefore, Fig.1.6 depicts equally well also the variation of U with T (with v fixed). Its slope should, therefore, be a measure of the specific heat $C_V(T)$ of the gas. We readily observe that this parameter is vanishingly small at low temperatures, rising with T until reaching a maximum at $T = T_c$. Thereafter, it

decreases, tending asymptotically to the constant classical value. Analytically, for $T \leq T_c$, we obtain:

$$\frac{C_v}{Nk} = \frac{1}{Nk} \left(\frac{\partial U}{\partial T} \right)_{N,V} = \frac{3}{2} \frac{V}{N} \zeta \left(\frac{5}{2} \right) \frac{d}{dT} \left(\frac{T}{\lambda^3} \right) = \frac{15}{4} \zeta \left(\frac{5}{2} \right) \frac{v}{\lambda^3}, \quad (1.6.29)$$

which is proportional to $T^{3/2}$. At $T = T_c$, we have

$$\frac{C_v(T_c)}{Nk} = \frac{15}{4} \frac{\zeta(5/2)}{\zeta(3/2)} \simeq 1.925, \quad (1.6.30)$$

which is significantly higher than the classical value 1.5.

For the case of $T > T_c$, we may obtain an implicit formula. First of all,

$$\frac{C_v}{Nk} = \left[\frac{\partial}{\partial T} \left(\frac{3}{2} T \frac{g_{5/2}(z)}{g_{3/2}(z)} \right) \right]_v. \quad (1.6.31)$$

To carry out the differentiation, we need to know $(\partial z / \partial T)_v$. This can be obtained from (1.6.21) with the help of the recurrence relation, satisfied by the Bose-Einstein functions:

$$z \frac{\partial}{\partial z} [g_\nu(z)] = g_{\nu-1}(z). \quad (1.6.32)$$

On one hand, since $g_{3/2}(z) \sim T^{-3/2}$,

$$\left[\frac{\partial}{\partial T} g_{3/2}(z) \right]_v = -\frac{3}{2T} g_{3/2}(z). \quad (1.6.33)$$

On the other hand,

$$z \frac{\partial}{\partial z} [g_{3/2}(z)] = g_{1/2}(z). \quad (1.6.34)$$

Combining this two results, we obtain:

$$\frac{1}{z} \left(\frac{\partial}{\partial T} \right)_v = -\frac{3}{2T} \frac{g_{3/2}(z)}{g_{1/2}(z)}. \quad (1.6.35)$$

Therefore, equation (1.6.31) now gives:

$$\frac{C_v}{Nk} = \frac{15}{4} \frac{g_{5/2}(z)}{g_{3/2}(z)} - \frac{9}{4} \frac{g_{3/2}(z)}{g_{1/2}(z)}. \quad (1.6.36)$$

Here the value of z as a function of T is again to be determined from (1.6.21). In the limit $z \rightarrow 1$, the second term in (1.6.36) vanishes because of the divergence of $g_{1/2}(z)$, while the first term gives exactly the result appearing in (1.6.30). The specific heat is, therefore, continuous at the transition point. Its derivative, however, is discontinuous, with the magnitude of discontinuity being equal to

$$\left(\frac{\partial C_v}{\partial T} \right)_{T=T_c-0} - \left(\frac{\partial C_v}{\partial T} \right)_{T=T_c+0} = \frac{27Nk}{16\pi T_c} \left[\zeta \left(\frac{3}{2} \right) \right]^2 \simeq 3.665 \frac{Nk}{T_c}. \quad (1.6.37)$$

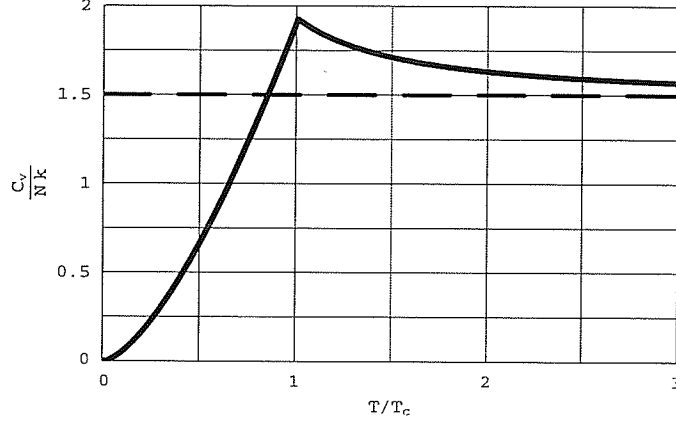


Figure 1.7: The specific heat per particle of an ideal Bose gas as a function of the temperature parameter T/T_c . Dashed line indicates the classical value.

For $T > T_c$, the specific heat decreases steadily towards the limiting value

$$\left(\frac{C_v}{Nk} \right)_{z \rightarrow 0} = \frac{15}{4} - \frac{9}{4} = \frac{3}{2}. \quad (1.6.38)$$

Figure 1.7 shows all the features of the (C_v, T) -relationships.

We shall now look at the isotherms of the ideal Bose gas, i.e. the variation of the pressure with the volume for fixed T . The Bose-Einstein condensation now sets in a characteristic volume v_c , given by

$$v_c = \lambda^3 / \zeta(3/2) \quad (1.6.39)$$

(see (1.6.18)). We note that $v_c \sim T^{-3/2}$. For $v < v_c$, the pressure is independent of v and is given by

$$P_0 = \frac{kT}{\lambda^3} \zeta\left(\frac{5}{2}\right) \quad (1.6.40)$$

(see (1.6.22)).

In Fig.1.8 the region, where two phases coexist, is marked by a boundary line (called the transition line), given by the equation

$$P_0 v_c^{5/3} = \frac{h^2}{2\pi m} \frac{\zeta(5/2)^{5/3}}{\zeta(3/2)} = \text{const.} \quad (1.6.41)$$

Clearly, the region to the left of this line belongs to the mixed phase, while the region to the right belongs to the normal phase alone.

Finally, we examine the adiabats of the ideal Bose gas. For this, we need an expression for the entropy of the system. Using the thermodynamic formula

$$U - TS + PV = N\mu \quad (1.6.42)$$

and the expressions for U and P obtained above, we get:

$$\frac{S}{Nk} \equiv \frac{U + PV}{NkT} - \frac{\mu}{kT} = \begin{cases} \frac{5}{2} \frac{g_{5/2}(z)}{g_{3/2}(z)} - \ln z & \text{for } T > T_c, \\ \frac{5}{2} \frac{v}{\lambda^3} \zeta\left(\frac{5}{2}\right) & \text{for } T \leq T_c. \end{cases} \quad (1.6.43)$$

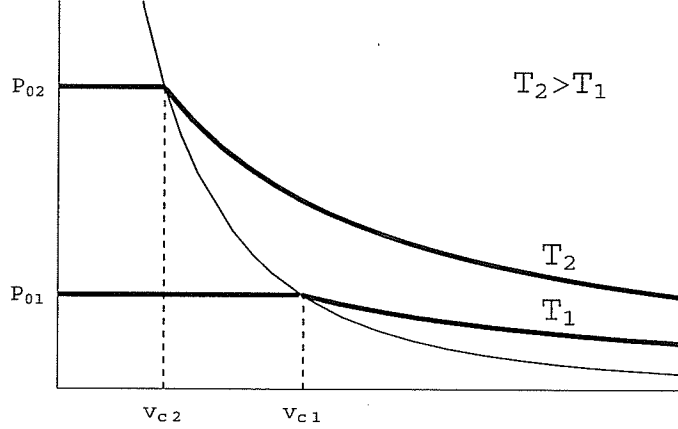


Figure 1.8: Isotherms of an ideal Bose gas. Thin solid line corresponds to the transition line given by (1.6.41).

Once again, the value of $z(T)$, for $T > T_c$, is to be obtained from (1.6.21).

A reversible adiabatic process implies the constancy of S and N . For $T > T_c$, this implies the constancy of z , as well as the constancy of (v/λ^3) by (1.6.21). For $T \leq T_c$, it again implies the same. Thus, we obtain, quite generally, the following relationship between the volume and the temperature of the system, when it undergoes a reversible adiabatic process:

$$vT^{3/2} = \text{const.} \quad (1.6.44)$$

The corresponding relationship between the pressure and the temperature is

$$P/T^{5/2} = \text{const.} \quad (1.6.45)$$

Eliminating T , we obtain

$$Pv^{5/3} = \text{const} \quad (1.6.46)$$

as the equation for an adiabat of the ideal Bose gas.

Incidentally, the foregoing results are exactly the same as for an ideal classical gas. There is, however, a significant difference between the two. While the exponent $5/3$ in formula (1.6.46) is identically equal to the ratio of the specific heats C_P and C_V in the case of the ideal classical gas, it is not so in the case of the ideal Bose gas. For the latter, this ratio is given by

$$\gamma = \frac{C_P}{C_V} = 1 + \frac{4 C_V g_{1/2}(z)}{9 N k g_{3/2}(z)} = \frac{5 g_{5/2}(z) g_{1/2}(z)}{3 [g_{3/2}(z)]^2}. \quad (1.6.47)$$

It is only for $T \gg T_c$ that $\gamma \sim 5/3$. At any finite temperature, $\gamma > 5/3$ and as $T \rightarrow T_c$, $\gamma \rightarrow \infty$. Equation (1.6.46), on the other hand, holds for all T .

In the region of the mixed phase ($T < T_c$), the entropy of the gas may be written as

$$S = N_e \cdot \frac{5}{2} k \frac{\zeta(5/2)}{\zeta(3/2)} \propto N_e \quad (1.6.48)$$

As expected, the N_0 particles, that constitute the condensate, do not contribute towards the entropy of the system, while the N_e particles, that form the normal part, contribute the amount of $\frac{5}{2}k\zeta(\frac{5}{2})/\zeta(\frac{3}{2})$ per particle. Thus, as the temperature goes up, the entropy grows proportionally to the number of accessible excited states, i.e. $\sim T^{3/2}$ (see (1.6.21)).

1.7 The method of quantized fields

Previous sections were dedicated to the statistical mechanical investigation of the ideal Bose gas. However, if the gas is interacting, it is convenient to reformulate the problem on the language of quantum field theory. First, because it provides convenient tools necessary to calculate the interaction corrections. Second, because it will lead to the appearance of brand new ideas and concepts underlying the phenomenon of Bose-Einstein condensation.

Nowadays, quantum field theory is a highly elaborate subject. There are three equivalent roads to it [8]:

1. Operator secondary quantization technique.
2. Approach, based on Feynman diagrams (Green's function method).
3. Functional integral formulation.

Despite the recent trend in the literature to treat the degenerate gases within the third approach [14], most of the works use the secondary quantization technique as a tool.

In the secondary quantization formalism one considers a system of interest as a quantum field, represented by an infinite number of interacting harmonic oscillators, whose excitations are being identified with particles.

The special role of the harmonic oscillators is due to additivity of their spectra: if E_1, E_2 are the energy levels, then $E_1 + E_2$ is also an energy level. That is exactly what we expect from elementary particles. Therefore, we try to identify hamiltonians of particles with hamiltonians of interacting oscillators [9].

In addition, oscillators are considered to be indistinguishable, and, therefore, the state of the system is completely getting characterized by the occupation numbers of all accessible single-particle states.

Thus, the secondary quantization technique could be regarded as a far-reaching generalization of the statistical mechanical method, which we employed to derive the Bose-Einstein and Maxwell-Boltzmann distributions. It preserves all the virtues of the latter and extends its area of applicability to virtually any kind of physical system, closed or open, interacting or not.

With this introduction, let us now turn to a formal consideration of the subject.

1.7.1 The number representation

Consider a system of particles, whose single-particle states could be classified by a discrete index $i = 1, 2, 3, \dots$ [10]. To explain what the index i implies, let us recall

that, according to wave mechanics, the state of a single particle is represented by a normalizable wave function $\Psi(\mathbf{r})$:

$$\int d\mathbf{r} |\Psi(\mathbf{r})|^2 < \infty. \quad (1.7.1)$$

By this reason, $\Psi(\mathbf{r})$ cannot be a plane wave. It is a wave packet, i.e. any spatially localized wave function.

Any normalizable function $\Psi(\mathbf{r})$ can be expanded as

$$\Psi(\mathbf{r}) = \sum_i c_i \phi_i(\mathbf{r}), \quad (1.7.2)$$

where the functions $\phi_i(\mathbf{r})$ form a countable set $\{\phi_i(\mathbf{r}); i = 1, 2, \dots\}$ of orthonormalized functions, which satisfy the following conditions:

$$\int d\mathbf{r} \phi_i^*(\mathbf{r}) \phi_j(\mathbf{r}) = \delta_{ij}, \quad (1.7.3)$$

where the "star" denotes the operation of complex conjugation.

A well known example of an orthonormalized complete set $\{\phi_i\}$ are the aforementioned harmonic oscillator wave functions, which are classified by the principle quantum numbers.

The expansion coefficients c_i in (1.7.2) may depend on time.

Earlier, when deriving the ideal quantum gas distribution, we constructed a subsystem as a collection of particles of the same energy. Thus, the state of the subsystem turned out to be completely characterized by the occupation numbers of the single-particle quantum states. This kind of description can straightforwardly be generalized to the case of an arbitrary many-body system of interacting particles.

Indeed, let us consider a many-body quantum system which, unlike the previous consideration, comprises particles of different energies. Suppose n_i is the number of particles occupying the i th single-particle quantum state. Then a state of the whole system is identified when we specify n_i for all i . Thus, we will denote this state by $|n_1, n_2, \dots\rangle$.

Due to the interactions, the system state will evolve in time. Correspondingly, the numbers n_i will run through the whole sequence of possible values, which is limited only by certain restrictions specific to the system.

Assembling all such states, we construct the set $\{|n_1, n_2, \dots\rangle\}$. This set has interesting features, which will be investigated below.

In order to describe the interactions, it is convenient to introduce the annihilation and creation operators, $\hat{a}_i$ and $\hat{a}_i^\dagger$ respectively, as the following:

$$\hat{a}_i |n_1, \dots, n_i, \dots\rangle = \sqrt{n_i} |n_1, \dots, n_i - 1, \dots\rangle, \quad (1.7.4)$$

$$\hat{a}_i^\dagger |n_1, \dots, n_i, \dots\rangle = \sqrt{n_i + 1} |n_1, \dots, n_i + 1, \dots\rangle. \quad (1.7.5)$$

Thus, the operator $\hat{a}_i$ reduces the number of particles in state i by one, i.e. replaces n_i by $n_i - 1$. In contrast, the operator $\hat{a}_i^\dagger$ increases this number by one, i.e. replaces n_i by $n_i + 1$. Obviously, we can move from any state to another state in the set $\{|n_1, n_2, \dots\rangle\}$ by means of repeated applications of the creation and annihilation operators.

Definitions (1.7.4) and (1.7.5) allow one to introduce an important particle number operator as

$$\hat{N}_i |n_1, \dots, n_i, \dots\rangle = n_i |n_1, \dots, n_i, \dots\rangle, \quad (1.7.6)$$

where $\hat{N}_i$ is defined by

$$\hat{N}_i = \hat{a}_i^\dagger \hat{a}_i. \quad (1.7.7)$$

This operator gives the number of particles in the i th energy state. The total number of particles in the system is then represented by the sum

$$\hat{N} = \sum_i \hat{N}_i, \quad (1.7.8)$$

which is called the total number operator.

The actions of the $\hat{a}_i$ and $\hat{a}_i^\dagger$ operators on the system states are not independent. This fact can be expressed by the following Bose commutation relations, which might be read from (1.7.4) and (1.7.5):

$$[\hat{a}_i, \hat{a}_j^\dagger] |n_1, n_2, \dots\rangle = \delta_{ij} |n_1, n_2, \dots\rangle, \quad (1.7.9)$$

$$[\hat{a}_i, \hat{a}_j] |n_1, n_2, \dots\rangle = 0, \quad (1.7.10)$$

$$[\hat{a}_i^\dagger, \hat{a}_j^\dagger] |n_1, n_2, \dots\rangle = 0. \quad (1.7.11)$$

The creation/annihilation operators and states, introduced in that way, constitute the major ingredients of the secondary quantization formalism. However, the development, performed above, contains one feature, which is inherent to the systems of infinite number degrees of freedom and which, therefore, is absent in ordinary quantum mechanics. Let us discuss it in more detail.

1.7.2 Unitarily inequivalent representations

A significant feature of the set $\{|n_1, n_2, \dots\rangle\}$ is its non-countability. This property is easy to observe in the case of a fermion system, in which there are only two values of the occupation numbers possible, $n_i = 0$ and 1. Indeed, using the binary number system, we consider the set $A = 0, n_1 n_2 \dots n_i \dots$, in which $n_i = 0$ or 1. This sequence covers the interval $(0, 1)$ of the real line and has a one-to-one correspondence with the set $\{|n_1, n_2, \dots\rangle\}$. We thus conclude that $\{|n_1, n_2, \dots\rangle\}$ is not countable.

It is obvious that this conclusion also holds true in the case of a boson system, where there are no restrictions on the values of the occupation numbers.

Since the set $\{|n_1, n_2, \dots\rangle\}$ is not countable, we cannot use it as a base of a separable Hilbert space. For this purpose, it is necessary first to choose its countable subset. Obviously, there are infinitely many ways to do that. The problem, however, is that when two different subsets can be used as a base of representation for the operators $\hat{a}_i, \hat{a}_i^\dagger$, then these two representations turn out to be unitarily inequivalent to each other in the sense that a vector of one representation is not

a superposition of the base vectors of another representation. This creates a very deep difference between the situation in ordinary quantum mechanics and the one in quantum field theory. In quantum mechanics, one deals with finite-dimensional systems and does not have to worry about the choice of representations for canonical variables, because all representations are unitarily equivalent. This is not so in quantum field theory.

In the next section we will see why this happens and which physical consequences it reveals. But first we need to construct the Fock space.

1.7.3 The Fock space

At first glance, it seems probable, that the set $\{|n_1, n_2, \dots\rangle\}$ is unnecessarily large for the description of nature. After all, in all experiments only a finite number of quanta is excited, although this number can be arbitrarily large. Therefore, we shall assume that the following subset is sufficient for the description of physical processes:

$$[0]\text{-set} = \left\{ |n_1, n_2, \dots\rangle; \sum n_i = \text{finite} \right\}. \quad (1.7.12)$$

This set contains the state of no particles ($n_i = 0$ for all i), which is called the vacuum and denoted by $|0\rangle$:

$$|0\rangle = |0, 0, \dots\rangle. \quad (1.7.13)$$

On the other hand, it does not contain many states which were in the original set $\{|n_1, n_2, \dots\rangle\}$. For example, the state with $n_i = 1$ for all i is clearly not contained in the $[0]$ -set.

The vectors in the $[0]$ -set are constructed by repeated application of the creation operators $\hat{a}_i^\dagger$ on the vacuum state. In the case of the boson system, we may write a vector $|n_1, n_2, \dots\rangle$ as (see (1.7.5))

$$|n_1, n_2, \dots\rangle = \prod_i (n_i!)^{-1/2} (\hat{a}_i^\dagger)^{n_i} |0\rangle. \quad (1.7.14)$$

Construction of the conjugate vectors $\langle n_1, n_2, \dots|$ goes along the same lines. First, we suppose, that the inner product of vectors and conjugate vectors is well defined. We will denote it by $\langle n'_1, n'_2, \dots | n_1, n_2, \dots \rangle$. Additionally, for the inner product of the vacuum vector and its conjugate $\langle 0|$, the following normalization condition applies:

$$\langle 0|0\rangle = 1. \quad (1.7.15)$$

Second, we define the operation of $\hat{a}_i^\dagger$ and $\hat{a}_i$ on conjugate state vectors in such a way that $\hat{a}_i$ becomes the hermitian conjugate of $\hat{a}_i^\dagger$. Then (1.7.4) and (1.7.5) lead to

$$\langle n_1, \dots, n_i, \dots | \hat{a}_i^\dagger = \sqrt{n_i} \langle n_1, \dots, n_i - 1, \dots | \quad (1.7.16)$$

and

$$\langle n_1, \dots, n_i, \dots | \hat{a}_i = \sqrt{n_i + 1} \langle n_1, \dots, n_i + 1, \dots |. \quad (1.7.17)$$

Thus, the conjugate vectors could be constructed by the repeated application of the annihilation operators on the conjugate vacuum state:

$$\langle n_1, n_2, \dots | = \langle 0 | \prod_i (n_i!)^{-1/2} (\hat{a}_i)^{n_i}. \quad (1.7.18)$$

Now, from (1.7.4) and (1.7.16) we may observe the following obvious identities:

$$\hat{a}_i |0\rangle = 0, \quad (1.7.19)$$

$$\langle 0 | \hat{a}_i^\dagger = 0. \quad (1.7.20)$$

Furthermore, (1.7.4) and (1.7.5) lead to

$$\prod_i (1/n_i!) (\hat{a}_i)^{n_i} (\hat{a}_i^\dagger)^{n_i} |0\rangle = |0\rangle. \quad (1.7.21)$$

Equations (1.7.19-1.7.21) contain enough to show that the $[0]$ -set is an orthonormalized set:

$$\langle n'_1, n'_2, \dots | n_1, n_2, \dots \rangle = \prod_i \delta_{n_i n'_i}, \quad (1.7.22)$$

The Hilbert space, constructed as a linear superposition of the vectors of the $[0]$ -set and equipped with a norm, is called the Fock space.

We may also take a different look at the space just constructed. As one may observe, the relations (1.7.9-1.7.11) lead to

$$\langle a | [\hat{a}_i, \hat{a}_j^\dagger] | b \rangle = \delta_{ij} \langle a | b \rangle, \quad (1.7.23)$$

$$\langle a | [\hat{a}_i, \hat{a}_j] | b \rangle = \langle a | [\hat{a}_i^\dagger, \hat{a}_j^\dagger] | b \rangle = 0 \quad (1.7.24)$$

for any two vectors $|a\rangle$ and $|b\rangle$, which belong to the Fock space. These relations imply that this space is a representation of the operators $\hat{a}_i$ and $\hat{a}_i^\dagger$, the algebraic properties of which are defined by the Bose commutators:

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \quad (1.7.25)$$

$$[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0. \quad (1.7.26)$$

Thus, the construction of the Fock space could be realized purely empirically. One can set up a quantum-theoretical language, in terms of which the system of interest could be described without any reference to the specifics of its dynamic behavior. This "language", i.e. the Fock space, can therefore be used in any situations, where one deals with quantum systems, whose states could be specified by the number series. That is why the general framework, constructed here, can successfully be used in such diverse areas as condensed matter and high energy physics.

1.8 Long-range order, symmetry breaking and order parameter

In the previous section we have seen, how a broad class of physical systems could be represented by a Fock space, constructed by repeated applications of creation operators $\hat{a}_i^\dagger$ on its vacuum state.

It may seem that this representation is unique, i.e completely determined by the algebraic relations (1.7.25, 1.7.26) up to unitary equivalence. However, this is not so. It turns out, that the canonical transformations of the Fock space (the ones, which leave the commutation relations invariant) do not need to be unitarily implementable.

For instance, this kind of situation emerges, when a huge number of bosons condense into the ground state. The fact that a macroscopically large number of particles participates in this process suggests that, adding or extracting one of them from the vacuum, does not change the physical properties of the system just because it is impossible to detect this change. Therefore, those kinds of states are physically identical. Mathematically, however, they are distinct, since they contain different numbers of particles (which is a characteristic of the state and which cannot be changed by any mathematical transformation). Thus, in the thermodynamic limit, the number of mathematically different ground states tends to infinity together with the number of condensed bosons. Correspondingly, the Fock spaces, built on those vacua, are not unitarily equivalent, though they describe essentially the same physical situation.

The rigorous treatment of this issue within the secondary quantization framework is beyond the scope of this work. We will rather refer to the book [10], where this problem is elaborate in a great detail.

Instead, we will concentrate on physical consequences of the unitary nonequivalence, which appear in the problem we are interested in. These are the long-range order, spontaneous symmetry breaking and the order parameter [11]. All three concepts play a major role in the theory of Bose-Einstein condensation. Let's consider each of them separately.

1.8.1 One-body density matrix and long-range order

The object of our interest is the ideal uniform Bose gas. Within the secondary quantization framework, it can be considered as a field, each mode of which is represented by an independent oscillator with its own creation and annihilation operators $\hat{a}_\mathbf{p}^\dagger$ and $\hat{a}_\mathbf{p}$. With their help, the field operators, which create and annihilate a particle at point $\mathbf{r}$, could then be represented as a linear superposition of modes

$$\hat{\Psi}(\mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{1}{\sqrt{2\omega_\mathbf{p}}} (\hat{a}_\mathbf{p} e^{i\mathbf{r}\cdot\mathbf{p}} + \hat{a}_\mathbf{p}^\dagger e^{-i\mathbf{r}\cdot\mathbf{p}}), \quad (1.8.1)$$

where $\omega_\mathbf{p}$ is the frequency of the mode.

The field operators are subject to the Bose commutation relations:

$$[\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'), \quad [\hat{\Psi}(\mathbf{r}), \hat{\Psi}(\mathbf{r}')] = 0. \quad (1.8.2)$$

Correspondingly,

$$[\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}'}^\dagger] = (2\pi)^3 \delta^3(\mathbf{p} - \mathbf{p}'). \quad (1.8.3)$$

Important information about the system properties can be extracted from the so-called one-body density matrix. With the help of the field operators, it can be introduced as follows:

$$n^{(1)}(\mathbf{r}, \mathbf{r}') = \langle \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}') \rangle \quad (1.8.4)$$

With its help, one may directly obtain the density of the system by setting $\mathbf{r} = \mathbf{r}'$:

$$n(\mathbf{r}) = \langle \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \rangle = n^{(1)}(\mathbf{r}, \mathbf{r}). \quad (1.8.5)$$

The total number of particles is then equal to $N = \int d\mathbf{r} n(\mathbf{r}) = \int d\mathbf{r} n^{(1)}(\mathbf{r}, \mathbf{r})$, which defines the normalization of the one-body density matrix.

For the later considerations, it is useful to rewrite (1.8.5) in the momentum representation:

$$n(\mathbf{p}) = \langle \hat{\Psi}^\dagger(\mathbf{p}) \hat{\Psi}(\mathbf{p}) \rangle, \quad (1.8.6)$$

where $\hat{\Psi}(\mathbf{p}) = (2\pi\hbar)^{-3/2} \int d\mathbf{r} \exp[i\mathbf{p} \cdot \mathbf{r}/\hbar] \hat{\Psi}(\mathbf{r})$ is the field operator in the momentum space.

Now we are ready to explore the large distance properties of the ideal Bose gas. Suppose, it contains N particles and occupies a volume V . Since the gas is considered to be uniform, its one-body density matrix should depend only on the modulus of the relative distance $\mathbf{s} = \mathbf{r} - \mathbf{r}'$: $n^{(1)}(\mathbf{r}, \mathbf{r}') = n^{(1)}(s)$. Therefore, one can write:

$$n^{(1)}(s) = \frac{1}{V} \int d\mathbf{p} n(\mathbf{p}) e^{-i\mathbf{p} \cdot \mathbf{s}/\hbar}. \quad (1.8.7)$$

If the system contains only normal component, its momentum distribution has a smooth behavior at small momenta and, consequently, the one-body density vanishes, when $s \rightarrow \infty$.

The situation is different if, instead, the momentum distribution exhibits the singular behavior:

$$n(\mathbf{p}) = N_0 \delta(\mathbf{p}) + \tilde{n}(\mathbf{p}), \quad (1.8.8)$$

characterized by a δ -function term with a weight N_0 , proportional to the total number of particles. But this is exactly what happens due to the Bose condensation, when the single-particle state with momentum $\mathbf{p} = 0$ is getting occupied with macroscopic number of particles. Substituting this expression back into (1.8.7), we find that in the presence of BEC, the one-body density matrix does not vanish at large distances, but approaches a finite value

$$n^{(1)}(s)_{s \rightarrow \infty} \rightarrow n_0, \quad (1.8.9)$$

fixed by the condensate density $n_0 = N_0/V$.

This kind of behavior is quite expected. Indeed, qualitative treatment of the Bose-Einstein distribution, conducted earlier, showed, that bosons exhibit a tendency of “bunching” together as a manifestation of the positive correlation, existing between the particles. This correlation does not vanish at large distances and serves as a source of a long-range order.

1.8.2 Order parameter and spontaneous symmetry breaking

The long-range order exhibited by the one-body density matrix is strongly connected with the behavior of its eigenvalues n_i , defined by the solution of the following eigen equation:

$$\int d\mathbf{r}' n^{(1)}(\mathbf{r}, \mathbf{r}') \phi_i(\mathbf{r}') = n_i \phi_i(\mathbf{r}). \quad (1.8.10)$$

Solutions of (1.8.10) provide a natural basis of orthonormalized single-particle wave functions: $\int \phi_i^*(\mathbf{r}) \phi_j(\mathbf{r}) d\mathbf{r} = \delta_{ij}$. By multiplying (1.8.10) by $\phi_i^*(\mathbf{r})$ and integrating over $\mathbf{r}$, one finds the normalization condition $\sum_i n_i = N$, which follows from the completeness relation $\sum_i \phi_i^*(\mathbf{r}) \phi_i(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$ and from the normalization of the diagonal density.

The knowledge of the eigenfunctions $\phi_i(\mathbf{r})$ and eigenvalues n_i permits us to write the density matrix in a useful diagonal form:

$$n^{(1)}(\mathbf{r}, \mathbf{r}') = \sum_i n_i \phi_i^*(\mathbf{r}) \phi_i(\mathbf{r}'). \quad (1.8.11)$$

In the language of second quantization, the eigenvalues n_i provide the single-particle occupation numbers, relative to the single-particle states $\phi_i(\mathbf{r})$.

As we have seen above, in the presence of BEC different parts of the density matrix have different long-distance behavior. Therefore, it is a good idea to extract the condensate term from (1.8.11) and rewrite the resulting expression as

$$n^{(1)}(\mathbf{r}, \mathbf{r}') = N_0 \phi_0^*(\mathbf{r}) \phi_0(\mathbf{r}') + \sum_{i \neq 0} n_i \phi_i^*(\mathbf{r}) \phi_i(\mathbf{r}'). \quad (1.8.12)$$

In the thermodynamic limit, the sum with $i \neq 0$ can be replaced by a proper integration, which tends to zero at large distances $s = |\mathbf{r} - \mathbf{r}'|$. Vice versa, the contribution of the condensate remains finite up to distances $|\mathbf{r} - \mathbf{r}'|$, fixed by the extension of the function $\phi_0(\mathbf{r})$.

Now we are ready to introduce the order parameter. For this, we will use the single particle wave functions $\phi_i(\mathbf{r})$ to write the field operator $\hat{\Psi}(\mathbf{r})$ in the following form:

$$\hat{\Psi}(\mathbf{r}) = \sum_i \phi_i(\mathbf{r}) \hat{a}_i. \quad (1.8.13)$$

Here, as usual, $\hat{a}_i$ and $\hat{a}_i^\dagger$ are the creation and annihilation operators of a particle in a state $\phi_i(\mathbf{r})$. Separating the condensate term $i = 0$ as earlier, we obtain:

$$\hat{\Psi}(\mathbf{r}) = \phi_0(\mathbf{r}) \hat{a}_0 + \sum_{i \neq 0} \phi_i(\mathbf{r}) \hat{a}_i. \quad (1.8.14)$$

This equation provides the natural starting point to develop the *Bogoliubov approximation*, which consists of replacing the operators $\hat{a}_0$ and $\hat{a}_0^\dagger$ with the c -number $\sqrt{N_0}$. This is equivalent to ignoring the noncommutativity of the operators $\hat{a}_0$ and $\hat{a}_0^\dagger$ and is a good approximation for describing the macroscopic phenomena associated with BEC, for which $N_0 = \langle \hat{a}_0^\dagger \hat{a}_0 \rangle \gg 1$.

In fact, the commutator of $\hat{a}_0$ and $\hat{a}_0^\dagger$ is equal to 1, while the operators themselves are of order $\sqrt{N_0}$. Thus, the Bogoliubov approximation is equivalent to treating the macroscopic component $\phi_0\hat{a}_0$ of the field operator (1.8.14) as a classical field, so that (1.8.14) can be written as

$$\hat{\Psi}(\mathbf{r}) = \Psi_0(\mathbf{r}) + \delta\hat{\Psi}(\mathbf{r}), \quad (1.8.15)$$

where we have defined $\Psi_0 = \sqrt{N_0}\phi_0$ and $\delta\hat{\Psi} = \sum_{i \neq 0} \phi_i \hat{a}_i$. If one can neglect the noncondensate component $\delta\hat{\Psi}$, as happens, for example, in dilute Bose gases at very low temperatures, then the field operator coincides exactly with the classical field Ψ_0 and the system behaves like a classical object.

The function $\Psi_0(\mathbf{r})$ is called the wave function of the condensate and plays the role of an order parameter. It is a complex quantity, characterized by a modulus and a phase:

$$\Psi_0(\mathbf{r}) = |\Psi_0(\mathbf{r})| e^{iS(\mathbf{r})}. \quad (1.8.16)$$

The modulus determines the contribution of the condensate to the diagonal density (1.8.5). The phase $S(\mathbf{r})$ plays a major role in describing the coherence and superfluid phenomena.

The order parameter (1.8.16) characterizes the condensed phase and vanishes above the critical temperature. As one can readily observe, it is defined only up to a constant phase factor, so one can always multiply it by $e^{i\alpha}$ without changing any physical property. This reflects the gauge symmetry, manifested in all physical equations of the problem.

Making an explicit choice of the value of the order parameter (and hence of its phase) corresponds to a formal breaking of the gauge invariance.

The Bogoliubov ansatz can be interpreted by saying that the expectation value $\langle \hat{\Psi} \rangle$ is different from zero. This would not be possible, if the states on the left and on the right had exactly the same number of particles. From a physical point of view, this symmetry breaking means that the condensate plays the role of a reservoir. Since $N_0 \gg 1$, adding a particle to the condensate does not change the physical properties of the system. In other words, the state $|N\rangle$, containing N particles, and the states $|N+1\rangle \propto \hat{a}_0^\dagger |N\rangle$ and $|N-1\rangle \propto \hat{a}_0 |N\rangle$ are physically equivalent, apart from the corrections of order $1/N_0$. This provides the physical ground for the spontaneous symmetry breaking phenomenon.

One more interesting feature of the order parameter should be noted. If we take the average of the field operator $\langle \hat{\Psi} \rangle$ over the stationary states, whose time dependence is governed by the law $e^{-iEt/\hbar}$, then it is easy to see that the time dependence of the condensate wave function is given by

$$\Psi_0(\mathbf{r}, t) = \Psi_0(\mathbf{r}) e^{-i\mu t/\hbar}, \quad (1.8.17)$$

where the chemical potential μ is determined by the standard statistical mechanical formula: $\mu = E(N) - E(N-1) \sim \partial E / \partial N$. Thus, the time evolution of the order parameter turns out to be ruled not by the energy, as it happens with usual wave functions, but by the chemical potential, which emerges as a key parameter in the physics of BECs.

1.9 The weakly interacting Bose gas at zero temperature

The ideal Bose gas is a very peculiar system. It is sufficient to remember that, in the presence of BEC, it has infinite compressibility. Therefore, it is not surprising that the interactions between the particles affect the properties of the gas in a dramatic way, even for very dilute samples.

The problem of the almost ideal Bose gas is not trivial, since the ground state energy is equal to zero in the absence of interactions, and traditional perturbation techniques cannot be applied.

It was first solved by Bogoliubov [15]. His theory is based on a new perturbation technique and provides the basis for modern approaches to Bose-Einstein condensation in dilute gases. Below we review this theory and the physical predictions it makes.

1.9.1 Lowest-order interaction corrections: ground state energy and equation of state

In order to treat the influence of interaction on the properties of the ideal Bose gas, we have to make an additional assumption. Namely, we will treat the rarefied samples [11, 12, 13], so that the interactions between the atoms are weak enough and the convergence of corresponding perturbation expansions is guaranteed.

In such systems, the range r_0 of the interatomic forces is much smaller than the average distance $d = n^{-1/3}$ between the particles, which is fixed by the density $n = N/V$ of the gas. This allows one to consider only configurations involving pairs of interacting atoms, while configurations with three or more particles, interacting simultaneously, can be safely ignored.

A second important consequence is that the distance between two particles is always large enough to justify the use of the asymptotic expression for the wave function of their relative motion, fixed by the scattering amplitude. This implies that all physical properties of the system can be expressed in terms of the latter quantity and do not depend on more specific details of the two-body interaction. Furthermore, we shall always consider gases at temperatures smaller than the critical temperature for Bose-Einstein condensation. This suggests that the relevant values of momenta always satisfy the inequality

$$\frac{pr_0}{\hbar} \ll 1. \quad (1.9.1)$$

At such momenta, the scattering amplitude becomes independent of energy as well as of the scattering angle and can be safely replaced with its low-energy value which, according to standard scattering theory, is determined by the s -wave scattering length a , which characterizes all effects of interaction in Bose gases.

In particular, the condition of diluteness can be written as

$$|a| \ll n^{-1/3} \quad (1.9.2)$$

and should always be explicitly satisfied. It is equivalent to requiring that the value of the so-called gas parameter $n|a|^3$ be very small, i.e. $n|a|^3 \ll 1$.

Let us write the Hamiltonian of the system in terms of the field operators $\hat{\Psi}$:

$$\hat{H} = \int \left(\frac{\hbar^2}{2m} \nabla \hat{\Psi}^\dagger \nabla \hat{\Psi} \right) d\mathbf{r} + \frac{1}{2} \int \hat{\Psi}^\dagger \hat{\Psi}^\dagger U(\mathbf{r}' - \mathbf{r}) \hat{\Psi} \hat{\Psi} d\mathbf{r}' d\mathbf{r}. \quad (1.9.3)$$

Here $U(\mathbf{r})$ is the two-body interaction potential.

For a uniform gas occupying a volume V , the field operators can be conveniently written as a superposition of the plane wave functions:

$$\hat{\Psi}(\mathbf{r}) = \sum_{\mathbf{p}} \hat{a}_{\mathbf{p}} \frac{1}{\sqrt{V}} e^{i\mathbf{r} \cdot \mathbf{p} / \hbar}. \quad (1.9.4)$$

Substitution of (1.9.4) into (1.9.3) gives an equivalent expression for the Hamiltonian

$$\hat{H} = \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{1}{2V} \sum_{\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}} U_{\mathbf{q}} \hat{a}_{\mathbf{p}_1 + \mathbf{q}}^\dagger \hat{a}_{\mathbf{p}_2 - \mathbf{q}}^\dagger \hat{a}_{\mathbf{p}_2} \hat{a}_{\mathbf{p}_1}, \quad (1.9.5)$$

in which $U_{\mathbf{p}} = \int U(\mathbf{r}) \exp[-i\mathbf{q} \cdot \mathbf{r}] d\mathbf{r}$.

In the real systems the interatomic potential always contains a short-range term, which makes it difficult to obtain the solution of the Schrodinger equation at the microscopic level. In particular, the scattering of slow particles cannot be worked out using perturbation theory. On the other hand, in virtue of the above discussion on the diluteness criteria, we conclude, that the actual form of the two-body potential is not important for describing the macroscopic properties of the gas, if it gives the correct value of the s -wave scattering length.

In order to work out the many-body formalism in the simplest way, it is therefore convenient to replace the microscopic potential U with an effective soft potential U_{eff} , to which perturbation theory can be safely applied. Since the physical properties must depend uniquely on the values of the scattering length, this procedure will provide the correct answer to the many-body problem as far as the macroscopic properties of the system are concerned.

Since only small momenta are involved in the solution of the many-body problem, we are only allowed to consider the value $q = 0$ of the Fourier transform of U_{eff} :

$$U_0 = \int U_{eff} d\mathbf{r}. \quad (1.9.6)$$

With this ansatz, the Hamiltonian (1.9.5) takes the following form:

$$\hat{H} = \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{1}{2V} U_0 \sum_{\mathbf{p}_1 + \mathbf{q}} \hat{a}_{\mathbf{p}_1 + \mathbf{q}}^\dagger \hat{a}_{\mathbf{p}_2 - \mathbf{q}}^\dagger \hat{a}_{\mathbf{p}_2} \hat{a}_{\mathbf{p}_1}. \quad (1.9.7)$$

The crucial point of the theory now is to use the Bogoliubov prescription, i.e. to replace the operator $\hat{a}_0$ with a c -number

$$\hat{a}_0 = \sqrt{N} \quad (1.9.8)$$

in the Hamiltonian (1.9.7).

This operation is perfectly justified. Indeed, in a dilute gas at $T = 0$, the occupation numbers of states with $\mathbf{p} \neq 0$ are finite but small. This means that

in the first approximation we can neglect all the terms in the Hamiltonian (1.9.7) containing the operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$ with $\mathbf{p} \neq 0$. Since in the same approximation $N_0 \approx N$, one can replace $\hat{a}_0$ with $\sqrt{N}$. Consequently, the ground state energy takes the following form:

$$E_0 = \frac{N^2 U_0}{2V}. \quad (1.9.9)$$

To the same order of approximation one can easily express the parameter U_0 of (1.9.9) in terms of the scattering length a , using the result $U_0 = 4\pi\hbar^2 a/m$ of the Born approximation. The ground state energy (1.9.9) can then be written as

$$E_0 = \frac{1}{2} N n g, \quad (1.9.10)$$

where $n = N/V$ is the density of the gas and the relevant interaction coupling constant

$$g = \frac{4\pi\hbar^2 a}{m}, \quad (1.9.11)$$

is fixed by the s -wave scattering length a .

Equation (1.9.10) shows that, unlike the ideal gas case, the pressure of a weakly interacting Bose gas does not vanish at zero temperature:

$$P = -\frac{\partial E_0}{\partial V} = \frac{g n^2}{2}. \quad (1.9.12)$$

Accordingly, the compressibility is also finite

$$\frac{\partial n}{\partial P} = \frac{1}{g n} \quad (1.9.13)$$

and tends to infinity when $g \rightarrow 0$. With the help of the hydrodynamic relation

$$\frac{1}{m c^2} = \frac{\partial n}{\partial P} \quad (1.9.14)$$

one obtains the following expression for the sound velocity:

$$c = \sqrt{\frac{g n}{m}} \quad (1.9.15)$$

In the next section we will prove that this result for c coincides with the value obtained by starting from the dispersion relation of the elementary excitations in the long wavelength limit.

The condition of thermodynamic stability implies that the quantity $\partial n / \partial P$ must be positive, i.e. $a > 0$. We then arrive at the important conclusion, that a dilute Bose-Einstein condensed gas can exist only if the value of the s -wave scattering length is positive.

It is finally important to remark that, unlike the ideal gas, the chemical potential of the interacting gas is not equal to zero, but is given by

$$\mu = \frac{\partial E_0}{\partial N} = g n \quad (1.9.16)$$

and is always positive at zero temperature. Using the result (1.9.15) for the sound velocity, one can always write the chemical potential of a dilute Bose gas as

$$\mu = mc^2. \quad (1.9.17)$$

These kinds of curious parallels with relativistic physics will frequently emerge in the future.

1.9.2 Higher order approximation: excitation spectrum and quantum fluctuations

Result (1.9.10) for the ground state energy has been obtained by taking into account in (1.9.7) only the particle operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$ with $\mathbf{p} = 0$. Terms, containing only one particle operator with $\mathbf{p} \neq 0$, do not enter the Hamiltonian (1.9.7) because of the momentum conservation. Therefore, by retaining all the quadratic contributions in the particle operators with $\mathbf{p} \neq 0$, one obtains the following decomposition of the Hamiltonian:

$$\begin{aligned} \hat{H} = & \frac{U_0}{2V} \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 + \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} \\ & + \frac{U_0}{2V} \sum_{\mathbf{p} \neq 0} \left(4\hat{a}_0^\dagger \hat{a}_{\mathbf{p}}^\dagger \hat{a}_0 \hat{a}_{\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger \hat{a}_0 \hat{a}_0 + \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}} \right) \end{aligned} \quad (1.9.18)$$

As previously, we can replace $\hat{a}_0^\dagger$ and $\hat{a}_0$ with $\sqrt{N}$ in the third term of (1.9.18). However, in the first term one has to work with higher accuracy by using the normalization relation $\hat{a}_0^\dagger \hat{a}_0 + \sum_{\mathbf{p} \neq 0} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} = N$ or, neglecting the higher-order terms,

$$\hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 = N^2 - 2N \sum_{\mathbf{p} \neq 0} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}}. \quad (1.9.19)$$

An analogous situation takes place when one looks for the relation between U_0 and the scattering length a beyond the lowest-order Born approximation. In this case, one has to calculate a up to quadratic terms in U_0 . Using higher-order perturbation theory, one finds the following result

$$a = \frac{m}{4\pi\hbar} \left(U_0 + \frac{U_0^2}{V} \sum_{\mathbf{p} \neq 0} \frac{m}{p^2} \right) \quad (1.9.20)$$

or, with equivalent accuracy,

$$U_0 = g \left(1 + \frac{g}{V} \sum_{\mathbf{p} \neq 0} \frac{m}{p^2} \right), \quad (1.9.21)$$

where g is related to the scattering length by (1.9.11).

Equation (1.9.21) renormalizes the relationship between the effective potential and the physical coupling constant g . The divergency occurring for large $\mathbf{p}$ in the summation of (1.9.21) is the consequence of the replacement of the matrix element $U_{\mathbf{q}}$ with the constant value U_0 . This term is crucial to assure a convergent result for the ground state energy calculated to the higher-order of approximation.

Substitution of (1.9.19) and (1.9.21) into (1.9.18) yields the following expression for the Hamiltonian:

$$\hat{H} = g \frac{N^2}{2V} + \sum \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{1}{2} g n \sum_{\mathbf{p} \neq 0} \left(2 \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger + \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}} + \frac{m g n}{p^2} \right) \quad (1.9.22)$$

which turns out to be uniquely fixed by the interaction coupling constant g .

The Hamiltonian (1.9.22) is quadratic in the operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$ and can be diagonalized by a linear transformation

$$\hat{a}_{\mathbf{p}} = u_{\mathbf{p}} \hat{b}_{\mathbf{p}} + v_{-\mathbf{p}}^* \hat{b}_{-\mathbf{p}}^\dagger, \quad \hat{a}_{\mathbf{p}}^\dagger = u_{\mathbf{p}}^* \hat{b}_{\mathbf{p}}^\dagger + v_{-\mathbf{p}} \hat{b}_{-\mathbf{p}}, \quad (1.9.23)$$

known as the Bogoliubov transformation. This transformation introduces a new set of operators, $\hat{b}_{\mathbf{p}}$ and $\hat{b}_{\mathbf{p}}^\dagger$, to which we impose the same Bose commutation relations $\hat{b}_{\mathbf{p}} \hat{b}_{\mathbf{p}'}^\dagger - \hat{b}_{\mathbf{p}}^\dagger \hat{b}_{\mathbf{p}'} = \delta_{\mathbf{p}\mathbf{p}'}$, obeyed by the original particle operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$.

It is easily verified, that the commutation relations are satisfied, if

$$|u_{\mathbf{p}}|^2 - |v_{-\mathbf{p}}|^2 = 1, \quad (1.9.24)$$

i.e. if one can write

$$u_{\mathbf{p}} = \cosh \alpha_{\mathbf{p}}, \quad v_{-\mathbf{p}} = \sinh \alpha_{\mathbf{p}}. \quad (1.9.25)$$

The value of the parameter $\alpha_{\mathbf{p}}$ will be chosen such that the coefficients of the non-diagonal terms $\hat{b}_{\mathbf{p}}^\dagger \hat{b}_{-\mathbf{p}}^\dagger$ and $\hat{b}_{\mathbf{p}} \hat{b}_{\mathbf{p}}$ in the Hamiltonian (1.9.22) vanish. The corresponding condition has the form:

$$\frac{g n}{2} (|u_{\mathbf{p}}|^2 + |v_{-\mathbf{p}}|^2) + \left(\frac{p^2}{2m} + g n \right) u_{\mathbf{p}} v_{-\mathbf{p}} = 0. \quad (1.9.26)$$

Using the properties $\cosh 2\alpha = \cosh^2 \alpha + \sinh^2 \alpha$ and $\sinh 2\alpha = 2 \cosh \alpha \sinh \alpha$, one immediately finds, that (1.9.26) is solved by choosing

$$\coth 2\alpha_{\mathbf{p}} = -\frac{p^2/2m + g n}{g n} \quad (1.9.27)$$

and that the explicit form of the coefficients $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$ becomes

$$u_{\mathbf{p}}, v_{-\mathbf{p}} = \pm \left(\frac{p^2/2m + g n}{2\varepsilon(\mathbf{p})} \pm \frac{1}{2} \right)^{1/2}, \quad (1.9.28)$$

where $\varepsilon(\mathbf{p})$ is given by (1.9.31) below.

By virtue of the Bogoliubov transformation (1.9.23) and of result (1.9.28) for $u_{\mathbf{p}}$ and $v_{\mathbf{p}}$, the Hamiltonian (1.9.22) can be finally reduced to the diagonal form:

$$\hat{H} = E_0 + \sum \varepsilon(\mathbf{p}) \hat{b}_{\mathbf{p}}^\dagger \hat{b}_{\mathbf{p}}, \quad (1.9.29)$$

where

$$E_0 = g \frac{N^2}{2V} + \frac{1}{2} \sum_{\mathbf{p} \neq 0} \left[\varepsilon(\mathbf{p}) - g n - \frac{p^2}{2m} + \frac{m(g n)^2}{p^2} \right] \quad (1.9.30)$$

is the ground state energy calculated to the higher-order of approximation and

$$\varepsilon(\mathbf{p}) = \left[\frac{gn}{m} p^2 + \left(\frac{p^2}{2m} \right)^2 \right]^{1/2} \quad (1.9.31)$$

is the famous Bogoliubov dispersion law for the elementary excitations of the system.

Results (1.9.29)-(1.9.31) have a deep physical meaning. They show that the original system of interacting particles can be described in terms of a Hamiltonian of independent quasi-particles having energy $\varepsilon(\mathbf{p})$, and whose annihilation and creation operators are given, respectively, by $\hat{b}_{\mathbf{p}}$ and $\hat{b}_{\mathbf{p}}^\dagger$. The ground state of the interacting system then corresponds to the vacuum of quasi-particles

$$\hat{b}_{\mathbf{p}}|\text{vac}\rangle = 0 \quad (1.9.32)$$

for any $\mathbf{p} \neq 0$.

The ground state energy (1.9.30) can be easily calculated by replacing the sum with an integral in the momentum space. The result is

$$E_0 = g \frac{N^2}{2V} \left[1 + \frac{128}{15\sqrt{\pi}} (na^3)^{1/2} \right], \quad (1.9.33)$$

while the chemical potential $\mu = \partial E_0 / \partial N$ is given by

$$\mu = gn \left[1 + \frac{32}{3\sqrt{\pi}} (na^3)^{1/2} \right]. \quad (1.9.34)$$

The condensate density

$$n_0 \equiv \frac{N_0}{V} = n \left[1 - \frac{8}{3\sqrt{\pi}} (na^3)^{1/2} \right] \quad (1.9.35)$$

reveals that the quantum depletion of the condensate is fixed by the same parameter $\sqrt{na^3}$, which characterizes the first corrections to the ground state energy.

It is not difficult to see that in the integration, yielding the above results, only values $p \sim \sqrt{mgn} = mc$ are important. For such momenta, the parameter $pa/\hbar \sim (na^3)^{1/2}$ is very small compared to the unity, which is consistent with our initial assumptions. This justifies a posteriori the replacement of $U_{\mathbf{q}}$ with U_0 made in the calculation of the renormalized scattering length (1.9.20).

It is also worth pointing out that the perturbation parameter of the expansion (1.9.33) is given by $(na^3)^{1/2}$. One can show that the next term in the expansion is proportional to $na^3 \ln(na^3)$. The coefficient in front of the logarithm can also be calculated with a proper accuracy. The term inside the logarithm, however, depends on the details of the interaction.

1.9.3 Particles and elementary excitations

Thus, the excited states of an interacting Bose gas can be described in terms of a gas of noninteracting quasi-particles (see (1.9.29)).

For small momenta $p \ll mc$ the dispersion law (1.9.31) of quasi-particles takes the phonon-like form

$$\varepsilon(p) = cp, \quad (1.9.36)$$

where $c = \sqrt{gn/m}$ is the sound velocity. This coincides with the result (1.9.15), derived by starting from the equation of state (1.9.12). The Bogoliubov theory then predicts that the long wavelength excitations of an interacting Bose gas are sound waves.

It is also worth noticing that in the phonon regime the coefficients (1.9.28), characterizing the Bogoliubov transformation (1.9.23), exhibit a divergent infrared behavior: $u_{\mathbf{p}} \rightarrow -v_{-\mathbf{p}} \rightarrow (mc/2p)^{1/2}$. This reflects the fact that in this regime the Bogoliubov transformation introduces a drastic modification in the nature of elementary excitations with respect to the ideal gas.

In the opposite limit $p \gg mc$, the dispersion law approaches the free particle law:

$$\varepsilon(p) \approx \frac{p^2}{2m} + gn. \quad (1.9.37)$$

Correspondingly, one has $|v_{-\mathbf{p}}| \ll |u_{\mathbf{p}}| \sim 1$ and $a_{\mathbf{p}} \sim b_{\mathbf{p}}$.

The transition between the phonon and particle regimes takes place when $p^2/2m \sim gn = mc^2$, i.e. for $p \sim mc$ (see Fig.1.9). By setting $p^2/2m = gn$ with $p = \hbar/\xi$, one can define the characteristic interaction length

$$\xi = \sqrt{\frac{\hbar^2}{2mgn}} = \frac{1}{\sqrt{2}} \frac{\hbar}{mc}, \quad (1.9.38)$$

also called the healing length, which plays important role in theory of non-uniform Bose gases.

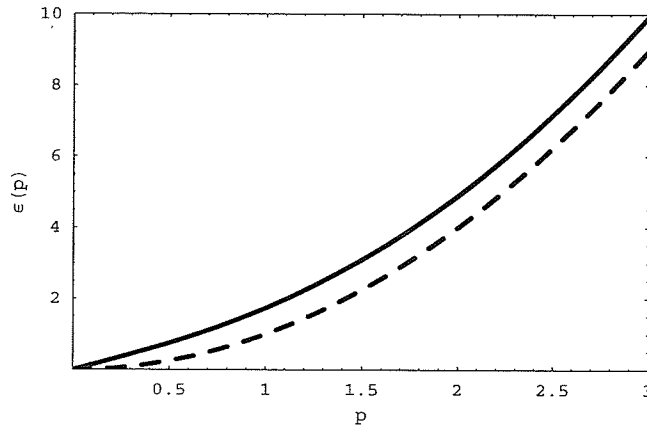


Figure 1.9: Bogoliubov dispersion of elementary excitations (see (1.9.31) with $gn = mc^2$). Solid line is the actual curve $\varepsilon(p)$, dashed line corresponds to free particle regime ($p^2/2m$). It is well seen that the physics at small momenta is determined by the phonon excitations (cp). The transition between the phonon and the free particle regimes takes place at $p \sim \hbar/\xi$. Energy is given in units of mc^2 , momentum in units of $\hbar/\xi$.

1.10 The weakly-interacting Bose gas at finite temperatures

The theory of weakly interacting Bose gases at zero temperature is a well established subject. Many of the questions of interest have been settled years ago and have become a standard topic of numerous textbooks. In contrast, the treatment of finite-temperature behavior of these systems is still far from being elaborate.

In the next few sections we will review the current progress being made in the area followed by the formulation of our approach to the investigation of the thermal properties of weakly interacting uniform Bose gases at temperatures below critical.

1.10.1 Thermo-field dynamics

In order to incorporate the temperature effects into consideration, one has to treat the systems under study as open ones, exchanging the energy and matter freely with the thermal reservoir. That requires the use of the techniques of the field theory at finite temperature and density (FTFT), or statistical field theory.

One especially physically transparent approach from this family is the *thermo-field dynamics* (TFD) [10]. It is essentially the extension of the secondary quantization formalism used earlier to treat the zero-temperature problems.

Below, we will review this method and will subsequently use it to perform calculations of the interaction corrections to the thermal properties of ideal Bose gases. The equivalence between the TFD framework and modern finite-temperature path integral formulation is exposed in Appendix A.

Quantum excitations at finite temperature

Let us imagine an open system, freely exchanging the particles and energy with a reservoir, maintained at constant inverse temperature β . As usual, the process of annihilation of a quantum of energy $\omega(\mathbf{k}, \beta)$ in such a system can be regarded as the action of an operator $a(\mathbf{k})$, which satisfies the familiar Bose commutation relation:

$$[a(\mathbf{k}), a^\dagger(\mathbf{p})] = \delta(\mathbf{k} - \mathbf{p}). \quad (1.10.1)$$

However, as distinct from the zero temperature case, the operator $a(\mathbf{k})$ now has an internal structure, which incorporates two independent kinds of thermal effects:

1. annihilation of quanta in the system, and
2. creation of the (Dirac) "holes" of particles maintained by the reservoir.

When the latter process takes place, we say that an $\tilde{\alpha}^\dagger(\mathbf{k}, \beta)$ -quantum (hole) with a negative energy $[-\hbar\omega(\mathbf{k})]$ and negative momentum $[-\hbar\mathbf{k}]$ is created. Correspondingly, the former process will be described by the temperature dependent annihilation operator $\alpha(\mathbf{k}, \beta)$.

Since $a(\mathbf{k})$ now performs two independent operations, it should be represented as the following linear combination:

$$a(\mathbf{k}) = c(\mathbf{k}, \beta)\alpha(\mathbf{k}, \beta) + d(\mathbf{k}, \beta)\tilde{\alpha}^\dagger(\mathbf{k}, \beta), \quad (1.10.2)$$

where $c(\mathbf{k}, \beta)$ and $d(\mathbf{k}, \beta)$ are certain c -number functions. Similarly, the creation operator is

$$a^\dagger(\mathbf{k}) = c^*(\mathbf{k}, \beta)\alpha^\dagger(\mathbf{k}, \beta) + d^*(\mathbf{k}, \beta)\tilde{\alpha}(\mathbf{k}, \beta). \quad (1.10.3)$$

By construction, the introduced α -operators satisfy the Bose commutation relations. This suggests, that the relations (1.10.2-1.10.3) could be regarded as the canonical transformation, which implies

$$c(\mathbf{k}, \beta)c^*(\mathbf{k}, \beta) - d(\mathbf{k}, \beta)d^*(\mathbf{k}, \beta) = 1. \quad (1.10.4)$$

Additionally, the phase factors of the above coefficients could be absorbed by those of the respective operators, so we can choose $c(\mathbf{k}, \beta)$ and $d(\mathbf{k}, \beta)$ to be real.

Thus, the need to incorporate the thermal effects leads, in fact, to the doubling of degrees of freedom. The resulting Fock space has twice as many dimensions as its zero temperature counterpart and could be constructed by the action of the $\alpha^\dagger(\mathbf{k}, \beta)$ and $\tilde{\alpha}^\dagger(\mathbf{k}, \beta)$ operators on the thermal vacuum $|0, \beta\rangle$, parameterized by the inverse temperature β .

In order to establish the explicit form of the coefficients $c(\mathbf{k}, \beta)$ and $d(\mathbf{k}, \beta)$, subject to constraint (1.10.4), the following reasoning is used. Since the operator $a^\dagger(\mathbf{k})$ in our construction takes care of the excitations in the system, the corresponding quantum number density operator is given by:

$$N(\mathbf{k}) = a^\dagger(\mathbf{k})a(\mathbf{k}). \quad (1.10.5)$$

Then, since the model we consider is nothing else but the grand canonical ensemble, we may require, that the vacuum average of $N(\mathbf{k})$ should be equal to the corresponding value of the number density in statistical mechanics, i.e.

$$n(\mathbf{k}) = \frac{(2\pi)^3}{V} \langle 0, \beta | N(\mathbf{k}) | 0, \beta \rangle = f(\omega), \quad (1.10.6)$$

where

$$f(\omega) = \frac{1}{e^{\beta\omega(\mathbf{k},\beta)} - 1}. \quad (1.10.7)$$

This results in the following coefficient values:

$$c(\mathbf{k}, \beta) = \sqrt{1 + f(\omega)}, \quad d(\mathbf{k}, \beta) = \sqrt{f(\omega)}. \quad (1.10.8)$$

The relation (1.10.6) constitutes the axiom, which determines the density of the system in a thermal equilibrium state. It can easily be extended to any compound operator, consisting of α and $\alpha^\dagger$, say $A(\alpha, \alpha^\dagger)$. Thus, the vacuum expectation value of the field operator $\langle 0, \beta | A(\alpha, \alpha^\dagger) | 0, \beta \rangle$ becomes equal to the ensemble average of the function $A(\alpha, \alpha^\dagger)$. In this way, the statistical mechanics of a quantum many-body system becomes a quantum field theory realized in the temperature-dependent Fock space. This formalism is called *thermo field dynamics*.

The form of relations (1.10.2) and (1.10.3) suggests, that the tilde and non-tilde operators are related to each other. Indeed, there is a general TFD "tilde-conjugation" operation, which is valid not only for the elementary creation and annihilation operators, but also for their arbitrary compound functions O_1 and O_2 :

$$\widetilde{\widetilde{O_1 O_2}} = \widetilde{O_1} \widetilde{O_2}, \quad (1.10.9)$$

$$c_1 \widetilde{\widetilde{O_1}} + c_2 \widetilde{\widetilde{O_2}} = c_1^* \widetilde{O_1} + c_2^* \widetilde{O_2}, \quad (1.10.10)$$

$$\widetilde{\widetilde{O}} = O. \quad (1.10.11)$$

Constructing the free TFD Hamiltonian $\hat{H}_0$ is now straightforward. It could be written as the following:

$$\hat{H}_0 = H_0 - \tilde{H}_0, \quad (1.10.12)$$

with

$$H_0 = \hbar \int d\mathbf{k} \omega(\mathbf{k}) \alpha^\dagger(\mathbf{k}, \beta) \alpha(\mathbf{k}, \beta), \quad (1.10.13)$$

$$\tilde{H}_0 = \hbar \int d\mathbf{k} \omega(\mathbf{k}) \tilde{\alpha}^\dagger(\mathbf{k}, \beta) \tilde{\alpha}(\mathbf{k}, \beta) \quad (1.10.14)$$

or, equivalently, with the use of the canonical transformation,

$$H_0 = \hbar \int d\mathbf{k} \omega(\mathbf{k}) a^\dagger(\mathbf{k}) a(\mathbf{k}), \quad (1.10.15)$$

$$\tilde{H}_0 = \hbar \int d\mathbf{k} \omega(\mathbf{k}) \tilde{a}^\dagger(\mathbf{k}) \tilde{a}(\mathbf{k}). \quad (1.10.16)$$

The minus sign in (1.10.12) takes care of the fact, that the tilde-excitations carry negative energy and momenta.

The examples of TFD free fields and their two-point functions

Let us now consider a simple example of the TFD free field. Since in non-relativistic many-body theory one has to deal with the Schrodinger equation in operator form, the latter will be the point of our interest.

Suppose that a free field Ψ_0 satisfies the equation $\lambda(\partial)\Psi_0 = 0$ with the following $\lambda(\partial)$ operator:

$$\lambda(\partial) = i \frac{\partial}{\partial t} - \omega(\nabla). \quad (1.10.17)$$

Then the expressions for the tilde- and non-tilde Hamiltonians read:

$$H_0 = \int dx \Psi_0^\dagger \omega(\nabla) \Psi_0, \quad (1.10.18)$$

$$\tilde{H}_0 = \int dx \tilde{\Psi}_0^\dagger \omega(-\nabla) \tilde{\Psi}_0. \quad (1.10.19)$$

Here the relation $\omega^*(\nabla) = \omega(-\nabla)$ due to the tilde-conjugation rules (1.10.9-1.10.11) was considered. Corresponding equations of motion

$$i \frac{\partial}{\partial t} \Psi_0(\mathbf{x}) = [\Psi_0(\mathbf{x}), H_0], \quad (1.10.20)$$

$$i \frac{\partial}{\partial t} \tilde{\Psi}_0(\mathbf{x}) = - [\tilde{\Psi}_0(\mathbf{x}), \tilde{H}_0]. \quad (1.10.21)$$

have the following formal solutions:

$$\Psi_0(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{k} a(\mathbf{k}) \exp[i\mathbf{k} \cdot \mathbf{x} - i\omega(\mathbf{k})t], \quad (1.10.22)$$

$$\tilde{\Psi}_0(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{k} \tilde{a}(\mathbf{k}) \exp[-i\mathbf{k} \cdot \mathbf{x} + i\omega(\mathbf{k})t]. \quad (1.10.23)$$

In order to operate with two functional degrees of freedom more conveniently, it is useful to simplify the notation by introducing the following thermal doublet symbol:

$$\begin{pmatrix} \Psi^1 \\ \Psi^2 \end{pmatrix} = \begin{pmatrix} \Psi_0 \\ \tilde{\Psi}_0^\dagger \end{pmatrix}. \quad (1.10.24)$$

The free causal two-point function is then defined by

$$G^{(0)\alpha\beta}(x-y) = \langle 0, \beta | T[\Psi^\alpha(x), \Psi^{\beta\dagger}(y)] | 0, \beta \rangle \quad (1.10.25)$$

$$\begin{aligned} &= \theta(t_x - t_y) \langle 0, \beta | \Psi^\alpha(x) \Psi^{\beta\dagger}(y) | 0, \beta \rangle \\ &+ \theta(t_y - t_x) \langle 0, \beta | \Psi^{\beta\dagger}(y) \Psi^\alpha(x) | 0, \beta \rangle, \end{aligned} \quad (1.10.26)$$

where the symbol T denotes the ordering along the time path. Using (1.10.22), (1.10.23) and considering the canonical transformations (1.10.2) and (1.10.3), one may find, that in the momentum representation this function reads:

$$G^{(0)\alpha\beta}(k_0, \mathbf{k}) = \begin{pmatrix} \frac{c^2(\omega)}{k_0 - \omega + i\epsilon} - \frac{d^2(\omega)}{k_0 - \omega - i\epsilon}, & \frac{c(\omega)d(\omega)}{k_0 - \omega + i\epsilon} - \frac{c(\omega)d(\omega)}{k_0 - \omega - i\epsilon} \\ \frac{c(\omega)d(\omega)}{k_0 - \omega + i\epsilon} - \frac{d^2(\omega)}{k_0 - \omega - i\epsilon}, & \frac{c^2(\omega)}{k_0 - \omega + i\epsilon} - \frac{d^2(\omega)}{k_0 - \omega - i\epsilon} \end{pmatrix} \quad (1.10.27)$$

where $\omega = \omega(\mathbf{k})$ and the coefficients $c(\omega), d(\omega)$ are given by (1.10.8).

The free propagator (1.10.27) will be the major building block in further developments.

Field theory calculations in TFD

Perturbative calculations in TFD are very similar to those in vacuum field theory.

The doubling of degrees of freedom alluded to above leads to a 2×2 matrix structure of propagators and self energies. This feature implies that in higher orders a much larger number of diagrams has to be taken into account as compared to the vacuum theory and calculations may become cumbersome.

The Feynman diagrams, however, turn out to be topologically and combinatorically identical to those of the corresponding zero-temperature quantum field theory, but generalized to a two-component formalism. The first (type 1) component represents, by construction, the physical field, describing propagation of excitations in the system. The second (type 2) component corresponds to a “thermal ghost field”, corresponding to holes, maintained by the reservoir.

In TFD, two types of vertices occur, one type describing the interactions of the type 1 fields and the other of the type 2 fields. The Feynman rules for these two types of fields differ only by a sign in the case of even interactions. There is no direct coupling between the two types of fields, but they can propagate into each other because of the non-diagonal elements of the propagator matrix. Its 11 and 22 components correspond to physical and ghost propagators. Therefore, external lines of *physical* Green’s function are always of type 1.

In order to find a particular n -point Green’s function in momentum space, one must draw all topologically distinct diagrams with n external points of type 1 and corresponding number of vertices of type 1,2. These two types of vertices are connected to each other by propagator lines representing the elements of the free propagator matrix. As in the vacuum theory, disconnected blobs without external legs can be ignored.

To conclude, the perturbative calculations in TFD are technically the same as in vacuum field theory. Generally, their goal is to compute the 11 component of the matrix propagator, which could subsequently be used to calculate the physical parameters of interest.

Weakly interacting gas in TFD

Now we are ready to formulate the general statement of the problem of the weakly interacting Bose gas within the TFD formalism.

The system we are concerned with represents a dilute gas, consisting of N atoms obeying Bose statistics, enclosed in a box of volume V and interacting through the two-body potential $U(\mathbf{x} - \mathbf{x}')$. Interaction is assumed to be weak, which, together with the low density of the gas, allows one to neglect higher-order interactions and treat the system properties perturbatively.

For simplicity, the atoms are assumed to have zero net spin. They are described by the boson field operators $\Psi(\mathbf{x})$, $\Psi^\dagger(\mathbf{x})$ subject to the Bose commutation relations:

$$[\Psi(\mathbf{x}), \Psi(\mathbf{x}')] = 0, \quad [\Psi^\dagger(\mathbf{x}), \Psi^\dagger(\mathbf{x}')] = 0, \quad [\Psi(\mathbf{x}), \Psi^\dagger(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}'). \quad (1.10.28)$$

The system is immersed into a large heat reservoir, with which it can freely exchange both energy and particles. In the state of equilibrium both system and reservoir possess the same chemical potential μ and inverse temperature β .

The reservoir, unlike the system, maintains the negative-energy holes, represented by the operators, obtained from the ordinary ones with the help of the tilde-conjugation operation, defined in (1.10.9-1.10.11). They satisfy the same commutation relations as the regular operators, while all commutators between the tilde- and non-tilde operators vanish by construction.

In the state of equilibrium, the system contains a mixture of particles and holes. Therefore, its Hamiltonian $\hat{H}$ is given by

$$\hat{H} = K - \tilde{K}, \quad (1.10.29)$$

where

$$\begin{aligned} K = H_0 - \mu N &= \int d\mathbf{x} \Psi^\dagger(\mathbf{x}) \left[-\frac{\hbar^2}{2m} \nabla^2 - \mu \right] \Psi(\mathbf{x}) \\ &+ \frac{1}{2} \int d\mathbf{x} \int d\mathbf{x}' \Psi^\dagger(\mathbf{x}) \Psi^\dagger(\mathbf{x}') U(\mathbf{x} - \mathbf{x}') \Psi(\mathbf{x}') \Psi(\mathbf{x}) \end{aligned} \quad (1.10.30)$$

is the regular zero-temperature Hamiltonian describing the particles of the system and $\tilde{K}$ is its tilde-conjugate, describing the holes:

$$\begin{aligned} \tilde{K} = \tilde{H}_0 - \mu \tilde{N} &= \int d\mathbf{x} \tilde{\Psi}^\dagger(\mathbf{x}) \left[-\frac{\hbar^2}{2m} \nabla^2 - \mu \right] \tilde{\Psi}(\mathbf{x}) \\ &+ \frac{1}{2} \int d\mathbf{x} \int d\mathbf{x}' \tilde{\Psi}^\dagger(\mathbf{x}) \tilde{\Psi}^\dagger(\mathbf{x}') U(\mathbf{x} - \mathbf{x}') \tilde{\Psi}(\mathbf{x}') \tilde{\Psi}(\mathbf{x}). \end{aligned} \quad (1.10.31)$$

The chemical potential μ is chosen such that the vacuum average of the atom number operator is equal to the total number of particles in the system:

$$\langle \hat{N} \rangle = N. \quad (1.10.32)$$

With the Hamiltonian $\hat{H}$, one may introduce the time-dependent Heisenberg picture for any Schrodinger operator $O(\mathbf{x})$ and its tilde-conjugate $\tilde{O}(\mathbf{x})$:

$$O(\mathbf{x}, t) \equiv e^{iKt} O(\mathbf{x}) e^{-iKt}, \quad (1.10.33)$$

$$\tilde{O}(\mathbf{x}, t) \equiv e^{-i\tilde{K}t} \tilde{O}(\mathbf{x}) e^{i\tilde{K}t}. \quad (1.10.34)$$

In particular, the field operators have a time-dependence given by

$$\Psi(\mathbf{x}, t) = e^{iKt} \Psi(\mathbf{x}) e^{-iKt}, \quad \Psi^\dagger(\mathbf{x}, t) = e^{-iKt} \Psi^\dagger(\mathbf{x}) e^{iKt}, \quad (1.10.35)$$

$$\tilde{\Psi}(\mathbf{x}, t) = e^{-i\tilde{K}t} \tilde{\Psi}(\mathbf{x}) e^{i\tilde{K}t}, \quad \tilde{\Psi}^\dagger(\mathbf{x}, t) = e^{i\tilde{K}t} \tilde{\Psi}^\dagger(\mathbf{x}) e^{-i\tilde{K}t}. \quad (1.10.36)$$

In order to simplify the notation, we introduce the following thermal doublet symbol (see (1.10.24)):

$$\begin{pmatrix} \Psi^1(\mathbf{x}, t) \\ \Psi^2(\mathbf{x}, t) \end{pmatrix} = \begin{pmatrix} \Psi(\mathbf{x}, t) \\ \tilde{\Psi}^\dagger(\mathbf{x}, t) \end{pmatrix}. \quad (1.10.37)$$

The single-particle Green's function is then defined as

$$G^{\alpha\beta}(\mathbf{x}, t; \mathbf{x}', t') = \langle 0, \beta | T[\Psi^\alpha(\mathbf{x}, t), \Psi^{\beta\dagger}(\mathbf{x}', t')] | 0, \beta \rangle. \quad (1.10.38)$$

For our purposes, it is more convenient to work in the single-particle momentum representation. In this representation, the field operators $\Psi(\mathbf{x})$, $\tilde{\Psi}(\mathbf{x})$ can be written as

$$\Psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{k} a_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{x}), \quad (1.10.39)$$

$$\tilde{\Psi}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{k} \tilde{a}_{\mathbf{k}} \tilde{\phi}_{\mathbf{k}}(\mathbf{x}) \quad (1.10.40)$$

where $a_{\mathbf{k}}(a_{\mathbf{k}}^{\dagger})$ and $\tilde{a}_{\mathbf{k}}(\tilde{a}_{\mathbf{k}}^{\dagger})$ are the annihilation (creation) operators for a particle and a hole in single-particle states $\phi_{\mathbf{k}}(\mathbf{x})$ and $\tilde{\phi}_{\mathbf{k}}(\mathbf{x})$ correspondingly, obeying the following Bose commutation relations:

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}] = 0, \quad [a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}, \mathbf{k}'}; \quad (1.10.41)$$

$$[\tilde{a}_{\mathbf{k}}, \tilde{a}_{\mathbf{k}'}] = 0, \quad [\tilde{a}_{\mathbf{k}}, \tilde{a}_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}, \mathbf{k}'} \quad (1.10.42)$$

with all commutators between the tilde and non-tilde operators vanishing.

Just as in the case of fields, we may introduce the thermal doublet notation for the operators $a_{\mathbf{k}}$ and $\tilde{a}_{\mathbf{k}}$ and then write the Green's function $G^{\alpha\beta}(\mathbf{x}, t; \mathbf{x}', t')$ in the single-particle momentum representation as

$$G^{\alpha\beta}(\mathbf{x}, t; \mathbf{x}', t') = \frac{1}{(2\pi)^3} \int d\mathbf{k} \int d\mathbf{k}' \phi_{\mathbf{k}}^{\alpha}(\mathbf{x}) \phi_{\mathbf{k}'}^{\beta\dagger}(\mathbf{x}') \langle 0, \beta | T[a_{\mathbf{k}}^{\alpha}(t), a_{\mathbf{k}'}^{\beta\dagger}(t')] | 0, \beta \rangle. \quad (1.10.43)$$

In case of a uniform system governed by a time-independent Hamiltonian, the single-particle states are the plane waves

$$\phi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{V}} \exp(i\mathbf{k}\mathbf{r}), \quad (1.10.44)$$

$$\tilde{\phi}_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{V}} \exp(-i\mathbf{k}\mathbf{r}). \quad (1.10.45)$$

Similarly, $G^{\alpha\beta}(\mathbf{x}, t; \mathbf{x}', t')$ now depends only on the differences $\mathbf{x} - \mathbf{x}'$ and $t - t'$, so that

$$G^{\alpha\beta}(\mathbf{x}, t) = \int d\mathbf{k} e^{i\mathbf{k}\mathbf{x}} G^{\alpha\beta}(\mathbf{k}, t), \quad (1.10.46)$$

where

$$G^{\alpha\beta}(\mathbf{k}, t) \equiv \langle 0, \beta | T[a_{\mathbf{k}}^{\alpha}(t), a_{\mathbf{k}}^{\beta\dagger}(0)] | 0, \beta \rangle \quad (1.10.47)$$

is a single-particle Green's function in the momentum representation.

The remaining task is to calculate the Green's function $G^{\alpha\beta}(\mathbf{k}, t)$. It is complicated by a possible phase transition to a Bose-condensed state. This is signaled by a non-vanishing average of the field operator:

$$\langle 0, \beta | \Psi^{\alpha}(\mathbf{x}) | 0, \beta \rangle = \Phi_0^{\alpha}(\mathbf{x}) \neq 0. \quad (1.10.48)$$

As discussed in sect. 1.8.2, the function $\Phi_0^{\alpha}(\mathbf{x})$ is often referred to as the macroscopic wave function of the condensate and in general has an amplitude and phase.

In a uniform system, we can take $\Phi_0^\alpha(\mathbf{x})$ to be real and independent of position. In this case, $\Phi_0^\alpha(\mathbf{x})$ equals to the square root of the condensate density n_0 . We are then led to separate the boson field operator $\Psi^\alpha(\mathbf{x})$ into two parts:

$$\Psi^\alpha(\mathbf{x}) \equiv a_0^\alpha/\sqrt{V} + \bar{\Psi}^\alpha(\mathbf{x}), \quad (1.10.49)$$

$$\Psi^{\alpha\dagger}(\mathbf{x}) \equiv a_0^{\alpha\dagger}/\sqrt{V} + \bar{\Psi}^{\alpha\dagger}(\mathbf{x}). \quad (1.10.50)$$

Then, just like in the zero temperature case, we may apply the Bogoliubov prescription and replace the operators a_0^α and $a_0^{\alpha\dagger}$ by the c -number $\sqrt{N_0}$. Clearly, the new field operators $\bar{\Psi}^\alpha(\mathbf{x})$ and $\bar{\Psi}^{\alpha\dagger}(\mathbf{x})$ describe the normal phase atoms. They satisfy the Bose commutation relations and have vanishing vacuum averages:

$$\langle 0, \beta | \bar{\Psi}^\alpha(\mathbf{x}) | 0, \beta \rangle = \langle 0, \beta | \bar{\Psi}^{\alpha\dagger}(\mathbf{x}) | 0, \beta \rangle = 0. \quad (1.10.51)$$

With this modification, the thermal Green's function now becomes

$$G^{\alpha\beta}(\mathbf{x}, t; \mathbf{x}', t') = -n_0 + \bar{G}^{\alpha\beta}(\mathbf{x}, t; \mathbf{x}', t'), \quad (1.10.52)$$

where $\bar{G}^{\alpha\beta}(\mathbf{x}, t; \mathbf{x}', t')$ is its non-condensate part defined by

$$\bar{G}^{\alpha\beta}(\mathbf{x}, t; \mathbf{x}', t') \equiv -\langle 0, \beta | T[\bar{\Psi}^\alpha(\mathbf{x}, t), \bar{\Psi}^{\beta\dagger}(\mathbf{x}', t')] | 0, \beta \rangle. \quad (1.10.53)$$

Correspondingly, in the momentum representation we have, for $\mathbf{k} \neq 0$,

$$\bar{G}^{\alpha\beta}(\mathbf{k}, t) = -\langle 0, \beta | T[a_{\mathbf{k}}^\alpha(t), a_{\mathbf{k}}^{\beta\dagger}(0)] | 0, \beta \rangle. \quad (1.10.54)$$

The Bogoliubov prescription modifies the Hamiltonian (1.10.29) fundamentally. In order to simplify the consideration, we will concentrate for a while on its zero-temperature part K only, making a straightforward generalization to TFD later on. After all of the above transformations, K reads

$$K = E_0 - \mu N_0 + \frac{1}{V} \sum_{\mathbf{k} \neq 0} (\varepsilon_{\mathbf{k}} - \mu) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{j=1}^7 \hat{V}_j, \quad (1.10.55)$$

where the interaction term $\hat{V}$ can be separated into the following eight distinct

parts:

$$E_0 = \frac{1}{2} n_0^2 V U(0), \quad (1.10.56)$$

$$\hat{V}_1 = \frac{1}{2} n_0 \sum_{\mathbf{k}} U(\mathbf{k}) a_{\mathbf{k}} a_{-\mathbf{k}}, \quad (1.10.57)$$

$$\hat{V}_2 = \frac{1}{2} n_0 \sum_{\mathbf{k}} U(\mathbf{k}) a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}, \quad (1.10.58)$$

$$\hat{V}_3 = n_0 \sum_{\mathbf{k}} U(\mathbf{k}) a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \quad (1.10.59)$$

$$\hat{V}_4 = n_0 \sum_{\mathbf{k}} U(0) a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \quad (1.10.60)$$

$$\hat{V}_5 = \frac{n_0^{1/2}}{V^{1/2}} \sum_{\mathbf{k}, \mathbf{q}} U(\mathbf{q}) a_{\mathbf{k}+\mathbf{q}} a_{\mathbf{k}} a_{\mathbf{q}}, \quad (1.10.61)$$

$$\hat{V}_6 = \frac{n_0^{1/2}}{V^{1/2}} \sum_{\mathbf{k}, \mathbf{q}} U(\mathbf{q}) a_{\mathbf{k}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{k}+\mathbf{q}}, \quad (1.10.62)$$

$$\hat{V}_7 = \frac{1}{2V} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} U(\mathbf{q}) a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger a_{\mathbf{k}'} a_{\mathbf{k}} \quad (1.10.63)$$

with

$$U(\mathbf{q}) \equiv \int d\mathbf{x} e^{i\mathbf{q} \cdot \mathbf{x}} U(\mathbf{x}). \quad (1.10.64)$$

In a normal system ($n_0 = 0$) only $\hat{V}_7$ is present. Also, K has no terms containing a single operator $a_{\mathbf{k}}^\dagger$ or $a_{\mathbf{k}}$, because that would violate the momentum conservation. This is in agreement with (1.10.51), which gives, in momentum representation,

$$\langle 0, \beta | a_{\mathbf{k}} | 0, \beta \rangle = \langle 0, \beta | a_{\mathbf{k}}^\dagger | 0, \beta \rangle = 0, \quad (\mathbf{k} \neq 0). \quad (1.10.65)$$

The fact that there exist interaction terms such as $\hat{V}_1$ implies the non-conservation of particles due to exchanges between the phases. This changes the way the proper self-energies are defined. There are three distinct types of them now, indicated in Fig.1.10. The first of these (Σ_{11}) has one particle line coming in and one coming

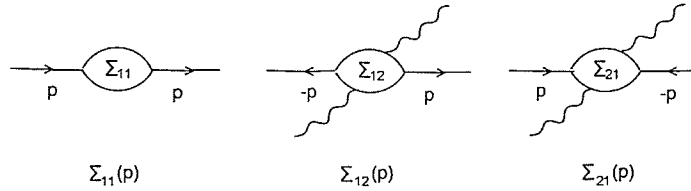


Figure 1.10: Proper self-energies for a Bose-condensed system. Straight lines correspond to normal phase particles, wave lines to condensed phase' ones.

out. The others, correspondingly, have two particle lines either coming out (Σ_{12})

or going in (Σ_{21}) simultaneously. This reflects the new features associated with the existence of a Bose condensate.

Thus, we must also introduce two new types of Green's functions:

$$G_{12}(\mathbf{k}, t) \equiv -\langle 0, \beta | T a_{-\mathbf{k}}(t) a_{\mathbf{k}}(0) | 0, \beta \rangle, \quad (1.10.66)$$

$$G_{21}(\mathbf{k}, t) \equiv -\langle 0, \beta | T a_{\mathbf{k}}^\dagger(t) a_{-\mathbf{k}}^\dagger(0) | 0, \beta \rangle. \quad (1.10.67)$$

Functions G_{12} and G_{21} are usually called the anomalous Green's functions and represent the disappearance and appearance of two non-condensate particles respectively. The normal Green's function is denoted as G_{11} and represents the propagation of a single particle

$$G_{11}(\mathbf{k}, t) \equiv -\langle 0, \beta | T a_{\mathbf{k}}(t) a_{\mathbf{k}}^\dagger(0) | 0, \beta \rangle. \quad (1.10.68)$$

These three Green's functions are shown in Fig.1.11, where the arrows indicate the direction of momentum of the atoms involved.

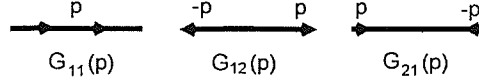


Figure 1.11: Green's functions for a Bose-condensed system.

The Dyson equations, connecting the above self-energies and propagators, are a subject of many textbooks. For the case of zero-temperature, they were first written down by Beliaev [17] and illustrated diagrammatically in Fig.1.12.

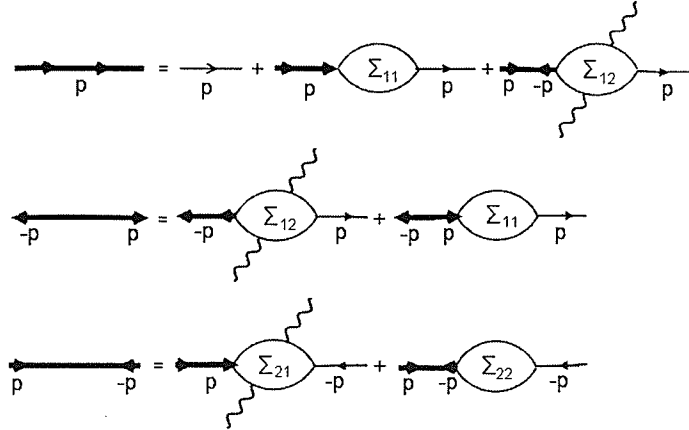


Figure 1.12: Dyson-Beliaev equations for a Bose-condensed system. Thin and thick straight lines denote, correspondingly, the free and resummed propagators of the normal phase particles.

Their generalization to TFD is straightforward and in the momentum repre-

sensation reads:

$$\begin{aligned} G_{11}^{\alpha\beta}(p) &= G^{(0)\alpha\beta}(p) + G_{11}^{\alpha\gamma}(p)\Sigma_{11}^{\gamma\delta}(p)G^{(0)\delta\beta}(p) + G_{21}^{\alpha\gamma}(p)\Sigma_{12}^{\gamma\delta}(p)G^{(0)\delta\beta}(p), \\ G_{12}^{\alpha\beta}(p) &= G_{11}^{\alpha\gamma}(-p)\Sigma_{12}^{\gamma\delta}(p)G^{(0)\delta\beta}(p) + G_{12}^{\alpha\gamma}(p)\Sigma_{11}^{\gamma\delta}(p)G^{(0)\delta\beta}(p), \\ G_{21}^{\alpha\beta}(p) &= G_{11}^{\alpha\gamma}(p)\Sigma_{21}^{\gamma\delta}(p)G^{(0)\delta\beta}(-p) + G_{21}^{\alpha\gamma}(p)\Sigma_{22}^{\gamma\delta}(-p)G^{(0)\delta\beta}(p), \end{aligned} \quad (1.10.69)$$

Here the TFD indices $\{\alpha, \beta\}$ may take the values $\{1, 2\}$ and summation over the repeated indices is implied. The obvious shortcut notation $p = (p_0, \mathbf{p})$ was employed. The free TFD Green's function $G^{(0)\alpha\beta}(p)$ is given by (1.10.27).

The structure of Beliaev equations can be simplified considerably by introducing the matrix notation [18], namely

$$\mathbf{G}(p) = \mathbf{G}(p) + \mathbf{G}^{(0)}(p) \cdot \Sigma(p) \cdot \mathbf{G}^{(0)}(p), \quad (1.10.70)$$

where

$$\mathbf{G}^{\alpha\beta}(p) = \begin{bmatrix} G_{11}^{\alpha\beta}(p) & G_{12}^{\alpha\beta}(p) \\ G_{21}^{\alpha\beta}(p) & G_{22}^{\alpha\beta}(p) \end{bmatrix}, \quad (1.10.71)$$

$$\mathbf{G}^{(0)\alpha\beta}(p) = \begin{bmatrix} G^{(0)\alpha\beta}(p) & 0 \\ 0 & G^{(0)\alpha\beta}(p) \end{bmatrix}, \quad (1.10.72)$$

$$\Sigma^{\alpha\beta}(p) = \begin{bmatrix} \Sigma_{11}^{\alpha\beta}(p) & \Sigma_{12}^{\alpha\beta}(p) \\ \Sigma_{21}^{\alpha\beta}(p) & \Sigma_{22}^{\alpha\beta}(p) \end{bmatrix}. \quad (1.10.73)$$

Not all of the above components are independent. For instance, as one may readily observe from Figs.1.10-1.12, the matrix elements $\Sigma_{22}^{\alpha\beta}(p)$, which appear in the equations above, are simply

$$\Sigma_{22}^{\alpha\beta}(p) = \Sigma_{11}^{\alpha\beta}(-p). \quad (1.10.74)$$

Similarly, there are useful relations between the anomalous proper self-energies and propagators correspondingly:

$$G_{12}^{\alpha\beta}(p) = G_{21}^{\alpha\beta}(-p), \quad \Sigma_{12}^{\alpha\beta}(p) = \Sigma_{21}^{\alpha\beta}(-p), \quad G_{22}^{\alpha\beta}(p) = G_{11}^{\alpha\beta}(-p). \quad (1.10.75)$$

With their help, the equations (1.10.70) could be solved with respect to the propagators in terms of the exact proper self-energies and unperturbed Green's functions.

In deriving Beliaev equations, we did not make any approximations. The only fact, that we recognized, is that the underlying system consists of two coexisting phases. Therefore, these equations are completely general and can be safely applied to any uniform Bose-condensed fluid, liquid or gas without any reference to whether the underlying system is weakly interacting or not.

Most of the approximation schemes, including ours, discussed below, use Beliaev equations as a starting point for consideration.

As we will see later, complete characterization of thermodynamic properties of a Bose-condensed system requires an additional constraint, independent of the formalism developed above. It is necessary in order to determine the chemical potential. Such a constraint could be provided by the Hugenholtz-Pines theorem [19], which states, that

$$\mu = \Sigma_{11}^{11}(0, 0) - \Sigma_{12}^{11}(0, 0). \quad (1.10.76)$$

This theorem holds both in zero and finite temperature cases and assures that the single particle excitations have no energy gap in the long-wavelength limit.

Now that we have formulated the general statement of the problem, we are ready to discuss in detail two of the most popular approximations involved, namely the Bogoliubov and the first-order Popov ones, both within the framework we have developed. This will be followed by the review of other notable results, obtained in the area until now.

1.10.2 The Bogoliubov approximation

In order to illustrate the consistency of the formalism, we will use it to rederive the physics of Bogoliubov approximation, which was substantially investigated in sect.1.9.

As it was noted there, the fundamental assumption, made in this approximation, is that the majority of atoms are in the $\mathbf{k} = 0$ state, only a few of them being "kicked" out of the condensate by the interactions, i.e. $N_0 \approx N$. This condition, obviously, holds at low enough temperatures, so that the restriction

$$T \ll T_c \quad (1.10.77)$$

is compatible with the assumption made.

The number of non-condensate atoms is usually called the "depletion". If the depletion is small, the interaction between two non-condensate atoms will not be important, which allows one to neglect the terms $\hat{V}_5$, $\hat{V}_6$ and $\hat{V}_7$ in the Hamiltonian (1.10.55). The terms that remain turn out to be quadratic and diagonalizable by a canonical transformation (see sect.1.9.2).

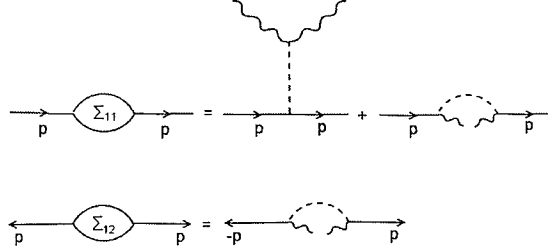


Figure 1.13: Self-energy diagrams in the Bogoliubov approximation.

In the Green's function language, the Bogoliubov approximation consists of keeping the lowest-order self-energy diagrams that contain two condensate lines, as shown in Fig.1.13. These can be written as

$$\Sigma_{11} = n_0[U(0) + U(\mathbf{k})], \quad (1.10.78)$$

$$\Sigma_{12} = n_0 U(\mathbf{k}). \quad (1.10.79)$$

Low temperature of the system makes it possible to safely replace the condensate density n_0 by the total gas density n , so that $n_0 \equiv N/V$. Due to the same reason, particle momenta should be considered to be small. Therefore, the Fourier components $U(\mathbf{p})$ could be replaced by their value $U(0)$ at $\mathbf{p} = 0$.

Then, according to the Hugenholtz-Pines theorem (1.10.76), the lowest-order contribution to the chemical potential is given by

$$\mu = nU(0). \quad (1.10.80)$$

As the temperature of the system nears zero, the TFD formalism smoothly converges to that of the regular zero-temperature field theory. When working in the Bogoliubov approximation, we may set $\beta = \infty$. This effectively cancels the non-diagonal elements of the propagator (1.10.27). Physically, it is equivalent to the decoupling of the system from the heat reservoir.

This allows one to neglect the matrix structure of the self-energies and propagators involved and to consider only their 11-components thereafter. Thus, substituting (1.10.78-1.10.80) into (1.10.69) and solving with respect to $G_{11}^{11}(p)$ and $G_{12}^{11}(p)$, we obtain

$$G_{11}^{11}(p) = \frac{p_0 + \varepsilon_{\mathbf{p}} + nU(\mathbf{p})}{p_0^2 - \varepsilon_{\mathbf{p}}^2 - 2nU(\mathbf{p})\varepsilon_{\mathbf{p}}}, \quad (1.10.81)$$

$$G_{12}^{11}(p) = \frac{-nU(\mathbf{p})}{p_0^2 - \varepsilon_{\mathbf{p}}^2 - 2nU(\mathbf{p})\varepsilon_{\mathbf{p}}}, \quad (1.10.82)$$

where $\varepsilon_{\mathbf{p}} = \frac{p^2}{2m}$ is the kinetic energy of the atoms.

The Bogoliubov dispersion law follows from the poles of either $G_{11}^{11}(p)$ or $G_{12}^{11}(p)$ propagators:

$$E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + 2nU(\mathbf{k})\varepsilon_{\mathbf{k}}}, \quad (1.10.83)$$

This is in complete agreement with the result obtained earlier within the secondary quantization formalism (see (1.9.31)). Additionally, the ground state energy could be observed directly from (1.10.56). It reads:

$$E_0 = \frac{1}{2}(N^2/V)U(0), \quad (1.10.84)$$

which coincides with (1.9.9).

The rest of the thermodynamic relations of interest follow straightforwardly from the last two equations. Thus, the TFD framework allowed us to correctly describe the behavior of dilute Bose gas in the zero temperature limit.

1.10.3 The first order Popov approximation

Now we are going to discuss another first-order self-energy approximation for the weakly interacting Bose gas at finite temperatures. It was first introduced in 1965 by Popov [21]. Unlike the Bogoliubov approximation, the Popov approximation takes into account interactions between the excited atoms. It does not make any assumptions about the density of the normal phase and, therefore, is valid in the whole range of temperatures, both below and above the critical.

The self-energy diagrams in the Popov approximation include all possible first-order diagrams of a Bose-condensed system (see Fig.1.14). Among them, only those (a, b, e), containing two condensate lines, are included in the Bogoliubov approximation. The new ones (c and d) are the Hartree-Fock diagrams which

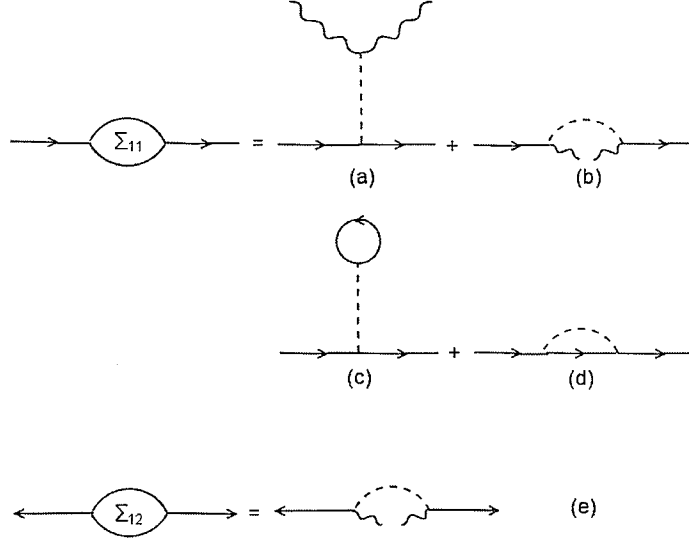


Figure 1.14: Self-energy diagrams in the Popov approximation.

include excited atoms.

The self-energies Σ_{11} and Σ_{12} of Fig.1.14 can be explicitly written as

$$\Sigma_{11} = \begin{bmatrix} 2(n_0 + \tilde{n}^{(0)})U_0 & 0 \\ 0 & -2(n_0 + \tilde{n}^{(0)})U_0 \end{bmatrix}, \quad (1.10.85)$$

$$\Sigma_{12} = \begin{bmatrix} n_0 U_0 & 0 \\ 0 & -n_0 U_0 \end{bmatrix}. \quad (1.10.86)$$

The quantity $\tilde{n}^{(0)}$ in (1.10.85) and (1.10.86) is the temperature-dependent density of excited atoms in a non-interacting Bose gas, given by

$$\tilde{n}^{(0)} \equiv i \int \frac{dp_0 d\mathbf{p}}{(2\pi)^4} G^{(0)11}(p_0, \mathbf{p}). \quad (1.10.87)$$

In this paragraph, we will use the superscript "(0)" as a reminder that the quantity corresponds to a non-interacting case.

With the self-energies (1.10.85-1.10.86), one can calculate the normal and anomalous Green's functions and use these to evaluate various physical quantities. It is convenient to discuss the normal phase ($T > T_c$) and the condensed phase ($T < T_c$) separately.

Normal phase ($T > T_c$)

In the normal phase, we have $n_0 = 0$, and, therefore, (1.10.85-1.10.86) reduce to

$$\Sigma_{11} = \begin{bmatrix} 2\tilde{n}^{(0)}U_0 & 0 \\ 0 & -2\tilde{n}^{(0)}U_0 \end{bmatrix}, \quad (1.10.88)$$

$$\Sigma_{12} = \begin{bmatrix} \tilde{n}^{(0)}U_0 & 0 \\ 0 & -\tilde{n}^{(0)}U_0 \end{bmatrix}. \quad (1.10.89)$$

Solving (1.10.70) using (1.10.88-1.10.89) with respect to $G_{11}^{(11)}(p)$, we get

$$G_{11}^{(11)}(p) = \frac{1 + d^2(p_0)}{p_0 - \varepsilon_{\mathbf{p}} + \mu - 2\tilde{n}^{(0)}U_0 + i\epsilon} - \frac{d^2(p_0)}{p_0 - \varepsilon_{\mathbf{p}} + \mu - 2\tilde{n}^{(0)}U_0 - i\epsilon}, \quad (1.10.90)$$

where the thermal weight factor $d^2(p_0)$ is defined in (1.10.8).

With (1.10.90), the density of the excited atoms as a function of the chemical potential μ and temperature T is given by

$$\tilde{n}(\mu, T) \equiv \int \frac{dp_0 d\mathbf{p}}{(2\pi)^4} G_{11}^{(11)}(p_0, \mathbf{p}) = \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{1}{e^{\beta(\varepsilon_{\mathbf{p}} - \mu + 2\tilde{n}^{(0)}U_0)} - 1}. \quad (1.10.91)$$

If the total density n and the temperature T are given, the chemical potential is determined by the usual condition

$$\tilde{n}(\mu, T) = n \quad \text{normal system.} \quad (1.10.92)$$

Similarly, the chemical potential $\mu^{(0)}$ of a non-interacting Bose gas at $T > T_c$ is determined by

$$\tilde{n}^{(0)}(\mu^{(0)}, T) = n. \quad (1.10.93)$$

Comparing (1.10.93) and (1.10.91), one sees that for a given n and T we have

$$\mu = \mu^{(0)} + 2nU_0 \quad (T > T_c), \quad (1.10.94)$$

i.e., the chemical potential is increased by $2nU_0$ due to the effectively repulsive interaction between the atoms [22].

The energy spectrum $E_{\mathbf{p}}$ of single-particle excitations (or quasiparticles) in the normal phase is determined by the poles of the Green's function $G_{11}^{(11)}(p)$, that is,

$$E_{\mathbf{p}} = \varepsilon_{\mathbf{p}} - \mu + 2nU_0 = \varepsilon_{\mathbf{p}} - \mu^{(0)}. \quad (1.10.95)$$

This shows that in the present first-order approximation the quasiparticles above T_c act just like free particles in a non-interacting Bose gas. Because the quasiparticles determine the thermodynamic properties of a system, we conclude that in the Popov approximation the normal properties of a dilute Bose gas are unchanged compared to that of the non-interacting Bose gas and, in particular, the phase transition temperature is the same.

Bose-condensed phase $T < T_c$

Just like in the normal phase, the Green's functions in the Bose-condensed phase are obtained by solving the Dyson-Beliaev equations (1.10.69). For that, we have to substitute the self-energies (1.10.88-1.10.89) and notice that the chemical potential μ satisfies the finite-temperature version of the Hugenholtz-Pines theorem:

$$\mu = \Sigma_{11}^{(11)}(0, 0) - \Sigma_{12}^{(11)}(0, 0) = 2\tilde{n}^{(0)}U_0 + n_0U_0. \quad (1.10.96)$$

Thus, we find:

$$\begin{aligned} G_{11}^{(11)}(p_0, \mathbf{p}) &= \frac{(1 + d^2(p_0))(p_0 + \varepsilon_{\mathbf{p}} + n_0U_0)}{p_0^2 - \varepsilon_{\mathbf{p}}^2 - 2\varepsilon_{\mathbf{p}}n_0U_0 + i\epsilon} \\ &+ \frac{d^2(p_0)(p_0 + \varepsilon_{\mathbf{p}} + n_0U_0)}{p_0^2 - \varepsilon_{\mathbf{p}}^2 - 2\varepsilon_{\mathbf{p}}n_0U_0 - i\epsilon}. \end{aligned} \quad (1.10.97)$$

Function $G_{11}^{(11)}(p_0, \mathbf{p})$ has the poles at $p_0 \pm E_{\mathbf{p}}$, where

$$E_{\mathbf{p}} = \sqrt{\varepsilon_{\mathbf{p}}^2 + 2\varepsilon_{\mathbf{p}}n_0(T)U_0}. \quad (1.10.98)$$

This gives the energy spectrum of elementary excitations for $T < T_c$.

The spectrum is formally identical to that of the $T = 0$ Bogoliubov approximation. However, in contrast to the Bogoliubov model, where $n_0 \simeq n$, the condensate density $n_0(T)$ in the Popov approximation is strongly dependent on temperature and becomes very small in the vicinity of the phase transition.

On the other hand, one should not over-interpret the formal similarity between the excitation spectrum in the Popov and Bogoliubov models. At first glance, it seems to imply that one can generalize the Bogoliubov model to finite temperatures simply by taking into account the temperature dependence of n_0 of an ideal gas. Although this gives the correct excitation spectrum, it gives an incorrect expression for the chemical potential, namely $\mu = n_0(T)U_0$ instead of the correct result (1.10.96).

We see that the Popov-Bogoliubov spectrum in (1.10.98) has quite different limits:

$$E_{\mathbf{p}} \sim \varepsilon_{\mathbf{p}} + n_0(T)U_0, \quad |\mathbf{p}| \gg \hbar^{-1}\sqrt{mn_0U_0}, \quad (1.10.99)$$

$$E_{\mathbf{p}} \sim \hbar c|\mathbf{p}|, \quad |\mathbf{p}| \ll \hbar^{-1}\sqrt{mn_0U_0}. \quad (1.10.100)$$

The energy $E_{\mathbf{p}}$ is free-particle like in the short-wavelength limit, and phonon-like in the long-wavelength limit, with the phonon velocity c given by

$$c \equiv \sqrt{n_0(T)U_0/m}. \quad (1.10.101)$$

The single-particle excitation spectrum in (1.10.100) is proportional to $\mathbf{p}$ in the long-wavelength limit. As we noted in sect.1.9, this linear dependence is expected to hold in any Bose-condensed fluid to all orders in perturbation theory. Although the Popov approximation is only the lowest-order approximation, we see that it gives gapless phonon excitations in the lowest-energy limit in a Bose gas at finite temperatures. Moreover, $c(T) \rightarrow 0$ as $T \rightarrow T_c$, i.e., the phonons in the Popov theory are the "broken-symmetry" soft modes of the Bose-condensed phase. However, unlike the zero temperature case, there is no established correspondence between the excitation phonon velocity and the compressional speed of sound at finite temperature.

With the Green's function (1.10.97), one can now calculate the condensate density. For a given total density n , we have

$$n = n_0 + \tilde{n}, \quad (1.10.102)$$

where

$$\begin{aligned} \tilde{n} &= \int \frac{dp_0 d\mathbf{p}}{(2\pi)^4} G_{11}^{(11)}(p_0, \mathbf{p}) \\ &= \int \frac{d\mathbf{p}}{(2\pi)^3} \left(1 + \frac{1}{\exp(\beta E_{\mathbf{p}}) - 1} \right) \frac{\varepsilon_{\mathbf{p}} + E_{\mathbf{p}} + n_0 U_0}{2E_{\mathbf{p}}} \quad (T < T_c). \end{aligned} \quad (1.10.103)$$

Equations (1.10.102) and (1.10.103) are the coupled equations for n_0 , since $\tilde{n}$ depends on $E_{\mathbf{p}}$ and $(n_0 U_0)$, which are themselves functions of n_0 . In general, they

must be solved numerically. However, in two important special cases analytical results can be obtained.

We first consider the low-temperature limit ($kT \ll n_0 U_0$). In this case, the integral in (1.10.103) can be approximated as

$$\begin{aligned}\tilde{n} &= \int \frac{d\mathbf{p}}{(2\pi)^3} \left(\frac{\varepsilon_{\mathbf{p}} + n_0 U_0}{2E_{\mathbf{p}}} + \frac{1}{2} \right) + \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{1}{\exp(\beta E_{\mathbf{p}}) - 1} \left(\frac{\varepsilon_{\mathbf{p}} + n_0 U_0}{2E_{\mathbf{p}}} + \frac{1}{2} \right) \\ &\simeq \frac{1}{3\pi^2} \left(\frac{m n_0 U_0}{\hbar^2} \right)^{3/2} + \frac{1}{12} \left(\frac{m}{\hbar^2} \right)^{3/2} (n_0 U_0)^{-1/2} (kT)^2,\end{aligned}\quad (1.10.104)$$

where in the second step we have assumed that $\frac{1}{\exp(\beta E_{\mathbf{p}}) - 1} \sim e^{-\beta E_{\mathbf{p}}}$ and regularized the ultraviolet divergent integral with a method of dimensional regularization (see Appendix B for details). With (1.10.102) and (1.10.104), we obtain

$$n_0 \simeq n - \frac{8n_0}{3} \left(\frac{n_0 a^3}{\pi} \right)^{1/2} - \frac{1}{12} \frac{m}{\hbar^3 c} (kT)^2, \quad (1.10.105)$$

where c is the phonon velocity defined in (1.10.101).

For a low-density gas at low temperatures, the second and third terms in (1.10.105) are small, implying $n_0 \sim n$. Therefore, when calculating the depletion $\tilde{n} \equiv n - n_0$ at $T = 0$, we can drop the third term and replace n_0 by n on the right-hand side of (1.10.105) to obtain

$$\frac{\tilde{n}}{n} \equiv \frac{n - n_0}{n} = \frac{8}{3} \left(\frac{n a^3}{\pi} \right)^{1/2} \ll 1. \quad (1.10.106)$$

The error introduced by the replacement of n_0 by n in obtaining (1.10.106) is of higher order in a . Equation (1.10.106) is a well-known result for the fractional depletion of the condensate in a dilute gas at absolute zero, which was previously derived in sect.1.9 (see (1.9.35)).

The T^2 law for an interacting Bose gas is quite different from the $T^{3/2}$ law of an ideal gas given by (1.6.20). This remind us that the introduction of even a small interaction between the particles can dramatically change the properties of a Bose gas at low temperatures, where the phonon part of the spectrum completely determines the thermodynamics.

As is seen from (1.10.104), the T -dependent part of $\tilde{n}$ tends to decrease with increasing values of n_0 , in contrast to the $T = 0$ part, which increases with n_0 . As a result, one expects a "crossover" between $n_0(T)$ of an interacting gas and $n_0^{(0)}(T)$ of a non-interacting gas. This crossover means that at sufficiently high temperatures the effect of repulsive interactions between the atoms in a dilute weakly interacting Bose gas is, in contrast to the $T = 0$ case, to put more atoms in the condensate. It seems to imply that the thermal effects are not as significant in a dilute Bose gas as in an ideal gas.

The "crossover" temperature T_x can be estimated by comparing $\tilde{n}$ for a weakly interacting gas in (1.10.104) with $\tilde{n}^{(0)}$ for an ideal gas, yielding

$$kT_x \sim 0.46 n_0 U_0 \sim 0.46 (4\pi \hbar^2 a/m)n \quad (1.10.107)$$

or

$$T_x/T \sim 1.74 (n^{1/3} a) \ll 1, \quad (1.10.108)$$

where the last step follows from (1.9.2).

We next discuss the region close to the transition, $T \approx T_c$. It is convenient to calculate the difference

$$\begin{aligned}\tilde{n} - n_{cr} &= \\ &= \int \frac{d\mathbf{p}}{(2\pi)^3} \left[\left(1 + \frac{1}{e^{\beta E_{\mathbf{p}}} - 1} \right) \left(\frac{\varepsilon_{\mathbf{p}} + E_{\mathbf{p}} + n_0 U_0}{2E_{\mathbf{p}}} \right) - \frac{1}{e^{\beta E_{\mathbf{p}}} - 1} \right],\end{aligned}\quad (1.10.109)$$

where n_{cr} is defined by

$$n_{cr} \equiv \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{1}{e^{\beta E_{\mathbf{p}}} - 1} = 2.61 \left(\frac{mkT}{2\pi\hbar} \right)^{3/2}. \quad (1.10.110)$$

This is the density of excited atoms of an ideal gas at a given temperature T . The dominant contribution to the difference $\tilde{n} - n_{cr}$ comes from the energy region, where the excitation spectrum $E_{\mathbf{p}}$ differs significantly from the free-particle energy $\varepsilon_{\mathbf{p}}$, which is the region $\varepsilon_{\mathbf{p}} \sim n_0 U_0$ in our case. We note that $n_0 U_0$ is very small near T_c , namely

$$n_0 U_0 / kT \sim n_0 U_0 / kT_c \ll 1. \quad (1.10.111)$$

Therefore, we can approximate $1/(e^{\beta E_{\mathbf{p}}} - 1)$ by $1/\beta E_{\mathbf{p}}$ and $1/(e^{\beta \varepsilon_{\mathbf{p}}} - 1)$ by $1/\beta \varepsilon_{\mathbf{p}}$ and carry out the integration analytically to obtain

$$\begin{aligned}\tilde{n} - n_{cr} &\simeq \int \frac{d\mathbf{p}}{(2\pi)^3} \left[\frac{\varepsilon_{\mathbf{p}} + n_0 U_0}{\beta E_{\mathbf{p}}^2} - \frac{1}{\varepsilon_{\mathbf{p}}} \right] = -\frac{kT}{2\pi^2} \int_0^\infty dp \, p^2 \frac{n_0 U_0}{\varepsilon_p(\varepsilon_p + 2n_0 U_0)} \\ &= -\frac{1}{8\pi} \left(\frac{2m}{\hbar} \right)^{3/2} kT (2n_0 U_0)^{1/2}.\end{aligned}\quad (1.10.112)$$

Combining this result with (1.10.102), we find

$$n \simeq n_0 + n_{cr} - (1/8\pi)(2m/\hbar^2)^{3/2} kT (2n_0 U_0)^{1/2}. \quad (1.10.113)$$

For given n and T , (1.10.113) is a quadratic equation for n_0 which has two solutions:

$$\sqrt{n_{0,\pm}} = \frac{1}{2} \left[\sqrt{n_g(T)} \pm \sqrt{n_g(T) + 4(n - n_{cr})} \right]. \quad (1.10.114)$$

Here $\sqrt{n_g(T)}$ is the coefficient of $\sqrt{n_0}$ in the third term of (1.10.113),

$$\sqrt{n_g(T)} \equiv (1/8\pi)(2m/\hbar^2)^{3/2} kT (2U_0)^{1/2}, \quad (1.10.115)$$

or

$$n_g(T) = (4\pi/(2.612)^{4/3})(n^{1/3} a)n. \quad (1.10.116)$$

Since $n > n_{cr}$ below the critical temperature, the solution $n_{0,-}$ in (1.10.114) is negative and, thus unphysical. Therefore, the condensate density is given by the other solution $n_{0,+}$, which yields a finite value at $T \rightarrow T_c^-$, namely

$$\begin{cases} n_g(T), & T \rightarrow T_c^-, \\ 0, & T \rightarrow T_c^+. \end{cases} \quad (1.10.117)$$

This clearly indicates a finite jump in the condensate density n_0 at the transition point. This jump is small compared to the total density n in a dilute Bose gas ($n^{1/3}a \ll 1$). Nevertheless, the finite jump in the order parameter is the characteristics of the first-order phase transition. This, however, contradicts to the fact that Bose condensation in an interacting Bose system involves a second-order phase transition.

The unphysical behavior near the phase transition point implies that the Popov approximation breaks down in this region. As was estimated by Popov, the self-energies in (1.10.88-1.10.89) are linear in n_0U_0 , while the largest diagrams dropped in the approximation are of the order $(m/\hbar^2)^{3/2}kTU_0(n_0U_0)^{1/2}$. As T approaches T_c from below, the neglected diagrams become larger than the first-order diagrams, since the former (proportional to $(n_0U_0)^{1/2}$) decrease at a slower rate than n_0U_0 . Therefore, the Popov approximation is valid, if

$$(m/\hbar^2)^{3/2}kTU_0(n_0U_0)^{1/2} \ll n_0U_0, \quad (1.10.118)$$

or, equivalently,

$$T_c - T \gg (n^{1/3}a)T_c. \quad (1.10.119)$$

The temperature region defined by $(n^{1/3}a)T_c$ is very small in the actual dilute Bose gases.

1.10.4 Other approximations

The Bogoliubov and Popov approximations are the most widely used ones when treating the thermal properties of rarefied Bose gases and related problems. Below we briefly review certain extensions of theirs along with some other recent notable developments in the field.

The Hartree-Fock-Bogoliubov approximation

The HFB approximation upgrades the Bogoliubov interactions by taking into account the parts of the interaction Hamiltonian, that contain three or four-operator terms, such as $\hat{a}^\dagger\hat{a}\hat{a}$ and $\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}$, which can be approximated by various terms containing the normal average $\langle\hat{a}^\dagger\hat{a}\rangle$, and the anomalous averages $\langle\hat{a}^\dagger\hat{a}^\dagger\rangle$ and $\langle\hat{a}\hat{a}\rangle$ [4, 23, 24]. Any average, that includes three or more operators, is neglected in the HFB approximation.

Thus, the Hamiltonian can again be diagonalized, defining a new set of quasiparticles. These quasiparticles are no longer Bogoliubov quasiparticles, since they are "dressed" by the mean-field effects on excited atoms. The latter are taken into account by the HFB self-energy contributions, shown diagrammatically in Fig.1.15.

One of the attractive features of the HFB approximation is that it is a conserving approximation, that respects the conservation laws following from the underlying symmetries of the field theory. One of the problems with the HFB approximation is that it predicts a gap in the quasiparticle spectrum, which is a consequence of the spontaneously broken symmetry. Thus, the HFB approximation violates the Goldstone theorem [14]. In [4] it was argued that the problem of a gap in the HFB approximation is due to the overcounting of diagrams that

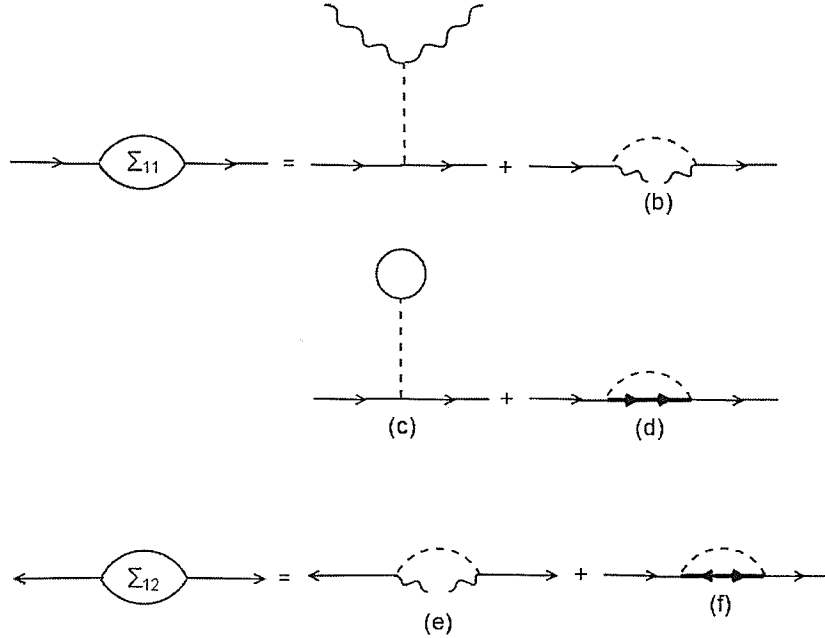


Figure 1.15: The HFB self-energy diagrams. Thick lines denote the resummed propagators.

contribute to the anomalous self-energy and that are of the second order in the interaction. Thus, the HFB approximation is inconsistent with that order in the interaction.

The many-body t -matrix approximation

As was discussed in the previous paragraph, the Popov approximation breaks down near the phase transition point. In an attempt to fix this problem, it was proposed to use a many-body t -matrix approximation, which employs the self-consistent propagator G_{11} in the Popov self-energy diagrams [4, 25].

The self-energy diagrams in the many-body t -matrix approximation are shown in Fig.1.16. They look the same as those in Fig.1.14. However, the gray-filled square now represents the multiple scattering of two "dressed" particles, whose propagators G_{11} are to be self-consistently determined.

The modified t -matrix Γ is defined by the integral equation, illustrated by the ladder diagrams in Fig.1.17.

Close examination of the problem reveals that the t -matrix becomes very temperature-dependent and displays the following properties:

1. In a low-temperature and low density limit the t -matrix approximation reduces to the simpler Popov approximation.
2. In the finite-temperature region just below the critical the t -matrix Γ goes to zero in the same way as does the condensed phase density of the ideal Bose gas, i.e. as $1 - (T/T_c)^{3/2}$.

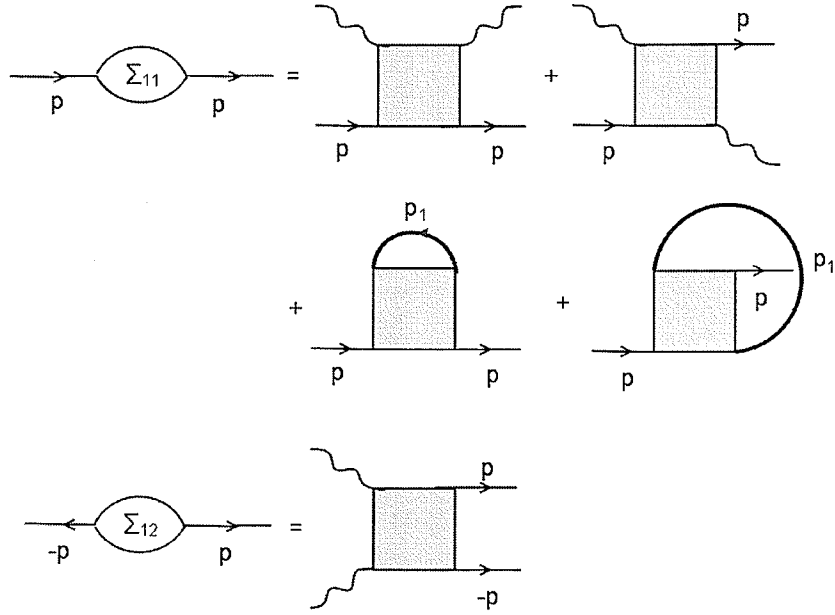


Figure 1.16: Self-energy diagrams in the many-body t -matrix approximation.

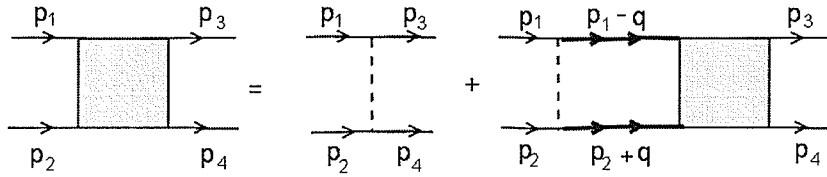


Figure 1.17: Integral equation for the many-body t -matrix Γ . A gray-filled square with four "legs" represents Γ , a solid line with two arrows represents a "dressed" particle or G_{11} , and a dashed line represents the interaction potential.

3. In the region just above the critical the t -matrix depends on temperature as $(T/T_c)^{3/2} - 1$.

The last two points suggest that the t -matrix vanishes as T approaches T_c from above or below in a systematic way. This leads to a smooth change of a condensate fraction n_0 at T_c and, thus, to the correct order of the phase transition. However, it also shows that T_c of an ideal Bose gas is unchanged in the many-body t -matrix approximation, which shows its insufficiency to explore the critical phenomena. This is not unexpected, since in using the many-body t -matrix in the Popov approximation, one is clearly including a class of higher order self-energy diagrams built out of the normal propagator G_{11} , but still omitting any contribution of other higher-order diagrams, especially those built out of the anomalous propagators G_{12} and G_{21} .

Breakdown of perturbation expansions

Approximation schemes reviewed so far are based on the perturbation expansions. They give a reasonable description of the elementary excitations in Bose gases as well as allow to evaluate the major features of the thermodynamic parameters of the system. However, they suffer from a serious common drawback. Namely, they are infrared divergent in the critical region and, therefore, lose validity near the phase transition point [14].

There are two possible ways to overcome this issue.

One consists of performing the selective resummations of the certain class of Feynman diagrams from all orders of perturbation series. This will lead to mutual cancellations of divergencies, which are screened in the actual physical systems. We will dedicate to this kind of techniques a separate chapter later on.

The second way is to use the renormalization group approach. It was specifically invented to deal with the problems of this particular type.

Renormalization group approach

The basic idea of the renormalization group is to separate the momentum modes in the path integral into fast modes and slow modes by a cutoff. One then integrates out the fast modes. This yields an effective action for the slow modes, in which the coefficients of the original operators are renormalized and new operators are introduced. By lowering the cutoff infinitesimally, one obtains a set of differential equations for the parameters in the effective action. Integrating out all modes down to $\mathbf{k} = 0$ yields the full effective action.

Renormalization group techniques have been applied to the homogenous Bose gas at finite temperatures by several authors [26, 27, 28]. In the most notable work [26], it was shown, that

1. the phase transition is clearly of the second order;
2. the effective chemical potential as well as the effective quartic coupling constant vanish at the critical point;
3. the critical exponents are the same as in the $O(2)$ -symmetric scalar theory in three dimensions.

1.10.5 Calculations of the critical temperature T_c

The question, that we did not cover so far, can be formulated as follows: what is the effect of weak interactions on the critical temperature of an ideal Bose gas?

Despite its apparent simplicity, the answer was causing a considerable amount of confusion for decades and settled down only very recently [29, 30].

The problem was attacked with the use of different methods. Initially, most of them, one way or another, involved perturbation expansions. Afterwards, when invalidity of the latter became obvious, various nonperturbative techniques, such as Monte Carlo simulations, $1/N$ expansions, self-consistent calculations involving summation of bubble and ladder diagrams, were utilized.

At the moment, there seems to be an overall agreement that the critical temperature of the ideal Bose gas is marginally increased by the weak interactions.

$\frac{\Delta T_c}{T_0} = 2.33n^{1/3}a,$	Leading order $1/N$ [39]
$\frac{\Delta T_c}{T_0} = 1.71n^{1/3}a$	Next-to-leading order $1/N$ [40]
$\frac{\Delta T_c}{T_0} = (1.32 \pm 0.02)n^{1/3}a$	Lattice [41].
$\frac{\Delta T_c}{T_0} = (1.29 \pm 0.05)n^{1/3}a$	Lattice [42].
$\frac{\Delta T_c}{T_0} = 0.7n^{1/3}a$	One-bubble approximation [43]
$\frac{\Delta T_c}{T_0} = 3.8n^{1/3}a$	One-bubble self-consistent approximation [29]
$\frac{\Delta T_c}{T_0} = 2.5n^{1/3}a$	Ladder-summation approximation [29]
$\frac{\Delta T_c}{T_0} = 1.6n^{1/3}a$	Bubble summation approximation [29]
$\frac{\Delta T_c}{T_0} = (1.27 \pm 0.11)n^{1/3}a$	7-loop VPT [44].
$\frac{\Delta T_c}{T_0} = 1.23n^{1/3}a$	RG in three dimensions [45]
$\frac{\Delta T_c}{T_0} = (1.3 \pm 0.4)n^{1/3}a$	Simulations of classical field theory [46]

Table 1.1: The critical temperature for a dilute Bose gas obtained by various analytical and numerical methods.

The magnitude of this margin depends parametrically on the gas density n and the s -wave scattering length a as follows:

$$\frac{\Delta T_c}{T_c^0} = c n^{1/3}a. \quad (1.10.120)$$

The results of many notable developments with explicit values of the coefficient c are outlined in Table 1.1.

1.11 Interaction corrections to the properties of ideal Bose gas at temperatures below critical

Motivation

In the previous sections we have reviewed common approaches used to investigate the influence of the interaction corrections on the properties of an ideal Bose gas. All of them capture essential features of the system's behavior, although each has some drawbacks or inconsistencies with experimental data.

Probably the major downside of the approximations involved is that they either do not allow to investigate the problem in the whole range of temperatures,

being concentrated in the region infinitesimally close to $T = 0$, or technically complicated, which makes solving the problem a hard task.

Therefore, we think it is important to elaborate such a procedure which, on the one hand being simple and easily implementable, could on the other hand be based only on the most general physical principles and be capable of reproducing the essential features of the weakly interacting Bose gases in the whole range of temperatures below critical [47].

Procedure

We choose a TFD approach as a framework for performing the actual calculations. As was shown earlier on examples of the Bogoliubov and Popov approximations, this formalism allows one to straightforwardly get the same analytical expressions for the quantities of interest as does the imaginary time formalism, which used to be the primary tool in the field so far. The price one has to pay, though, is the doubling of degrees of freedom. This may cause certain technical complications when calculating higher order loop corrections due to the sharp increase of the number of Feynman diagrams involved, but does not represent any difficulty when only few leading terms are in focus. The merit, however, is that the TFD approach does not require one to perform the technically tedious analytical continuation in the complex time plane. Therefore, choosing a proper analytical machinery is mostly a matter of taste, determined by one's familiarity with the approach.

The starting point of our procedure are the TFD generalizations of the Beliaev equations (1.10.70). These equations should be solved with respect to the resummed propagators G_{11} and G_{12} , expressed in terms of the corresponding self-energy functions.

The latter, however, cannot be written down in a closed form and some kind of approximation is required. In this work, we take into account only the self-energy functions, which correspond to the Bogoliubov approximation (see Fig.1.13). Despite the fact, that this approximation is valid only in the range of temperatures infinitesimally close to zero, our procedure, as we will see later, helps to bypass this limitation.

Thus, we may solve (1.10.70) and find the propagators as functions of the two unknown parameters, namely the condensed phase density n_0 and the chemical potential μ .

In TFD, one may express any physical parameter of interest via the G_{11}^{11} matrix element of the propagator. In particular, the gas density n could be written as:

$$n = n_0 + \int d\omega d\mathbf{p} G_{11}^{11}(\omega, \mathbf{p}; n_0, \mu). \quad (1.11.1)$$

This equation gives an implicit dependence of n_0 on μ .

In order to completely characterize the system, we need, however, to find an independent way to determine the chemical potential itself. A common practice here is to use the Hugenholtz-Pines theorem [19], which relates this parameter to the self-energy functions of the system [4, 14], thus providing a necessary constraint. We, however, proceed in a different direction and use the requirement that the physical values of the condensate density and the chemical potential in a state of equilibrium should minimize the free energy F . In TFD formalism, interaction

corrections to this potential are given by a set of vacuum diagrams, in which all internal propagators are of $G_{11}^{(0)11}$ type [10]. As in the case of the self-energy, we maintain only the minimal possible subset of diagrams required. It is depicted in Fig.1.18. Thus, for example, in the first order of approximation the free energy

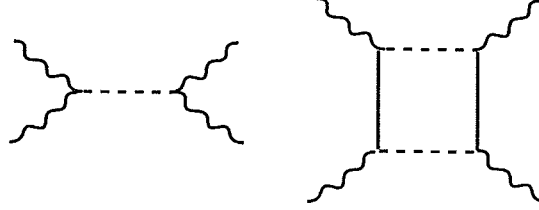


Figure 1.18: First and second order corrections to the free energy of the interacting Bose gas in Bogoliubov approximation.

reads:

$$F_1 = F_0 - \frac{1}{2}n_0(\mu)^2U, \quad (1.11.2)$$

where

$$F_0 = -\frac{kT}{\lambda^3}g_{5/2}(\exp(\mu)) \quad (1.11.3)$$

is the free energy of the ideal Bose gas. Here k is the Boltzmann constant, T is the temperature, U is the interaction potential, $g_{5/2}(x)$ is the Bose-Einstein function (see [7]) and $\lambda = h/(2\pi mkT)^{1/2}$ is the thermal wavelength, which, in turn, depends on the mass m of an atom.

In order to keep the procedure consistent, we take into account the interaction corrections to the self- and free energies which are of the same expansion order simultaneously. Therefore, the rest of the task consists of the following steps. First, given a subset of Feynman contributions to the self-energy, we iteratively solve (1.11.1) with respect to n_0 as a function of μ , T and n . Then, we use the value of n_0 found to determine the free energy F . As a last step, we adjust the chemical potential and repeat the whole process until the minimum of the free energy is found. The latter corresponds to the physical equilibrium.

Once the chemical potential and the condensed phase density are determined as functions of temperature, the rest of the parameters of interest follows straightforwardly by applying standard thermodynamic relations.

Discussion of the method

As one readily observes, our approach may suffer from the drawback we mentioned earlier. Namely, we use the Bogoliubov self-energies to explore the thermal properties of the system, which is only admissible in the vicinity of $T = 0$. On the other hand, however, the second part of the procedure, that is concerned with determining the chemical potential, is inherently non-perturbative.

In other approaches, one usually evaluates this parameter consistently, order by order, within the perturbation expansion process. First, the self-energy corrections

in a given order of approximation are being evaluated. Second, the Hugenholtz-Pines theorem is applied, which produces the value of the interaction correction to the chemical potential, consistent with this order.

In contrast, we first determine the expression for the free energy in a given order of approximation, and then determine μ by minimizing the function obtained. Therefore, a “series expansion” for the chemical potential does not happen.

For example, let F_n be the free energy in the n th order of approximation, given by the sum of the zero order free energy F_0 and corresponding loop corrections:

$$F_n(n_0, \mu) = F_0(n_0, \mu) + F^{(1)}(n_0, \mu) + \dots + F^{(n)}(n_0, \mu).$$

Then the chemical potential in our procedure is being determined by minimizing the whole right-hand side of this expression, in which it enters different-order terms on the same footing, without any additional expansions. Thus, some kind of order mixing occurs, that makes the entire procedure non-perturbative.

Therefore, we may expect that the explicit form of the self-energy contributions encountered is not the primary issue and regard the minimal possible subset of them (i.e. the Bogoliubov subset) as sufficient for our purposes.

Moreover, minimizing the free energy to obtain physical parameters makes the outcome of the procedure thermodynamically consistent.

Model parameters

When investigating the properties of interacting Bose gases, it is a common practice to choose the parameters of the liquid He⁴ when performing the formal quantitative estimations. We follow the same line and suppose, that the atom masses and molar volume of the system involved are $m = 6.65 \times 10^{-24}$ g and $V = 27.6$ cm³/mole correspondingly [7].

Since the momenta involved in the problem, are sufficiently small due to the low temperature of the system, we assume, as in previous chapters, that the Fourier components of the pair-interaction potential $U(\mathbf{p})$ could be replaced by their value U_0 at $\mathbf{p} = 0$. Thus, the form of the repulsive interaction potential is getting fixed by (see (1.9.11))

$$U_0 = \frac{4\pi\hbar^2 a}{m}. \quad (1.11.4)$$

In order to use U_0 safely as a loop expansion parameter, the s -wave scattering length was chosen such, that

$$\frac{nU_0}{kT_c} \approx 0.02, \quad (1.11.5)$$

where $T_c \approx 3.13^\circ\text{K}$ is the critical temperature of the ideal Bose gas with the parameters specified. In other words, the interaction energy between the particles is assumed to be small compared with the thermal energy.

Further, unless otherwise stated, we will say that the value of U_0 is unit if it satisfies the estimate (1.11.5).

Results

We have calculated the first and second order interaction corrections to the thermodynamic functions of the ideal Bose gas within our framework. Let us now present the findings.

First we look at the dependence of the condensate density in the zeroth, first and second orders of approximation on the physical temperature (see Fig.1.19). Due to the overwhelming role played by the order parameter in the theory of

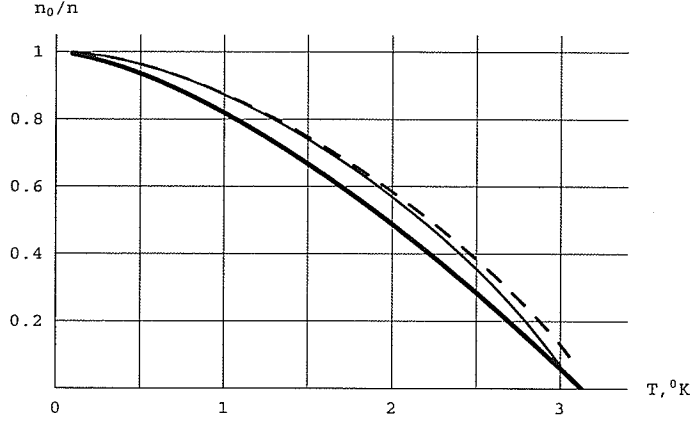


Figure 1.19: Order parameter as a function of the physical temperature. Thick solid, dashed and thin solid lines correspond to the value of the parameter in the zeroth, first and second orders of interaction corrections at unit interaction strength.

Bose condensation, its close inspection is enough for a preliminary account of all physical effects taking place in the system.

Two points of interest may be noted, observing Fig.1.19. First consists of the fact that the second order correction does not vary the overall picture too much compared with the first order one in the whole range of temperatures excluding, possibly, the region close to the critical. This is actually what one expects from the higher-order loop corrections.

The second point, however, is that we found it hard to draw any definite conclusions about the system properties in the critical region, since the procedure we have followed did not perform stably. This issue is not concerned with the particular calculation algorithms, but reflects the overall drawback of all theories that try to approach the critical region perturbatively or take only a limited subset of self-energy diagrams into account [14]. As was discussed earlier, all of them break down near the phase transition point due to the infrared divergencies. This problem can be cured by selective resummations of the diagrams from all orders of perturbation theory. Since our procedure does not perform that, we will refrain from drawing any particular conclusions about the critical region, limiting ourselves to only the most general statements.

Therefore, we conclude that most of the information concerning the influence of the weak interaction on the order parameter in the whole range of temperatures, excluding critical, is contained already in the first order of approximation. Let us

now consider it in more detail.

In Fig.1.20 the first order interaction correction n_{01} to the condensed phase density as a function of the temperature parameter T/T_c is represented for three different values of the interaction parameter.

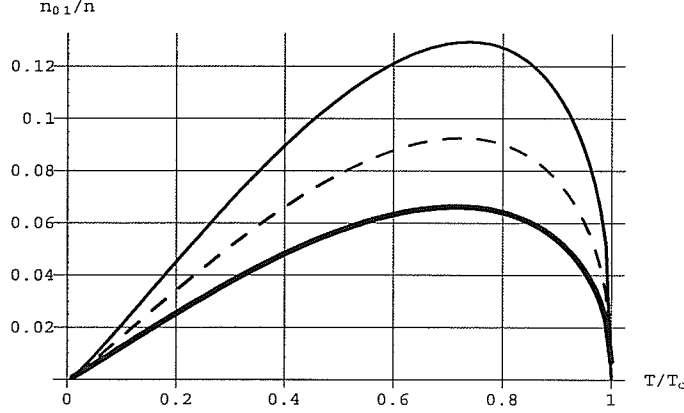


Figure 1.20: First order interaction correction to the condensed phase density as a function of the temperature parameter. Thick solid, dashed and thin solid lines correspond to the interaction parameter U_0 equal to $1/2$, 1 and 2 correspondingly.

First, we notice that the condensed phase density of the interacting gas is higher than that of its non-interacting counterpart in the whole range of temperatures. The explanation of this observation could be represented within the following general framework. The physics of non-ideal Bose gases is determined by the outcome of the competition between entropy and enthalpy. While the first favors more particles in a normal phase by increasing the number of accessible microstates as the temperature increases, the second tries to put more atoms into the condensate by the use of the repulsive interactions. The point, where these two mechanisms compensate each other, corresponds to the actual thermodynamic equilibrium.

Positiveness of n_{01} gives us a clue that the interaction term gives a greater contribution to the enthalpy than to the entropy. It seems to imply that the thermal effect is not as significant in an interacting Bose gas as it is in an ideal gas.

The dependence on the interaction strength is somewhat complicated. As it is clear from the plot, the bigger the interaction strength, the bigger the correction n_{01} . Qualitatively, the dependence is nonlinear. The nonlinearity, however, is two-fold. First, as we may observe directly from the plot, the increase in the magnitude of the interaction is not being accompanied by the proportional increase of the value of the correction itself. Second, the bigger the U_0 , the greater its change impacts the n_{01} . One may directly observe this effect from the relative distances between the curves while keeping the parameter T/T_c fixed.

It is also worth noticing that the maximum of n_{01} shifts slightly to the higher values of temperatures as U_0 increases. That suggests that the enthalpy is able to dominate the entropy the longer the stronger the interaction between the atoms.

Nonlinear dependence of n_{01} on the temperature parameter is obvious. What should be noticed here is the absence of symmetry of the curves with respect to a midpoint $T_c/2$. The bigger the interaction strength, the bigger the asymmetry. As was explained above, this is due to the nonlinear outcome of the competition of the entropy and enthalpy, which leads to the different slopes on the left and right sides of the maximum.

The plot of the dependence of n_{01} on T/T_c functionally and on U_0 parametrically captures the most part of the physics. What remains is to try to extract from the data the information about the system's behavior in the region close to the critical. The critical region itself, as we have already pointed out, cannot be accessed.

The best way to do that is to make a plot of the first order interaction correction to the specific heat C_{V1} per particle as a function of the temperature parameter T/T_c . It is represented in Fig.1.21. One may readily observe the sharp rise of

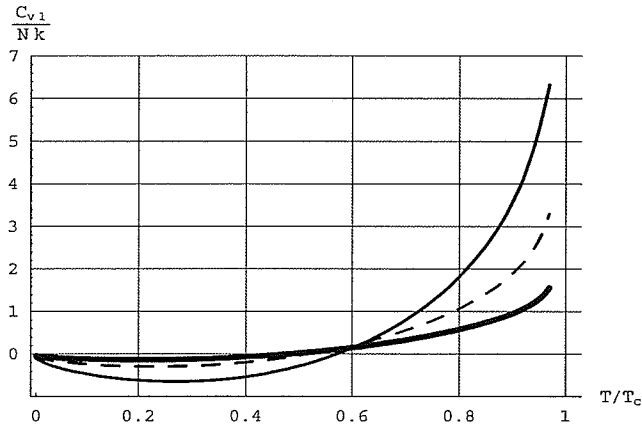


Figure 1.21: First order interaction correction to the specific heat per particle as a function of the temperature parameter. Thick solid, dashed and thin solid lines correspond to the interaction parameter U_0 equal to $1/2$, 1 and 2 correspondingly.

the specific heat as the temperature comes close to the critical. The bigger the interaction parameter, the sharper the rise. This is very similar to the behavior of the actual interacting systems near the phase transition point. Unfortunately, just like it was in the case with the condensate density, we were unable to estimate quantitatively the form of the curve due to the observed instability of the procedure near T_c .

Finally, one feature of our approach should be noted. It turns out, that in the first order of approximation we get the value of the chemical potential equal to zero. This diverges from the results obtained within other approaches, where the zero chemical potential of the ideal Bose gas acquires a small positive correction due to the interaction. However, the second-order correction appears to be useful in this case. It shows that the chemical potential acquires a small negative value, comparable in the order of magnitude to the interaction strength. Its magnitude is

maximal at $T = 0$ and quickly drops to zero in the absolute value as temperature goes up. This is depicted in Fig.1.22.

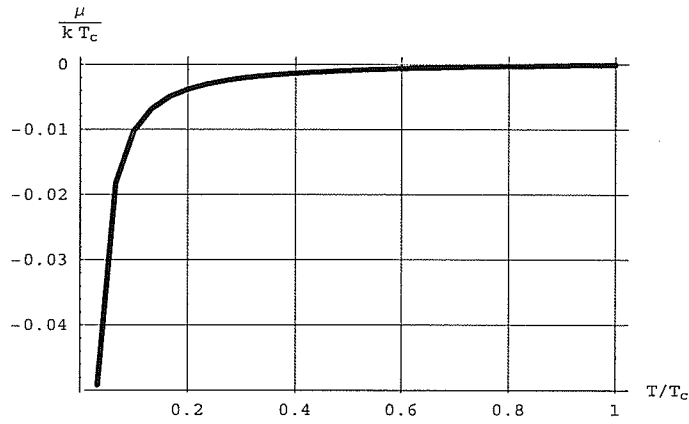


Figure 1.22: Chemical potential in the second order approximation with a unit interaction strength.

Conclusions

Thus, we have demonstrated, how the thermal properties of the weakly interacting Bose gas could be explored based on the approach developed. Despite the fact, that our procedure uses only the minimal subset of the self-energy and free energy contributions, it allows one to evaluate the major effects caused by the interaction already in the leading loop expansion order. The most notable of them are the increase of the condensate density, compared to the non-interacting case, in the whole temperature range, and a sharp rise of the specific heat near the phase transition point. These effects clearly demonstrate that the thermal properties of ideal Bose gases could be changed significantly by the interaction.

However, the most physically interesting region, the critical one, remains unaccessible for our method. Summation to all orders of a broad class of self-energy diagrams is required to make reliable conclusions about the phenomena taking place near the phase transition point [14].

Chapter 2

Two-particle irreducible effective action formalism

As we have observed in the previous chapter, the critical region of Bose condensed systems remains inaccessible for techniques based on perturbation series. The source of the problem is in infrared divergencies, which make the loop expansions unstable near the phase transition point. Physically, these infrared divergencies are screened, and this can be taken into account by summing certain classes of diagrams from all orders of perturbation theory. An example of this is the summation of bubble and ladder diagrams.

Surprisingly, the recent progress in theoretical physics allowed to develop an approach, which makes it possible to perform such summations in a self-consistent and economic manner. Additionally, it proved useful in exploring time-dependent and far-out-of-equilibrium phenomena in the systems of quantum fields, which was well beyond the scope of conventional formalisms.

This approach is based on efficient functional integral techniques, so-called n -particle irreducible (n PI) effective actions [48, 49, 50], for which powerful non-perturbative approximation schemes are available. The subject will be in the center of our attention in what follows.

Treating the Bose condensation phenomenon within the n PI framework is beyond the scope of this work. Instead, we will resolve an important question, concerning the gauge invariance breaking in the n PI theories. This issue is crucial for the internal consistency of the formalism as a whole.

In section 2.1 we overview the motivation which lies behind the n PI approach and discuss specifics of this formalism, which make its applicability area much wider than that of the conventional techniques.

Formal mathematical construction of the 2PI framework is presented in section 2.2.

In 2.3 we treat the simplest gauge theory, namely the quantum electrodynamics (QED), within the 2PI approach.

Section 2.4 is dedicated to the investigation of the issue of the gauge invariance breaking in truncated 2PI QED and contains our resolution of this problem.

2.1 Motivations and overview

Recent remarkable advances in astrophysics, heavy-ion collision experiments and observations of the Bose-Einstein condensates formation in the laboratory produced an abundance of data on matter in extreme conditions. Successful interpretation of that data requires a quantitative understanding of far-from-equilibrium quantum field theory.

On one hand, investigation of specific non-equilibrium effects is important by itself. On the other hand, connecting the far-from-equilibrium dynamics at early times with the approach to a thermal equilibrium at late times is a challenge for theory [52, 53, 54]. A curious problem from this category is prethermalization. This is a universal far-from-equilibrium phenomenon when different quantities thermalize on different time scales. For example, velocities of the atoms of an initially constrained classical gas, when released, relax to the equilibrium Maxwell distribution long before the gas as a whole is getting distributed uniformly over space. In the quantum case such prethermalized quantities approximately take on their final thermal values already at a time when the occupation numbers of individual momentum modes still show strong deviations from the late-time Bose-Einstein or Fermi-Dirac distributions. In order to explain such behavior, it is crucial to be able to compare between the time scales of prethermalization and thermal equilibration.

Moreover, a successful description of dynamics of quantum fields away from equilibrium is tightly related to the basic problem of how macroscopic irreversible behavior arises from time-reversal invariant dynamics of quantum fields. This is a fundamental question with most diverse applications in all areas of physics.

2.1.1 Standard approximation methods fail out of equilibrium

One may try to attack the problem of non-equilibrium quantum fields with the use of standard techniques and methods. There are several frequently employed strategies.

One of them, known as classical statistical field theory, consists of replacing the quantum field by a system of classical distinguishable oscillators. This approach gives important insights, when the number of field quanta per mode is sufficiently large, so that quantum fluctuations are suppressed compared to statistical fluctuations. However, this method is barely useful beyond the classical limit.

Another popular choice is a linear response theory, which is based on the assumption of small deviations from equilibrium and sufficient homogeneity in time of the underlying system. However, intensive exploration of this approach proved its inability to link the early and the late-time behavior in the case where the system is highly non-equilibrium.

Also, important theoretical progress is being made with effective descriptions based on a separation of scales in the weak coupling limit. These kind of problems frequently appear in complex biological systems, where different small and fast degrees of freedom coexist with the big and slow ones. However, there are situations, when there is typically no clear separation of scales which is valid at

all times and it is often difficult to identify a small expansion parameter.

Nevertheless, a successful out-of-equilibrium method should solve additional problems, which do not appear in conventional approaches.

The first problem is secularity. The perturbative expansion of time-dependent variables suffers from secular terms, which grow with time and make the expansion invalid even in the presence of a weak expansion parameter.

Another problem, which poses a severe constraint on a theory, is universality. The method, which pretends to give an adequate description of non-equilibrium systems, must produce universal late-time results, which are not sensitive to the initial conditions and uniquely determined only by the integrals of motion. In order to archive that, implementation of the necessary nonlinear dynamics is demanding.

An illustrative example from classical mechanics

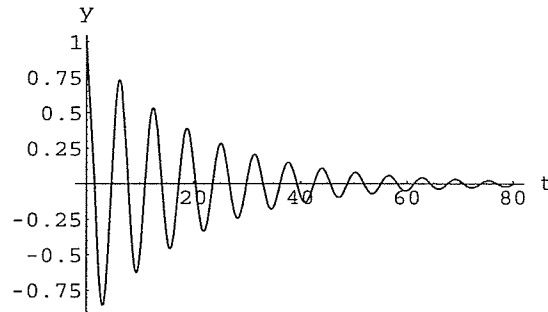
In order to develop intuition about the n PI effective actions, it is useful to consider an example of anharmonic classical oscillator. It is quite remarkable that such a simple system contains all the problems outlined above in their simplest form, and that the resolution of those problems could be straightforwardly translated into the case of nonequilibrium quantum fields.

Our damped oscillator with time-dependent amplitude $y(t)$ is characterized by an infinite number of anharmonic terms:

$$\ddot{y} + y = -\varepsilon \dot{y} - (\varepsilon y)^3 - (\varepsilon y)^5 - (\varepsilon y)^7 - \dots, \quad \varepsilon \ll 1 \quad (2.1.1)$$

Here each dot denotes a derivative with respect to time t . The presence of friction terms to arbitrarily high order resembles the situation in quantum field theory, where the presence of quantum fluctuations can induce self-interactions to high powers in the field. Its form is intentionally chosen in such a way that it results in a geometric series with $\sum_{n=3}^{\infty} (\varepsilon y)^n = (\varepsilon y)^3 / (1 - \varepsilon^2 y^2)$.

In order to solve the initial-value problem for the above second-order differential equation, we employ the following initial conditions: $y(0) = 1$, $\dot{y}(0) = -\varepsilon/2$ and consider the time evolution for $t \geq 0$. Thus, one finds the expected damped oscillator behavior displayed below for $\varepsilon = 0.1$:



What happens, when we neglect contributions from higher order friction terms and leave only a few leading order ones? It may seem quite obvious that such a solution will definitely be a good approximation of the full one in the case where the interaction parameter ε is small. However, this is not true.

Indeed, a perturbative expansion of y in ε ,

$$y_{\text{pert}}(t) = y_0(t) + \varepsilon y_1(t) + \frac{\varepsilon^2}{2} y_2(t) + \mathcal{O}(\varepsilon^3), \quad (2.1.2)$$

yields the standard hierarchy of equations:

$$\ddot{y}_0(t) + y_0(t) = 0 \quad , \quad \ddot{y}_1(t) + y_1(t) = -\dot{y}_0 \quad , \quad \dots \quad (2.1.3)$$

These can be iteratively solved as

$$y_0(t) = \frac{1}{2}e^{it} + \text{c.c.} \quad , \quad y_1(t) = -\frac{1}{4}e^{it}t + \text{c.c.} \quad , \quad \dots \quad (2.1.4)$$

Doing this to second order in ε , one finds:

$$y_{\text{pert}}(t) = \frac{1}{2}e^{it} \left(1 - \frac{\varepsilon}{2}t + \frac{\varepsilon^2}{8} [t^2 - it] \right) + \text{c.c.} \quad (2.1.5)$$

Beyond the lowest order, the solution contains secular terms which grow with powers of the time t , and one arrives at the important conclusion:

The perturbative expansion is only valid for $\varepsilon t \ll 1$.

Now consider an alternative, (“nPI type”) expansion. Unlike the previous case, we will not expand the amplitude $y(t)$ into a series, but rather classify the terms of the equation of motion (2.1.1) according to the powers of the small parameter ε . Since in the leading order of expansion the right-hand side does not contain any terms of order ε^0 , we obtain the same equation as in the conventional perturbation theory:

$$\ddot{y}_{n\text{PI}}^{(0)} + y_{n\text{PI}}^{(0)} = 0 \quad \Rightarrow \quad y_{n\text{PI}}^{(0)}(t) = \frac{1}{2}e^{it} + \text{c.c.} \quad (2.1.6)$$

The next order takes into account all terms of (2.1.1) to order ε^1 , i.e.

$$\ddot{y}_{n\text{PI}}^{(2)} + y_{n\text{PI}}^{(2)} = -\varepsilon \dot{y}_{n\text{PI}}^{(2)} \quad \Rightarrow \quad y_{n\text{PI}}^{(2)}(t) = \frac{1}{2}e^{it\sqrt{1-\varepsilon^2/4}-\varepsilon t/2} + \text{c.c.} \quad (2.1.7)$$

Since there are no ε^2 friction terms appearing in (2.1.1), the above equation also agrees with the second order of the expansion. The next order would take into account all terms of the equation to order ε^3 , and so on.

This provides a systematic approximation procedure in terms of powers of the small parameter ε . However, in contrast to the conventional perturbative expansion, the “nPI type” expansion turns out to be non-secular in time. Indeed, as one may explicitly observe from (2.1.6) and (2.1.7), both the lowest order approximation and $y_{n\text{PI}}^{(2)}(t)$ do not exceed $\mathcal{O}(\varepsilon^0)$ for all times. Thus, the result (2.1.7) provides a universally valid approximation to the equation (2.1.1) up to corrections of order ε^3 . The already very good agreement with the exact result can be checked explicitly.

It is instructive to compare the “nPI type” solution to the perturbative one by expanding (2.1.7) in powers of ε :

$$\begin{aligned} y_{n\text{PI}}^{(2)}(t) &= \frac{1}{2}e^{it} \left(1 - \frac{\varepsilon}{2}t + \frac{\varepsilon^2}{8} [t^2 - it] \right) + \mathcal{O}(\varepsilon^3) + \text{c.c.} \\ &\stackrel{(!)}{=} y_{\text{pert}}(t) + \mathcal{O}(\varepsilon^3) + \text{c.c.} \end{aligned}$$

This allows us to conclude that

- the “ n PI” result corresponds to the perturbative one up to the order of approximation (here up to $O(\varepsilon^3)$ corrections).
- the “ n PI” result resums all secular terms to infinite perturbative order in ε .

Stated differently: infinite summation of perturbative orders is required to obtain a uniform approximation to the exact solution, i.e. that the error stays of a given order at all times.

What made the alternative expansion so successful? In the case of the regular approximation, we started with breaking the variable y into degrees of freedom according to the powers of the expansion parameter ε . Thus, for example, the big and slow degree of freedom, y_0 , turned out to be separated from the small and fast one, y_1 , and served as its driving force, which led to secular divergence. In the second case, however, we did not expand y additionally, but rather preferred to define the degrees of freedom self-consistently, in terms of themselves. Therefore, those of them, including y_0 and y_1 , which were previously considered as separate, now got confined into a single object $y_{nPI}^{(2)}$, which behaves nicely.

Thus, in order to avoid secularity, we have to truncate the dynamics of a given variable according to powers of the small expansion parameter. The price to be paid is the necessity of having to deal with nonlinear equations. However, it is exactly the nonlinearity which will help us to obtain universality in the sense outlined above.

2.1.2 The way to describe nonequilibrium quantum fields from first principles.

Nonequilibrium dynamics requires the specification of an initial state at some given time t_0 . Once it is done, the subsequent time-evolution is completely determined by the Hamiltonian. Equivalently, the dynamics can be described in terms of a functional path integral with the classical action S . From the latter one obtains the effective action Γ , which is the generating functional for all correlation functions of the quantum theory. There are no further ingredients involved concerning the dynamics, than what is known from standard vacuum quantum field theory. There are no course graining, averaging or any other approximations or assumptions involved. The fact, that the dynamics is obtained from the effective action, guarantees a number of crucial properties for the time evolution. The most notable of them is the energy conservation, which in the classical limit is manifested by the absence of the friction terms in the equations of motion.

There is no loss of information during the thus derived nonequilibrium time evolution. In this respect it is quite remarkable that the evolution can come very close to the state of thermal equilibrium and remain there for an arbitrarily long time. Thus, the observed effective loss of details about the initial conditions can mimic very accurately the irreversible dynamics which is realized in the actual systems.

n -Particle irreducible expansions

Now we are ready to “translate” the above mechanical example into quantum field theory. Of course, this trick is intended to give only an intuitive insight and should

not to be regarded as a way to “quantize” the classical system.

In the language of field theory, the oscillator amplitude y plays the role of the one-point function, i.e. the field expectation value or macroscopic field. The squared amplitude is then, obviously, a two-point function, or propagator. The many-point functions are nothing else but vertices, etc.:

$$\begin{array}{lll}
y(t) & \rightsquigarrow & \phi(x) = \langle \hat{\Phi}(x) \rangle \\
& & \text{(macroscopic field)} \\
y^2(t) & \rightsquigarrow & G_2(x, y) = \langle T \hat{\Phi}(x) \hat{\Phi}(y) \rangle - \phi(x)\phi(y) \equiv G(x, y) \\
& & \text{(propagator)} \\
y^3(t) & \rightsquigarrow & G_3(x, y, z) \text{ or, with } G_3 \sim GGGV_3 : \\
& & V_3(x, y, z) \quad \text{(proper three-vertex)} \\
y^4(t) & \rightsquigarrow & V_4(x, y, z, w) \quad \text{(proper 4-vertex)} \\
& \vdots &
\end{array}$$

All of these are independent “degrees of freedom” and their knowledge provides a full description of the quantum field theory.

The equations of motion of n -point functions are conveniently encoded in an effective action Γ . There are different representations of this functional. The one, especially suitable for our needs, is the so-called n -particle irreducible effective action $\Gamma[\phi, G, V_3, \dots, V_n]$. It is parameterized by the degrees of freedom and serves as a starting point for powerful approximation schemes in non-equilibrium quantum field theory. It determines the equations of motion for $\phi, G, V_3, \dots, V_n$ by the following stationarity conditions:

$$\frac{\delta \Gamma[\phi, G, V_3, \dots]}{\delta \phi} = 0, \quad \frac{\delta \Gamma[\phi, G, V_3, \dots]}{\delta G} = 0, \quad \frac{\delta \Gamma[\phi, G, V_3, \dots]}{\delta V_3} = 0, \dots \quad (2.1.8)$$

Now the “ n PI” approximation scheme for the classical anharmonic oscillator introduced above can be translated into the quantum case as follows:

- Classify the contributions to $\Gamma[\phi, G, V_3, \dots]$ according to powers of a suitable expansion parameter or any other appropriate approximation scheme.
- Drop the higher order terms, thus performing truncation of the full effective action functional.
- Determine the equation of motion for $\phi, G, V_3, \dots, V_n$ from the truncated effective action according to (2.1.8) without any further assumptions.

It may seem that the full effective action $\Gamma[\phi, G, V_3, \dots, V_n]$ should be prohibitively complicated, since it depends on an infinite number of degrees of freedom. Fortunately, there exists an equivalence hierarchy between the n PI effective actions [48], which simplifies the task considerably. For instance, when performing the loop expansion, one has:

$$\begin{array}{l}
\Gamma^{(1\text{loop})}[\phi] = \Gamma^{(1\text{loop})}[\phi, D] = \dots, \\
\Gamma^{(2\text{loop})}[\phi] \neq \Gamma^{(2\text{loop})}[\phi, D] = \Gamma^{(2\text{loop})}[\phi, D, V_3] = \dots, \\
\Gamma^{(3\text{loop})}[\phi] \neq \Gamma^{(3\text{loop})}[\phi, D] \neq \Gamma^{(3\text{loop})}[\phi, D, V_3] = \Gamma^{(3\text{loop})}[\phi, D, V_3, V_4] = \dots, \\
\vdots
\end{array}$$

Here $\Gamma^{(n\text{loop})}$ denotes the truncation of the respective effective action to a given n -th loop order. In other words, if we are interested only in the effects of the second order in the interaction constant g , then all we need is to take the full 2PI effective action and truncate it to leave only two-loop diagrams. The resulting effective action will contain the same information about the effects of interest as any other higher order n PI functional with $n > 2$, truncated to the second order. On the other hand, if we want to explore the effects of order g^3 , then truncated to three loops 2PI and 3PI actions, respectively, will not give physically equivalent results. Thus, the higher order effects require higher order functionals to be introduced. Typically, one rarely needs to treat the processes beyond the fourth order. Therefore, the 2PI, 3PI and maybe 4PI effective actions are enough for most of the purposes.

In what follows, we will concentrate particularly on the 2PI functionals, briefly mentioning the 3PI ones when discussing the QED electrical conductivity.

Also, exploration of the non-equilibrium effects in the systems of quantum fields is beyond the scope of this review. Therefore, we will work completely within the equilibrium field theory, both vacuum and thermal, leaving discussion of the related subject for the concluding paragraph of the work.

2.2 Two-particle irreducible generating functionals

In this section we discuss a formal construction of the one-particle irreducible (1PI) and the two-particle irreducible (2PI) effective actions. The latter provides a powerful starting point for systematic approximations in non-equilibrium quantum field theory [49, 50]. To be specific, we consider first a quantum field theory for a real, N -component scalar field φ_a ($a = 1, \dots, N$) with the following classical action $S[\varphi]$:

$$S_{cl}[\varphi] = \frac{1}{2}(\partial_x \varphi_x)^2 - \frac{m^2}{2}(\varphi_x)^2 - \frac{\lambda}{4!N}(\varphi_x)^4. \quad (2.2.1)$$

Here the repeated index represents a summation over all discrete indices and an integral over space and time variables. The explicit time contour will be specified later.

The generating functional $W[J, R]$ for connected Green's functions in the presence of one-point J_1 and two-point R_{12} source terms is given by

$$\begin{aligned} Z[J, R] &= \text{Exp}(iW[J, R]) \\ &= \int D[\varphi] \text{Exp} \left[i \left(S_{cl}[\varphi] + J_x \varphi_x + \frac{1}{2} R_{xy} \varphi_x \varphi_y \right) \right]. \end{aligned} \quad (2.2.2)$$

We define the macroscopic field ϕ_1 and the connected two-point function G_{xy} by variation of $W[J, R]$ with respect to the source terms as the following:

$$\frac{\delta W[J, R]}{\delta J_x} = \phi_x; \quad \frac{\delta W[J, R]}{\delta R_{xy}} = \frac{1}{2}(\phi_x \phi_y + iG_{xy}). \quad (2.2.3)$$

Before constructing the 2PI effective action, it is convenient to consider the 1PI one, which is obtained by the Legendre transform of the generating functional

$W[J, R]$ with respect to the source J_1 :

$$\Gamma^R[\phi] = W[J, R] - \frac{\delta W[J, R]}{\delta J_x} J_x = W[J, R] - J_x \phi_x. \quad (2.2.4)$$

We note that:

1. $\Gamma^{R=0}[\phi]$ corresponds to the standard 1PI effective action.
2. For $R \neq 0$ it can be formally viewed as the 1PI effective action for a theory governed by the modified classical action, $S^R[\varphi]$, in the presence of a non-constant “mass term” $\sim R_{xy}$, quadratic in the fields:

$$S^R[\varphi] = S[\varphi] + \frac{1}{2} R_{xy} \varphi_x \varphi_y. \quad (2.2.5)$$

This can be directly observed from (2.2.2) and the fact that the standard 1PI effective action is obtained from the same defining functional integral in the presence of a term linear in the field. Correspondingly, it is a straightforward task to recover for $\Gamma^R[\phi]$ all the “textbook” relations for the 1PI effective action taking R into account. For instance, $\Gamma^R[\phi]$ to one-loop order is given by

$$\Gamma^{R(1\text{loop})}[\phi] = S^R[\phi] + \frac{i}{2} \text{Tr} \text{Ln} [(G_{xy}^0)^{-1} + R_{xy}], \quad (2.2.6)$$

which is the familiar result for the 1PI effective action with $S[\phi] \rightarrow S^R[\phi]$ and $(G_{xy}^0)^{-1} \rightarrow (G_{xy}^0)^{-1} + R_{xy}$. Similarly, one finds that the exact inverse propagator is obtained by taking double derivative over fields:

$$\frac{\delta^2 \Gamma^R[\phi]}{\delta \phi_x \delta \phi_y} = G_{xy}^{-1} = (G_{xy}^0)^{-1} + R_{xy} - \Sigma_{xy}^R. \quad (2.2.7)$$

Here the classical inverse propagator $(G_{xy}^0)^{-1} = \delta^2 S[\phi] / \delta \phi_x \delta \phi_y$ reads

$$(G_{xy}^0)^{-1} = - \left(\square + m^2 + \frac{\lambda}{6N} \phi_z \phi_z \right) \delta_{xy} - \frac{\lambda}{3N} \phi_x \phi_y \delta(\vec{x} - \vec{y}), \quad (2.2.8)$$

and Σ_{12}^R is the proper self-energy, to which only one-particle irreducible Feynman diagrams contribute, i.e. diagrams which cannot be separated by opening one propagator line.

The 2PI effective action is obtained by performing a further Legendre transform of $\Gamma^R[\phi]$ with respect to the two-point source R :

$$\begin{aligned} \Gamma[\phi, G] &= \Gamma^R[\phi] - \underbrace{\frac{\delta \Gamma^R[\phi]}{\delta R_{xy}}}_{\frac{\delta W[J, R]}{\delta R_{xy}}} R_{yx} \\ &= \Gamma^R[\phi] - \frac{1}{2} R_{xy} (\phi_x \phi_y + i G_{xy}). \end{aligned} \quad (2.2.9)$$

Here we have used the fact that the relation between ϕ and J is R -dependent, i.e. inverting $\phi = \delta W[J, R]/\delta J$ yields $J = J^R(\phi)$. From the above definition of $\Gamma^R[\phi]$ one therefore finds:

$$\begin{aligned}\frac{\delta \Gamma^R[\phi]}{\delta R_{xy}} &= \frac{\delta W[J, R]}{\delta R_{xy}} + \frac{\delta W[J, R]}{\delta J_z} \frac{\delta J_z}{\delta R_{xy}} - \frac{\delta J_z}{\delta R_{xy}} \phi_z \\ &= \frac{\delta W[J, R]}{\delta R_{xy}}.\end{aligned}\quad (2.2.10)$$

Of course, the two subsequent Legendre transforms of $W[J, R]$, which have been used to arrive at (2.2.9), could have been performed simultaneously like the following:

$$\begin{aligned}\Gamma[\phi, G] &= W[J, R] - \frac{\delta W[J, R]}{\delta J_x} J_x - \frac{\delta W[J, R]}{\delta R_{xy}} R_{xy} \\ &= W[J, R] - J_x \phi_x - \frac{1}{2} R_{xy} (\phi_x \phi_y + i G_{xy})\end{aligned}\quad (2.2.11)$$

From this one directly observes the stationarity conditions:

$$\frac{\delta \Gamma[\phi, G]}{\delta \phi_x} = -J_x - R_{xy} \phi_y, \quad (2.2.12)$$

$$\frac{\delta \Gamma[\phi, G]}{\delta G_{xy}} = -\frac{i}{2} R_{xy}, \quad (2.2.13)$$

which give the equations of motion for ϕ and G in the absence of the sources, i.e. $J = 0$ and $R = 0$.

To get familiar with equations (2.2.9) or (2.2.11), we may directly calculate $\Gamma[\phi, G]$ to one-loop order using the above results for $\Gamma^R[\phi]$. Plugging (2.2.6) into (2.2.9), one finds to this order:

$$\Gamma[\phi, G] \simeq S[\phi] + \frac{i}{2} \text{Tr} \text{Ln} [(G_{xy}^0)^{-1} + R_{xy}] - \frac{i}{2} R_{xy} G_{xy}. \quad (2.2.14)$$

If we set $G_{xy}^{-1} = (G_{xy}^0)^{-1} + R_{xy}$, then we can write

$$\Gamma[\phi, G] \simeq S[\phi] + \frac{i}{2} \text{Tr} \text{Ln} G^{-1} + \frac{i}{2} \text{Tr} [(G^0)^{-1} G] + \text{const}, \quad (2.2.15)$$

with $\text{Tr} [G^{-1} G] \sim \text{Tr} \mathbf{1} = \text{const}$. To verify this, one can check from the stationarity condition (2.2.12), that indeed to this order

$$\frac{\delta \Gamma[\phi, G]}{\delta G_{xy}} \simeq -\frac{i}{2} G_{xy}^{-1} + \frac{i}{2} (G_{xy}^0)^{-1} = -\frac{i}{2} R_{xy} \quad \Rightarrow \quad G_{xy}^{-1} = (G_{xy}^0)^{-1} + R_{xy}.$$

In order to go beyond the first order, it is convenient to write the exact functional $\Gamma[\phi, G]$ as the one-loop type expression (2.2.15) and a “rest”:

$$\Gamma[\phi, G] = S[\phi] + \frac{i}{2} \text{Tr} \text{Ln} G^{-1} + \frac{i}{2} \text{Tr} [(G^0)^{-1} (G - G^0)] + \Gamma_2[\phi, G]. \quad (2.2.16)$$

To get an understanding of the “rest” term $\Gamma_2[\phi, G]$, one may vary this expression with respect to G , which yields

$$G_{xy}^{-1} = (G_{xy}^0)^{-1} + R_{xy} - \Sigma_{xy}, \quad (2.2.17)$$

where we have written

$$\Sigma_{xy} \equiv 2i \frac{\delta \Gamma_2[\phi, G]}{\delta G_{yx}}. \quad (2.2.18)$$

Comparing this with the exact expression (2.2.7), one observes the equality

$$\Sigma_{xy} = \Sigma_{xy}^R, \quad (2.2.19)$$

which relates the functional G -derivative of $\Gamma_2[\phi, G]$ to the proper self-energy. As was mentioned earlier, the proper self-energy obtains contributions only from the 1PI diagrams in which propagator lines are associated with the effective classical propagator $((G^0)^{-1} - R)^{-1}$. The mapping between Σ and Σ^R is provided by (2.2.17), which can be used to express the full propagator G as an infinite series in terms of the classical propagator G^0 and Σ :

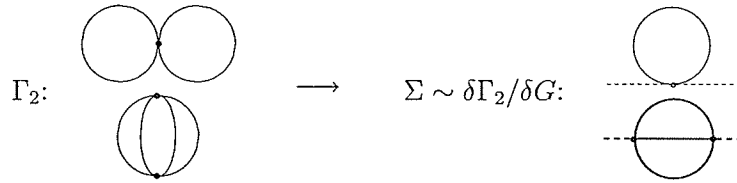
$$G = ((G^0)^{-1} - R)^{-1} + ((G^0)^{-1} - R)^{-1} \Sigma ((G^0)^{-1} - R)^{-1} + ((G^0)^{-1} - R)^{-1} \Sigma ((G^0)^{-1} - R)^{-1} \Sigma ((G^0)^{-1} - R)^{-1} + \dots \quad (2.2.20)$$

As a consequence, there is a direct correspondence between a 1PI diagram with propagator lines associated to G and an infinite set of 1PI diagrams with propagator lines associated to the classical propagator G^0 . Below we will consider some explicit examples. Most importantly, from the fact that only 1PI diagrams contribute to Σ , one can conclude that

- $\Gamma_2[\phi, G]$ only contains contributions from two-particle irreducible (2PI) diagrams.

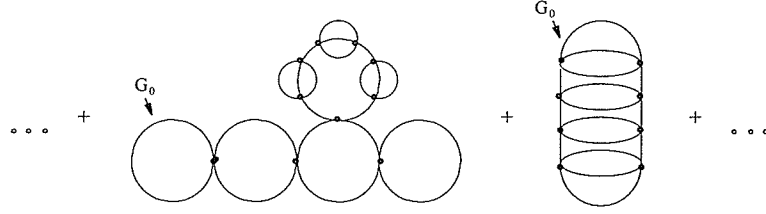
A diagram is said to be two-particle irreducible, if it cannot be disconnected into two parts upon opening two propagator lines. Suppose $\Gamma_2[\phi, G]$ has a two-particle reducible contribution. This means that the latter can be represented as $D G G \tilde{D}$, where G 's are the propagators connecting two separate parts, D and $\tilde{D}$, of the diagram. Then the self-energy Σ is obtained by differentiating $\Gamma_2[\phi, G]$ over G , i.e. opening one of the above G lines. The resulting diagram analytically reads as $D G \tilde{D}$ and is obviously one-particle reducible. Thus, it cannot occur as part of the self-energy and, therefore, the $\Gamma_2[\phi, G]$ functional is indeed 2PI.

Examples of the two- and three-loop diagrams, contributing to $\Gamma_2[\phi, G]$ and Σ in scalar ϕ^4 theory, are shown below:



Because of (2.2.20), each of the 2PI diagrams corresponds to an infinite series of 1PI diagrams. For example, the above 2PI diagrams contain the full series of so-called “daisies” and “ladder” resummations:

This kind of resummation is exactly what is required to get rid of the infrared divergencies in the problem of an interacting Bose gas near the phase transition point. Thus, one may expect, that the formalism of n PI effective actions will be a very successful tool to deal with critical phenomena issues.



2.2.1 Loop or coupling expansion of the 2PI effective action

Loop or coupling expansions of the 2PI effective action proceed along the same lines as the corresponding expansions for the standard 1PI effective action, with the only difference that

- the full propagator G is associated to propagator lines of a diagram
- and only 2PI graphs are kept.

The great advantage of the 2PI expansion scheme is that it produces much less topologically distinct diagrams than its 1PI counterpart. For instance, in the symmetric phase of the scalar ϕ^4 theory, there is only a single diagram that contributes at each order up to four loops. At fifth order there are two distinct diagrams, which are shown along with the lower-loop ones in Fig.2.1.

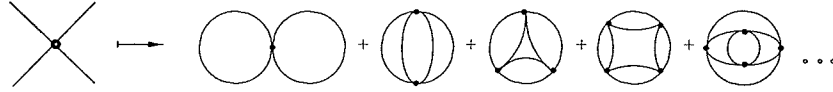


Figure 2.1: Topologically distinct diagrams in the 2PI loop expansion up to five-loop order for $\phi = 0$. All prefactors suppressed.

Such a quick convergence is unprecedented and cannot be archived by any other method.

2.3 Gauge invariance in 2PI effective action

The n PI expansions are known to be conserving, i.e. they are consistent with the global symmetries of the Lagrangian. However, they can violate the Ward-Takahashi identities (WTI) associated with the local symmetries [55, 56, 57]. This is a very serious issue that needs to be resolved for the sake of the consistency of the formalism itself.

Below, we will treat the problem of the gauge-invariance breaking on the example of the simplest possible 2PI gauge theory, namely the quantum electrodynamics (QED), based on the 2PI effective action. We will demonstrate that it is possible to construct a new effective theory on top of the 2PI formalism, which not only preserves all the properties of the latter, but is also free from the gauge-dependence issues [60, 61].

The approach to be developed is easily extendable not only to the more general gauge theories, but to higher order irreducible effective actions as well.

2.3.1 Definitions

The QED 2PI partition function is defined as [56]:

$$Z[J, \eta, \bar{\eta}, C, B] = \int D[\mathcal{A}\Psi\bar{\Psi}] \text{Exp} \left[i \left(S_{cl}[\mathcal{A}] + J_1 \mathcal{A}_1 + \bar{\eta}_1 \Psi_1 + \bar{\Psi}_1 \eta_1 + \frac{1}{2} C_{12} \mathcal{A}_1 \mathcal{A}_2 + B_{12} \Psi_1 \bar{\Psi}_2 \right) \right]. \quad (2.3.1)$$

It depends both on the one-point fermion $\bar{\eta}, \eta$ and photon J sources, as well as on two-point B and C ones.

The classical action $S_{cl}[\mathcal{A}]$ is the Maxwell action, which helps to define the lowest order inverse propagators for the electron and photon as

$$(S_{12}^0)^{-1} = \frac{\delta^2 S_{cl}}{\psi_2 \delta \psi_1}; \quad (D_{12}^0)^{-1} = \frac{\delta^2 S_{cl}}{\delta \mathcal{A}_2 \delta \mathcal{A}_1}. \quad (2.3.2)$$

As previously, we introduce the generating functional for connected fields:

$$W[J, \eta, \bar{\eta}, C, B] = -i \text{Ln} Z[J, \eta, \bar{\eta}, C, B]. \quad (2.3.3)$$

Taking functional derivatives of (2.3.3), we obtain:

$$\begin{aligned} \frac{\delta W}{\delta J_1} &= A_1; \quad \frac{\delta W}{\delta \bar{\eta}_1} = \psi_1; \quad \frac{\delta W}{\delta \eta_1} = -\bar{\psi}_1; \\ \frac{\delta W}{\delta C_{12}} &= \frac{1}{2} (A_1 A_2 + i D_{12}); \quad \frac{\delta W}{\delta B_{12}} = \psi_1 \bar{\psi}_2 + i S_{12}, \end{aligned} \quad (2.3.4)$$

where S and D are the resummed propagators

$$\begin{aligned} i D_{12} &= \langle \mathcal{A}_1 \mathcal{A}_2 \rangle - \langle \mathcal{A}_1 \rangle \langle \mathcal{A}_2 \rangle, \\ i S_{12} &= \langle \Psi_1 \bar{\Psi}_2 \rangle - \langle \Psi_1 \rangle \langle \bar{\Psi}_2 \rangle \end{aligned} \quad (2.3.5)$$

and A, ψ and $\bar{\psi}$ are the field expectation values:

$$\langle \mathcal{A} \rangle = A, \quad \langle \Psi \rangle = \psi, \quad \langle \bar{\Psi} \rangle = \bar{\psi}. \quad (2.3.6)$$

The QED 2PI effective action is now obtained by taking the double Legendre transform of $W[J, \eta, \bar{\eta}, C, B]$ with respect to the sources. The expression is explicitly constructed in such a way that its partial derivatives with respect to the sources are zero. Thus, we have:

$$\begin{aligned} \Gamma[\psi, \bar{\psi}, A, S, D] &= W[J, \eta, \bar{\eta}, C, B] - J_1 A_1 - \bar{\eta}_1 \psi_1 - \bar{\psi}_1 \eta_1 \\ &\quad - B_{12} (\psi_1 \bar{\psi}_2 + i S_{12}) - \frac{1}{2} C_{12} (A_1 A_2 + i D_{12}) \end{aligned} \quad (2.3.7)$$

with the following constraints:

$$\begin{aligned} \frac{\delta \Gamma}{\delta A_1} &= -J_1 - C_{12} A_2; \quad \frac{\delta \Gamma}{\delta \psi_1} = \bar{\eta}_1 - B_{12} \bar{\psi}_2; \quad \frac{\delta \Gamma}{\delta \bar{\psi}_1} = -\eta_1 + B_{21} \psi_2; \\ \frac{\delta \Gamma}{\delta D_{12}} &= -\frac{i}{2} C_{12}; \quad \frac{\delta \Gamma}{\delta S_{12}} = -i B_{12}. \end{aligned} \quad (2.3.8)$$

Using standard field theory techniques, expression (2.3.7) can be rewritten in a more convenient form, which yields

$$\begin{aligned}\Gamma[\psi, \bar{\psi}, A, S, D] &= S_{cl}[\psi, \bar{\psi}, A] + \frac{i}{2} \text{Tr} \text{Ln} D_{12}^{-1} + \frac{i}{2} \text{Tr} [(D_{12}^0)^{-1} (D_{21} - D_{21}^0)] \\ &\quad - i \text{Tr} \text{Ln} S_{12}^{-1} - i \text{Tr} [(S_{12}^0)^{-1} (S_{21} - S_{21}^0)] + \Phi[S, D].\end{aligned}\quad (2.3.9)$$

As we have already discussed in the previous chapter, the functional $\Phi[S, D]$ is the sum of all two-particle irreducible diagrams. It depends only on connected two-point functions S and D , but not on the expectation values of the fields $\{\psi, \bar{\psi}, A\}$.

The equations of motion of the mean fields and the propagators of the theory are obtained from conditions of the stationarity of the effective action. These are nothing else but the equations (2.3.8) in the absence of sources:

$$\begin{aligned}\frac{\delta \Gamma[\psi, \bar{\psi}, A, S, D]}{\delta A} &= 0; \quad \frac{\delta \Gamma[\psi, \bar{\psi}, A, S, D]}{\delta D} = 0 \\ \frac{\delta \Gamma[\psi, \bar{\psi}, A, S, D]}{\delta \psi} &= 0; \quad \frac{\delta \Gamma[\psi, \bar{\psi}, A, S, D]}{\delta \bar{\psi}} = 0; \quad \frac{\delta \Gamma[\psi, \bar{\psi}, A, S, D]}{\delta S} = 0\end{aligned}\quad (2.3.10)$$

2.3.2 Symmetry properties of the 2PI generating functionals

Let us now explore the symmetry properties of the 2PI functionals introduced above.

Local symmetries

Consider making in the functional integral (2.3.1) the following change of fermionic variables

$$\Psi_1 \rightarrow \Psi_1 - ie\Lambda_1 \bar{\Psi}_1; \quad \bar{\Psi}_1 \rightarrow \bar{\Psi}_1 + ie\Lambda_1 \bar{\Psi}_1 \quad \text{no sum} \quad (2.3.11)$$

without the corresponding term in the transformation law for $\mathcal{A}_1$ (which would make the Lagrangian invariant under such a transformation). The QED Lagrangian then transforms according to

$$L \rightarrow L - e\partial_1 \Lambda_1 \bar{\Psi}_1 \gamma^\mu \Psi_1. \quad (2.3.12)$$

Then, expanding (2.3.1) to the first order in Λ , we find that the infinitesimal change of the partition function, caused by the transformation (2.3.11), is

$$\begin{aligned}\Delta Z[J, \eta, \bar{\eta}, C, B] &= \\ &\int D[\mathcal{A}\Psi\bar{\Psi}] \left[\Lambda_1 \partial_1 j_1 + ie\Lambda_1 (\bar{\eta}_1 \Psi_1 - \bar{\Psi}_1 \eta_1) + ieB_{12}(\Lambda_1 - \Lambda_2) \Psi_1 \bar{\Psi}_2 \right] \\ &\cdot \text{Exp} \left[i \left(\int dx L + J_1 \mathcal{A}_1 + \bar{\eta}_1 \Psi_1 + \bar{\Psi}_1 \eta_1 + \frac{1}{2} C_{12} \mathcal{A}_1 \mathcal{A}_2 + B_{12} \Psi_1 \bar{\Psi}_2 \right) \right] = 0,\end{aligned}\quad (2.3.13)$$

where $j_1 = e\bar{\Psi}_1 \gamma \Psi_1$ is the local current.

This expression is not helpful in its present form. However, we may transform it by extracting the quantum fields from the path integral. To achieve that,

we replace them by derivatives with respect to the sources, which act on the exponential factor in (2.3.13) as the following:

$$\mathcal{A}_1 \rightarrow \frac{1}{i} \frac{\delta}{\delta J_1}; \quad \Psi_1 \rightarrow \frac{1}{i} \frac{\delta}{\delta \bar{\eta}_1}; \quad \bar{\Psi}_1 \rightarrow -\frac{1}{i} \frac{\delta}{\delta \eta_1}; \quad \Psi_1 \bar{\Psi}_2 \rightarrow \frac{1}{i} \frac{\delta}{\delta B_{12}}. \quad (2.3.14)$$

This gives

$$\begin{aligned} \Delta Z[J, \eta, \bar{\eta}, C, B] = & \quad (2.3.15) \\ & \int D[\mathcal{A}\Psi\bar{\Psi}] \left[\Lambda_1 \partial_1 j_1 + e\Lambda_1 (\bar{\eta}_1 \frac{\overrightarrow{\delta}}{\delta \bar{\eta}_1} + \frac{\overleftarrow{\delta}}{\delta \eta_1} \eta_1) + eB_{12} (\Lambda_1 - \Lambda_2) \frac{\overrightarrow{\delta}}{\delta B_{12}} \right] \\ & \cdot \text{Exp} \left[i \left(\int dx L + J_1 \mathcal{A}_1 + \bar{\eta}_1 \Psi_1 + \bar{\Psi}_1 \eta_1 + \frac{1}{2} C_{12} \mathcal{A}_1 \mathcal{A}_2 + B_{12} \Psi_1 \bar{\Psi}_2 \right) \right] = 0, \end{aligned}$$

where arrows indicate that the functional derivatives act on the partition function but not on the sources. This transformation leads straight to the WTI for the 2PI Z -functional:

$$\Lambda_1 \partial_1 j_1 Z + e\Lambda_1 \left(\bar{\eta}_1 \frac{\delta Z}{\delta \bar{\eta}_1} + \frac{\delta Z}{\delta \eta_1} \eta_1 \right) + e(\Lambda_1 - \Lambda_2) B_{12} \frac{\delta Z}{\delta B_{12}} = 0, \quad (2.3.16)$$

from which we observe that in the absence of sources the local current is conserved:

$$\partial_1 j_1 = 0. \quad (2.3.17)$$

For the sake of completeness, we may write the WTI for two other functionals of interest, namely W and Γ . Substituting $Z = \exp(iW)$ into (2.3.16) we obtain:

$$\Lambda_1 \partial_1 j_1 + ie\Lambda_1 (\bar{\eta}_1 \psi_1 - \bar{\psi}_1 \eta_1) + ie(\Lambda_1 - \Lambda_2) B_{12} (\psi_1 \bar{\psi}_2 + iS_{12}) = 0 \quad (2.3.18)$$

Once again, the absence of sources leads to the local current conservation.

Finally, we rewrite the above expression by replacing the sources with corresponding derivatives of the effective action, using (2.3.8). The result is:

$$\Lambda_1 \partial_1 j_1 + ie\Lambda_1 \left(\frac{\delta \Gamma}{\delta \psi_1} \psi_1 + \bar{\psi}_1 \frac{\delta \Gamma}{\delta \bar{\psi}_1} \right) + ie(\Lambda_1 - \Lambda_2) \frac{\delta \Gamma}{\delta S_{12}} S_{12} = 0 \quad (2.3.19)$$

Again, it follows immediately that for the solutions of the equations of motion, given by (2.3.10), the Noether current remains unchanged.

Global symmetries

Conservation of the global current comes straightforwardly from the scheme represented above. In this case the phase changes are the same in all points of space and we set $\Lambda_1 = \text{const}$. This means that the Lagrangian in (2.3.12) does not change and first terms in (2.3.16), (2.3.18) and (2.3.19) disappear. Third terms in the above equalities also vanish and what remains is the global form of the WTI

$$\frac{\delta \Gamma}{\delta \psi_1} \psi_1 + \bar{\psi}_1 \frac{\delta \Gamma}{\delta \bar{\psi}_1} = 0, \quad (2.3.20)$$

which is always satisfied for the physical solutions.

2.3.3 The Ward-Takahashi identity for the 2PI two-point function

Now let us turn to the WTI for the 2PI two-point function. The latter is defined as

$$\begin{aligned}\langle 0|T\Psi_a\bar{\Psi}_b|0\rangle &= \frac{1}{Z[J,\eta,\bar{\eta},C,B]}\left(-i\frac{\delta}{\delta\bar{\eta}_a}\right)\left(i\frac{\delta}{\delta\eta_b}\right)Z[J,\eta,\bar{\eta},C,B]\Big|_{J=\eta=\bar{\eta}}^{C=B=0} \\ &= \frac{1}{Z}\int D[\mathcal{A}\Psi\bar{\Psi}]\Psi_a\bar{\Psi}_b\exp(S_{cl}),\end{aligned}\quad (2.3.21)$$

where $Z = \int D[\mathcal{A}\Psi\bar{\Psi}]\exp(S_{cl})$. As earlier, transformation (2.3.11) leads to the following identity for the functional integral (2.3.21):

$$\begin{aligned}\frac{1}{Z}\int D[\mathcal{A}\Psi\bar{\Psi}]\exp(S_{cl})\Big\{ &-i\partial_1\Lambda_1[j_1\Psi_a\bar{\Psi}_b] \\ &+ie\Lambda_a\Psi_a\bar{\Psi}_b-ie\Psi_a\Lambda_b\bar{\Psi}_b\Big\}=0.\end{aligned}\quad (2.3.22)$$

As one may readily observe, (2.3.22) could be directly represented in terms of the vacuum averages of the quantum fields as follows:

$$\begin{aligned}i\partial_1\langle 0|Tj_1\Psi_a\bar{\Psi}_b|0\rangle &= -ie\delta(x-a)\langle 0|T\Psi_a\bar{\Psi}_b|0\rangle \\ &+ie\delta(x-b)\langle 0|T\Psi_a\bar{\Psi}_b|0\rangle \quad (\text{no integration})\end{aligned}\quad (2.3.23)$$

This is nothing else but the WTI for the 2PI two-point function.

Let us now take a closer look at the expression (2.3.23). The two-point functions on its right hand-side are the full fermion propagators. On the left side, in turn, there is a more complicated three-point structure. It can be rewritten as a product of the propagators for the entering and exiting electrons, times the amputated scattering diagram. In our case, the latter is just the 2PI vertex function Λ_{ab} , in which, in our notation, 1 stands for photon leg, and a and b stand for the oncoming and incoming fermion legs respectively.

In order to put (2.3.23) into a more familiar form, we compute its Fourier transform by integrating:

$$\int dx e^{-ik\cdot x} \int da e^{iq\cdot a} \int db e^{-ip\cdot b}.\quad (2.3.24)$$

Then the WTI for the two-point function reads:

$$S(p+k)[-iek_\mu\Lambda^\mu(p+k,p)]S(p) = e(S(p) + S(p+k)).\quad (2.3.25)$$

In order to simplify this equation, we multiply it on the left and right-hand sides by the following inverse propagators $S^{-1}(p+k)$ and $S^{-1}(p)$, respectively. This gives a familiar 1PI WTI:

$$-ik_\mu\Lambda^\mu(p+k,p) = S^{-1}(p+k) - S^{-1}(p).\quad (2.3.26)$$

2.3.4 Some qualitative considerations

Thus, the *full* 2PI effective theory turns out to be conserving, both locally and globally. Moreover, the WTI's assure that the gauge invariance of the theory is maintained at the correlator level and for the higher order vertex functions.

In order to illustrate the mechanisms of maintaining the gauge independence, let us consider the following example.

Suppose we have a full 2PI QED effective action (2.3.9). The first two Feynman diagrams from the infinite series, contributing to the functional $\Phi[S, D]$, are depicted in Fig.2.2. These are the leading and next-to-leading order terms with bare vertices and resummed propagators. Gauge invariance of the theory must be



Figure 2.2: First two contributions to the QED 2PI effective action. Thick solid lines represent full fermion propagators, thick dashed lines are the full photon propagators. All vertices are bare.

explicitly manifested by the transversality of the photon self-energy $\Pi^{\mu\nu}$. In order to obtain the latter, we have to open a photon line of all of the diagrams contributing to $\Phi[S, D]$ and then sum them up. Thus, for example, the leading and next-to-leading order contributions to the self energy could be straightforwardly inferred right from the Fig.2.2 (see Fig.2.3).



Figure 2.3: First two contributions to the photon self-energy function.

We will try to prove the gauge invariance of $\Pi^{\mu\nu}$ iteratively, order by order. To start with, we use the stationarity conditions (2.3.10) of the effective action (2.3.9) to derive the equations of motions of the full fermion and photon propagators. These equations have the form of Dyson equations and read:

$$S_{12}^{-1} = (S_{12}^0)^{-1} + i \frac{\delta \Phi[S, D]}{\delta S_{21}}, \quad (2.3.27)$$

$$D_{12}^{-1} = (D_{12}^0)^{-1} - 2i \frac{\delta \Phi[S, D]}{\delta D_{21}}. \quad (2.3.28)$$

Obviously, on the first iteration we have $S = S_0$ and $D = D_0$. Therefore, the leading order photon self-energy is nothing else but the vacuum polarization diagram of the conventional 1PI theory. It is shown in Fig.2.4, where all lines now are the usual bare propagators. Multiplying this diagram by the external momentum

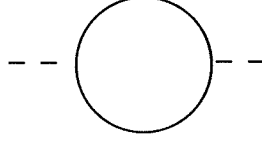


Figure 2.4: Lowest-order photon self-energy diagram. Thin solid lines are the ordinary bare fermion propagators.

vector k_μ , we get

$$k_\mu \Pi^{\mu\nu(0)}(k) = k_\mu \int dp \gamma^\mu S^0(p+k) S^0(p) \gamma^\nu. \quad (2.3.29)$$

The WTI (2.3.26) in the zeroth order of approximation is simply

$$k_\mu \gamma^\mu = (S^0)^{-1}(p+k) - (S^0)^{-1}(p). \quad (2.3.30)$$

Therefore, plugging this expression back into (2.3.29), we obtain

$$\begin{aligned} k_\mu \Pi^{\mu\nu(0)}(k) &= \int dp ((S^0)^{-1}(p+k) - (S^0)^{-1}(p)) S^0(p+k) S^0(p) \gamma^\nu \\ &= \int dp (S^0(p) - S^0(p+k)) \gamma^\nu = 0. \end{aligned} \quad (2.3.31)$$

Thus, in the lowest order of approximation the photon self-energy is transversal, as expected.

The next-to-leading order case proceeds along the same lines. First, the second iteration of equations (2.3.27) and (2.3.28) reveals, that the bare fermion propagators now obtain corresponding self-energy insertions $\Sigma^{(1)}$. Second, the two-loop contribution from $\Phi[S, D]$ comes into play. It could be regarded as the vacuum polarization diagram with the lowest-order vertex correction $\Lambda^{(1)}$. Thus, we have three diagrams combined, which are shown in Fig.2.5.

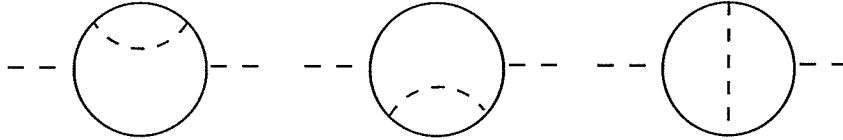


Figure 2.5: Next-to-leading order contributions to the photon self-energy.

The WTI (2.3.26) now reads:

$$k_\mu \Lambda^{(1)\mu}(p+k, k) = \Sigma^{(1)}(p) - \Sigma^{(1)}(p+k). \quad (2.3.32)$$

Multiplying each of the diagrams by k_μ and using relations (2.3.30) and (2.3.32), we get for the first of them:

$$\begin{aligned} k_\mu \Pi^{\mu\nu(1,1)}(k) &= k_\mu \int dp \gamma^\mu S^0(p) S^0(p+k) \Sigma^{(1)}(p+k) S^0(p+k) \gamma^\nu \\ &= \int dp ((S^0)^{-1}(p+k) - (S^0)^{-1}(p)) S^0(p) S^0(p+k) \Sigma^{(1)}(p+k) S^0(p+k) \gamma^\nu \\ &= \int dp S^0(p) \Sigma^{(1)}(p+k) S^0(p+k) \gamma^\nu - \int dp S^0(p+k) \Sigma^{(1)}(p+k) S^0(p+k) \gamma^\nu. \end{aligned} \quad (2.3.33)$$

Similarly, for the second

$$\begin{aligned}
k_\mu \Pi^{\mu\nu(1,2)}(k) &= k_\mu \int dp \gamma^\mu S^0(p+k) S^0(p) \Sigma^{(1)}(p) S^0(p) \gamma^\nu \quad (2.3.34) \\
&= \int dp ((S^0)^{-1}(p+k) - (S^0)^{-1}(p)) S^0(p+k) S^0(p) \Sigma^{(1)}(p) S^0(p) \gamma^\nu \\
&= \int dp S^0(p) \Sigma^{(1)}(p) S^0(p) \gamma^\nu - \int dp S^0(p+k) \Sigma^{(1)}(p) S^0(p) \gamma^\nu,
\end{aligned}$$

and for the third

$$\begin{aligned}
k_\mu \Pi^{\mu\nu(1,3)}(k) &= k_\mu \int dp \Lambda_1^\mu S^0(p+k) S^0(p) \gamma^\nu \quad (2.3.35) \\
&= \int dp (\Sigma^{(1)}(p) - \Sigma^{(1)}(p+k)) S^0(p+k) S^0(p) \gamma^\nu \\
&= \int dp S^0(k) \Sigma^{(1)}(p) S^0(p+k) \gamma^\nu - \int dp S^0(p+k) \Sigma^{(1)}(p+k) S^0(p) \gamma^\nu.
\end{aligned}$$

Summing up all three contributions, we get zero. This proves that the 2PI photon self-energy is transversal in the second loop expansion order.

It is clear that one could proceed the same way to any order one wishes.

This explicit example teaches one very important lesson. As we have just seen, the gauge invariance of the theory in the second order of approximation depends on the mutual cancellations of the diagrams of different topology. The same requirement, obviously, holds in higher orders. This does not pose any problem in the full 2PI theory, since it certainly contains all necessary diagrams by construction. Unfortunately, in truncated theory this is not already so. Let us investigate this question closely.

2.4 The modified effective action

The complete 2PI theory is well and good. It is conserving both locally and globally and produces gauge invariant results. However, when it comes to explicit calculations, one is inevitably stuck with accounting for the infinite number of 2PI Feynman diagrams, describing the interactions in the theory. This is obviously impossible; therefore, for all practical needs, one has to make certain simplifications of the underlying effective action. This is achieved by a truncation of the auxiliary functional $\Phi[S, D]$ in definition (2.3.9), while keeping the variational properties (2.3.10) untouched. Thus, one obtains a new generating functional $\Gamma_{\text{apprx}}[\psi, \bar{\psi}, A, S, D]$ and derives the equations of motion for the mean fields and propagators of the truncated theory from the following stationarity conditions:

$$\begin{aligned}
\frac{\delta \Gamma_{\text{apprx}}[\psi, \bar{\psi}, A, S, D]}{\delta A} &= 0; & \frac{\delta \Gamma_{\text{apprx}}[\psi, \bar{\psi}, A, S, D]}{\delta D} &= 0; \\
\frac{\delta \Gamma_{\text{apprx}}[\psi, \bar{\psi}, A, S, D]}{\delta \psi} &= 0; & \frac{\delta \Gamma_{\text{apprx}}[\psi, \bar{\psi}, A, S, D]}{\delta \bar{\psi}} &= 0; \\
\frac{\delta \Gamma_{\text{apprx}}[\psi, \bar{\psi}, A, S, D]}{\delta S} &= 0.
\end{aligned} \quad (2.4.1)$$

Those equations can be used to define the new self-energies in terms of the self-consistent propagators as

$$\begin{aligned} S_{12}^{-1} &= (S_{12}^0)^{-1} - \Sigma_{12}, & \Sigma_{12} &= -i \frac{\delta \Phi_{\text{apprx}}[S, D]}{\delta S_{21}}, \\ D_{12}^{-1} &= (D_{12}^0)^{-1} - \Pi_{12}, & \Pi_{12} &= 2i \frac{\delta \Phi_{\text{apprx}}[S, D]}{\delta D_{21}}. \end{aligned} \quad (2.4.2)$$

The way the functional Φ is truncated depends on the specifics of the problem. Different schemes could be employed, such as expansions in powers of the interaction constant, in loop orders or in powers of $1/N$, excluding the internal structure of the Green's functions from the counting.

The only requirement for the thus constructed $\Phi_{\text{apprx}}[S, D]$ is that it should preserve the symmetries of the classical action and be invariant under the classical background gauge field transformations. Therefore, the approximate 2PI effective action possesses the following properties of the exact formalism [59]:

- (1) The scheme is void of double counting and fulfills detailed balance relations and is thus thermodynamically consistent.
- (2) If the 2PI action is truncated in a systematic way (loop expansion, $1/N$ expansion, etc.) it fulfills the same symmetries as the classical action and is fully invariant with respect to external gauge fields;
- (3) However, it is not gauge invariant with respect to internal gauge transformations, which is explicitly manifested by the violation of the WTI's at the correlator level and for higher order vertex functions.

The latter problem is a serious issue that must be fixed.

Let us now demonstrate the mechanism of the gauge invariance breaking on a simple example of a truncated 2PI effective QED.

2.4.1 On gauge dependence of the truncated 2PI effective action

Suppose we truncate our full 2PI QED functional in the first order of the loop expansion. Thus, the only contribution which survives is given by the first diagram in Fig.2.2. Its analytical form reads:

$$\Phi_2[S, D] = \frac{1}{2} \int d^4x d^4y D_{\mu\nu}(x, x') \text{tr}\{(S(x, x')\gamma^\mu S(x', x)\gamma^\nu)\}. \quad (2.4.3)$$

As one may easily observe, the functional $\Phi_2[S, D]$ is invariant under the background field gauge transformation

$$A_\mu \rightarrow A_\mu + \partial_\mu \theta, \quad S^{-1} \rightarrow e^{-i\theta} S^{-1} e^{i\theta}, \quad (2.4.4)$$

which is assured by the cyclic property of the trace.

As earlier, we may treat the approximation order by order, by iteratively solving the equations of motion (2.4.2) and substituting the results back into the

corresponding self-energies. We find that, just like in the full theory, the first order photon self-energy is the ordinary one-loop vacuum polarization diagram with bare vertices and fermion propagators of the conventional 1PI theory (see Fig.2.4).

In the two-loop order, however, the difference with the full theory emerges. We discover that there is no way to get the third diagram of Fig.2.5, since its origin, the 2PI three-loop "mercedes" contribution (second in Fig.2.2), is truncated. Therefore, we have now only two diagrams, contributing to the photon self-energy in the next-to-leading order of approximation:

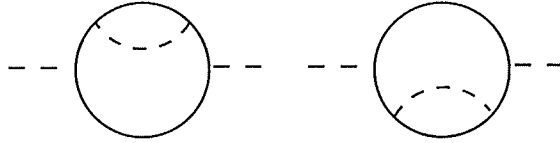


Figure 2.6: Next-to-leading order contributions to the photon self-energy in truncated theory. All propagators are bare.

The third diagram, with the cross photon propagator, which results in the vertex correction, is missing.

The same problem persists, obviously, in the higher loop expansion orders. Indeed, if we keep going with the iteration process, we will notice easily, that the vertex is never getting corrected and thus always remains bare, while the fermion propagators are getting dressed by acquiring the self-energy insertions. Therefore, the resulting WTI for our approximate theory would involve corrected propagators but bare vertices

$$k_\mu \gamma^\mu = S^{-1}(p+k) - S^{-1}(p) \quad (2.4.5)$$

and will never be satisfied, except of the lowest expansion order.

Thus, our approximate theory is *not* gauge invariant.

The problem, as we may observe, is that although the full 2PI representation is exact, any truncation scheme for $\Phi[S, D]$ in terms of skeleton diagrams, involving resummed photon and fermion propagators, leads to equations for these propagators that sum only a certain subset of higher loop diagrams with a *fixed* topology, determined by the choice of $\Phi[S, D]$, while the exact WTI requires cancelations at a given loop order between diagrams of *different* topology, which is not included in the same subset.

2.4.2 The modified effective action

The outlined pitfalls of the truncated 2PI theories look so severe, that there seems to be no way to coherently resolve them. On the other hand, such properties as resummation to all orders are too valuable to be lost. Therefore, we will take the mid-way strategy, which will allow us not only to resolve the gauge-dependence issues, but also retain the genuine properties of the full 2PI framework untouched.

The modified effective action

The idea behind our approach is simple. It is commonly known that the conventional 1PI QED is gauge invariant. So, it is worth trying to construct a special

1PI theory *on top* of the 2PI one, which, on one hand, could preserve the non-perturbative features of the latter, and would, on the other hand, be explicitly gauge invariant [58, 59, 60, 61].

The most obvious way to implement this program is the following. We introduce the new “tilde” propagators, fermion $\tilde{S}[\psi, \bar{\psi}, A]$ and photon $\tilde{D}[\psi, \bar{\psi}, A]$ ones, which are nothing else but the solutions of the familiar equations of motion

$$\left. \frac{\delta \Gamma_{\text{approx}}[\psi, \bar{\psi}, A, S, D]}{\delta S} \right|_{S=\tilde{S}[\psi, \bar{\psi}, A]} = 0; \quad \left. \frac{\delta \Gamma_{\text{approx}}[\psi, \bar{\psi}, A, S, D]}{\delta D} \right|_{D=\tilde{D}[\psi, \bar{\psi}, A]} = 0, \quad (2.4.6)$$

with $\Gamma_{\text{approx}}[\psi, \bar{\psi}, A, S, D]$ being the 2PI effective action, truncated in accord to some scheme. These equations have the form of Dyson equations:

$$\begin{aligned} \tilde{S}_{12}^{-1} &= (S_{12}^0)^{-1} - \Sigma_{12}; & \Sigma_{12} &= -i \left. \frac{\delta \Phi_{\text{approx}}[S, D]}{\delta S_{21}} \right|_{\tilde{S} \tilde{D}}; \\ \tilde{D}_{12}^{-1} &= (D_{12}^0)^{-1} - \Pi_{12}; & \Pi_{12} &= 2i \left. \frac{\delta \Phi_{\text{approx}}[S, D]}{\delta D_{21}} \right|_{\tilde{S} \tilde{D}}. \end{aligned} \quad (2.4.7)$$

The 2PI photon self-energy function Π_{12} , as we have seen above, is generally not transversal.

This stuff is still a regular 2PI theory. However, we are making another step forward and substitute the self-consistent solutions of equations (2.4.7) back into the truncated 2PI effective action. Thus, the following modified effective action emerges:

$$\tilde{\Gamma}[\psi, \bar{\psi}, A] = \Gamma[\psi, \bar{\psi}, A, \tilde{S}[\psi, \bar{\psi}, A], \tilde{D}[\psi, \bar{\psi}, A]]. \quad (2.4.8)$$

It can be shown [50] that (2.4.8) and (2.3.9) are equivalent at the exact level.

As one may observe, the action, thus constructed, is 1PI, since the propagators $\tilde{S}[\psi, \bar{\psi}, A]$ and $\tilde{D}[\psi, \bar{\psi}, A]$ are not independent entities, but functions of the mean-fields $A, \psi, \bar{\psi}$.

The many-point functions

Now we may use the action (2.4.8) as a generating functional of our new effective theory. Since it is 1PI, the many-point functions should be constructed in exactly the same way as in the regular field theory. We will call these functions *external* in order to distinguish them from the ones of the genuine 2PI theory.

We start with the propagators, which are defined as

$$(D_{12}^{\text{ext}})^{-1} = \frac{\delta^2}{\delta A_2 \delta A_1} \tilde{\Gamma}[\psi, \bar{\psi}, A]; \quad (S_{12}^{\text{ext}})^{-1} = \frac{\delta^2}{\delta \psi_2 \delta \bar{\psi}_1} \tilde{\Gamma}[\psi, \bar{\psi}, A]. \quad (2.4.9)$$

As one may readily observe, these expressions contain the implicit derivatives of the “tilde” propagators $\tilde{S}$ and $\tilde{D}$ with respect to the background fields. In order to avoid them, we first introduce the following three- and four-point functions:

$$\begin{aligned} \Lambda_{132}^0 &= -\frac{\delta (S_{12}^0)^{-1}}{\delta A_3}; & \Lambda_{132} &= -\frac{\delta \tilde{S}_{12}^{-1}}{\delta A_3}; & \Omega_{132} &= -\frac{1}{2} \frac{\delta \tilde{D}_{12}^{-1}}{\delta A_3} \\ M_{54;21}^{SS} &= -\frac{\delta^2 \Phi[\tilde{S}, \tilde{D}]}{\delta \tilde{S}_{12} \delta \tilde{S}_{45}}; & M_{54;21}^{SD} &= -2 \frac{\delta^2 \Phi[\tilde{S}, \tilde{D}]}{\delta \tilde{S}_{12} \delta \tilde{D}_{45}}; \\ M_{54;21}^{DS} &= -2 \frac{\delta^2 \Phi[\tilde{S}, \tilde{D}]}{\delta \tilde{D}_{12} \delta \tilde{S}_{45}}; & M_{54;21}^{DD} &= 4 \frac{\delta^2 \Phi[\tilde{S}, \tilde{D}]}{\delta \tilde{D}_{12} \delta \tilde{D}_{45}}. \end{aligned} \quad (2.4.10)$$

Second, we notice that some useful relations can be obtained from the following obvious identities:

$$\tilde{S}_{13}^{-1} \tilde{S}_{32} = \delta_{12}; \quad \tilde{D}_{13}^{-1} \tilde{D}_{32} = \delta_{12}. \quad (2.4.11)$$

Differentiating (2.4.11) with respect to A and using definitions (2.4.10), we obtain:

$$\frac{\delta \tilde{S}_{12}}{\delta A_3} = \tilde{S}_{11'} \Lambda_{1'32'} \tilde{S}_{2'2}; \quad \frac{\delta \tilde{D}_{12}}{\delta A_3} = 2 \tilde{D}_{11'} \Omega_{1'32'} \tilde{D}_{2'2}. \quad (2.4.12)$$

Thus, the derivatives of the “tilde” propagators could be conveniently expressed through the different types of vertex functions.

Additionally, the vertex functions themselves are subject to certain functional constraints. In order to determine them, we take derivatives of the Dyson equations (2.4.2) and obtain a set of Bethe-Salpeter type equations for the vertices. Using (2.4.10) and (2.4.12), we get:

$$\begin{aligned} \Lambda_{132} &= -\frac{\delta}{\delta A_3} ((S_{12}^0)^{-1} - \Sigma_{12}) \\ &= \Lambda_{132}^0 - i \left(\frac{\delta^2 \Phi[\tilde{S}, \tilde{D}]}{\delta \tilde{S}_{1'2'} \delta \tilde{S}_{21}} \frac{\delta \tilde{S}_{1'2'}}{\delta A_3} + \frac{\delta^2 \Phi[\tilde{S}, \tilde{D}]}{\delta \tilde{D}_{1'2'} \delta \tilde{S}_{21}} \frac{\delta \tilde{D}_{1'2'}}{\delta A_3} \right) \\ &= \Lambda_{132}^0 + i \left(M_{12;2'1'}^{SS} [\tilde{S}_{1'4} \Lambda_{435} \tilde{S}_{52'}] + M_{12;2'1'}^{SD} [\tilde{D}_{1'4} \Omega_{435} \tilde{D}_{52'}] \right) \\ \Omega_{132} &= -\frac{1}{2} \frac{\delta}{\delta A_3} ((D_{12}^0)^{-1} - \Pi_{12}) \\ &= i \left(\frac{\delta^2 \Phi[\tilde{S}, \tilde{D}]}{\delta \tilde{S}_{1'2'} \delta \tilde{D}_{21}} \frac{\delta \tilde{S}_{1'2'}}{\delta A_3} + \frac{\delta^2 \Phi[\tilde{S}, \tilde{D}]}{\delta \tilde{D}_{1'2'} \delta \tilde{D}_{21}} \frac{\delta \tilde{D}_{1'2'}}{\delta A_3} \right) \\ &= -\frac{i}{2} \left(M_{12;2'1'}^{DS} [\tilde{S}_{1'4} \Lambda_{435} \tilde{S}_{52'}] - M_{12;2'1'}^{DD} [\tilde{D}_{1'4} \Omega_{435} \tilde{D}_{52'}] \right) \end{aligned} \quad (2.4.13)$$

This system of equations is represented graphically in Fig.2.7. It incorporates the vertices (2.4.10) into a single structure, which could be easily solved iteratively when performing explicit calculations.

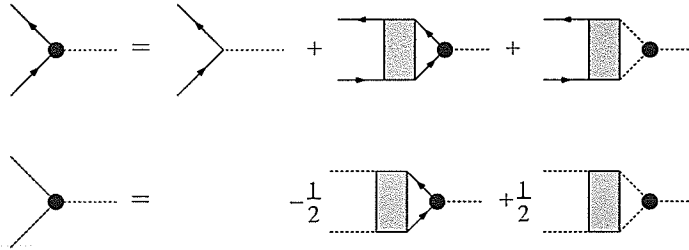


Figure 2.7: Graphical representation of Eqn. (2.4.13)

Now we are ready to write down the external propagator $(D_{12}^{\text{ext}})^{-1}$ in a closed analytic form. First we take the derivatives of the modified effective action (2.4.8)

using the chain rule. In the expression below we suppress the arguments and simply write $\Gamma[\psi, \bar{\psi}, A]$ as Γ . We obtain:

$$\begin{aligned}
(D_{12}^{\text{ext}})^{-1} = & \frac{\delta^2 \Gamma}{\delta A_2 \delta A_1} + \frac{\delta^2 \Gamma}{\delta D_{34} \delta D_{56}} \Big|_{\bar{s} \bar{D}} \frac{\delta \tilde{D}_{34}}{\delta A_2} \frac{\delta \tilde{D}_{56}}{\delta A_1} + \frac{\delta^2 \Gamma}{\delta S_{34} \delta S_{56}} \Big|_{\bar{s} \bar{D}} \frac{\delta \tilde{S}_{34}}{\delta A_2} \frac{\delta \tilde{S}_{56}}{\delta A_1} \\
& + \left(\frac{\delta^2 \Gamma}{\delta D_{34} \delta A_1} \Big|_{\bar{s} \bar{D}} \frac{\delta \tilde{D}_{34}}{\delta A_2} + \frac{\delta^2 \Gamma}{\delta S_{34} \delta A_1} \Big|_{\bar{s} \bar{D}} \frac{\delta \tilde{S}_{34}}{\delta A_2} \right. \\
& \left. + \frac{\delta^2 \Gamma}{\delta S_{34} \delta D_{56}} \Big|_{\bar{s} \bar{D}} \frac{\delta \tilde{D}_{34}}{\delta A_2} \frac{\delta \tilde{S}_{56}}{\delta A_1} + \{1 \leftrightarrow 2\} \right). \tag{2.4.14}
\end{aligned}$$

Each entry in this equation could be expressed via the many-point functions and free propagators with the help of (2.3.9), (2.3.2), (2.4.10) and (2.4.12). The result, separately for each of the terms, reads:

$$\begin{aligned}
\frac{\delta^2 \Gamma}{\delta A_2 \delta A_1} &= (D_{12}^0)^{-1} \\
\frac{\delta^2 \Gamma}{\delta D_{34} \delta D_{56}} \Big|_{\bar{s} \bar{D}} \frac{\delta \tilde{D}_{34}}{\delta A_2} \frac{\delta \tilde{D}_{56}}{\delta A_1} &= 2i\Omega_{413}[\tilde{D}_{33'}\Omega_{3'24'}\tilde{D}_{4'4}] \\
&+ M_{65;43}^{DD}[\tilde{D}_{55'}\Omega_{5'16'}\tilde{D}_{6'6}][\tilde{D}_{33'}\Omega_{3'24'}\tilde{D}_{4'4}] \\
\frac{\delta^2 \Gamma}{\delta S_{34} \delta S_{56}} \Big|_{\bar{s} \bar{D}} \frac{\delta \tilde{S}_{34}}{\delta A_2} \frac{\delta \tilde{S}_{56}}{\delta A_1} &= -i\Lambda_{413}[\tilde{S}_{33'}\Lambda_{3'24'}\tilde{S}_{4'4}] \\
&- M_{65;43}^{SS}[\tilde{S}_{55'}\Lambda_{5'16'}\tilde{S}_{6'6}][\tilde{S}_{33'}\Lambda_{3'24'}\tilde{S}_{4'4}] \\
\frac{\delta^2 \Gamma}{\delta D_{34} \delta A_1} \Big|_{\bar{s} \bar{D}} \frac{\delta \tilde{D}_{34}}{\delta A_2} + \{1 \leftrightarrow 2\} &= 0 \\
\frac{\delta^2 \Gamma}{\delta S_{34} \delta A_1} \Big|_{\bar{s} \bar{D}} \frac{\delta \tilde{S}_{34}}{\delta A_2} + \{1 \leftrightarrow 2\} &= i\Lambda_{413}^0[\tilde{S}_{33'}\Lambda_{3'24'}\tilde{S}_{4'4}] + \{1 \leftrightarrow 2\} \\
\frac{\delta^2 \Gamma}{\delta S_{34} \delta D_{56}} \Big|_{\bar{s} \bar{D}} \frac{\delta \tilde{D}_{34}}{\delta A_2} \frac{\delta \tilde{S}_{56}}{\delta A_1} + \{1 \leftrightarrow 2\} &= -M_{65;43}^{SS}[\tilde{S}_{55'}\Lambda_{5'16'}\tilde{S}_{6'6}][\tilde{D}_{33'}\Omega_{3'24'}\tilde{D}_{4'4}] \\
&+ \{1 \leftrightarrow 2\}
\end{aligned} \tag{2.4.15}$$

A great deal of this complicated set of terms is being mutually canceled out due to the Bethe-Salpeter equations derived above. Substituting (2.4.13) into (2.4.15), we finally arrive at the following compact result for the external propagator:

$$(D_{12}^{\text{ext}})^{-1} = (D_{12}^0)^{-1} + i(\Lambda_{314}^0 \tilde{S}_{44'} \Lambda_{4'23'} \tilde{S}_{3'3}). \tag{2.4.16}$$

Taking more functional derivatives of the modified action (2.4.8), one may define other external many-point functions of interest in the same way, as it was just made for the case of the external propagator.

The photon self-energy

In order to prove the gauge invariance of our theory, it is necessary to show the transversality of its photon self-energy. Unlike the 2PI approach, where this structure is determined as the corresponding derivative of the auxiliary functional $\Phi[S, D]$, in our framework it should be extracted directly from the expression for the external propagator. From (2.4.16) we get directly:

$$\Pi_{12}^{\text{ext}} = -i(\Lambda_{314}^0 \tilde{S}_{44'} \Lambda_{4'23'} \tilde{S}_{3'3}) := -i\text{Tr}[\Lambda_1^0 \tilde{S} \Lambda_2 \tilde{S}]. \tag{2.4.17}$$

$$\Pi_{12}^{\text{ext}} = -i \dots \text{(diagram of a bubble)} \dots$$
$$\partial_1(D_{12}^{\text{ext}})^{-1} = 0 \quad (2.4.18)$$

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We may proceed further and use definition (2.3.3) to get the equivalent identity for the functional W :

$$\Lambda_1 \partial_1 J_1 + ie\Lambda_1 \left(\bar{\eta}_1 \frac{\delta W}{\delta \bar{\eta}_1} + \frac{\delta W}{\delta \eta_1} \eta_1 \right) + \Lambda_1 \partial_1 C_{12} \frac{\delta W}{\delta J_2} + ieB_{12}(\Lambda_1 - \Lambda_2) \frac{\delta W}{\delta B_{12}} = 0. \quad (2.4.23)$$

The last expression could be directly represented in terms of the expectation values of the fields with the use of (2.3.4):

$$\begin{aligned} \Lambda_1 \partial_1 J_1 + ie\Lambda_1(\bar{\eta}_1 \psi_1 - \bar{\psi}_1 \eta_1) &+ \Lambda_1 \partial_1 C_{12} A_2 \\ &+ ieB_{12}(\Lambda_1 - \Lambda_2)(\psi_1 \bar{\psi}_2 + iS_{12}) = 0. \end{aligned} \quad (2.4.24)$$

Now, replacing the sources by the appropriate derivatives of the full 2PI effective action, as defined in (2.3.8), we obtain:

$$\Lambda_1 \partial_1 \frac{\delta \Gamma}{\delta A_1} - ie\Lambda_1 \left(\bar{\psi}_1 \frac{\delta \Gamma}{\delta \bar{\psi}_1} + \frac{\delta \Gamma}{\delta \psi_1} \psi_1 \right) + ie \frac{\delta \Gamma}{\delta S_{12}} (\Lambda_1 - \Lambda_2) S_{12} = 0. \quad (2.4.25)$$

Let us show that the above identity can be written as a total differential. Transformations (2.4.19) imply that

$$\begin{aligned} \Delta A_1 &= \partial_1 \Lambda_1; \quad \Delta \psi_1 = -ie\Lambda_1 \psi_1; \quad \Delta \bar{\psi}_1 = ie\Lambda_1 \bar{\psi}_1; \\ i\Delta S_{12} &= -ie(\Lambda_1 - \Lambda_2) iS_{12}; \quad i\Delta D_{12} = 0, \quad \text{no sum} \end{aligned} \quad (2.4.26)$$

where the last two equations come directly from definitions (2.3.5). Then (2.4.25) takes the following form:

$$\Delta \Gamma = \Delta A_1 \frac{\delta \Gamma}{\delta A_1} + \Delta D_{12} \frac{\delta \Gamma}{\delta D_{12}} + \Delta \bar{\psi}_1 \frac{\delta \Gamma}{\delta \bar{\psi}_1} + \Delta \psi_1 \frac{\delta \Gamma}{\delta \psi_1} + \Delta S_{12} \frac{\delta \Gamma}{\delta S_{12}} = 0. \quad (2.4.27)$$

From here one important conclusion could be drawn. If the functional derivatives of the 2PI effective action over the mean fields and propagators are evaluated at the points, corresponding to the physical solutions, the identity (2.4.27) is satisfied even in the case when the effective action itself is not exact, but truncated according to some scheme. The same conclusion holds true for our theory, with the only difference that the introduced effective action is 1PI, i.e. does not depend on two-point functions implicitly:

$$\Delta \tilde{\Gamma} = \Delta A_1 \frac{\delta \tilde{\Gamma}}{\delta A_1} + \Delta \bar{\psi}_1 \frac{\delta \tilde{\Gamma}}{\delta \bar{\psi}_1} + \Delta \psi_1 \frac{\delta \tilde{\Gamma}}{\delta \psi_1} = 0. \quad (2.4.28)$$

Thus, the functional $\tilde{\Gamma}$ is fully invariant under the local background gauge field transformations. In order to show that it also produces the gauge independent many-point functions, we transform (2.4.28) back with the use of (2.4.26) to get:

$$\partial_1 \frac{\delta \tilde{\Gamma}}{\delta A_1} - ie \left(\bar{\psi}_1 \frac{\delta \tilde{\Gamma}}{\delta \bar{\psi}_1} + \frac{\delta \tilde{\Gamma}}{\delta \psi_1} \psi_1 \right) = 0. \quad (2.4.29)$$

This relation could be employed as a starting point to derive the WTIs of interest by taking the functional derivatives with respect to the mean fields and setting

the remaining fields to zero. For example, differentiating with respect to A_2 and setting $\{A, \psi, \bar{\psi}\}$ to zero, explicitly shows the gauge invariance of the external propagator:

$$\partial_1 \frac{\delta^2 \tilde{\Gamma}}{\delta A_1 \delta A_2} = \partial_1 (D_{12}^{\text{ext}})^{-1} = 0. \quad (2.4.30)$$

This, in turn, implies that the corresponding photon self-energy Π_{12}^{ext} is transversal.

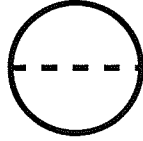
Qualitative treatment of the mechanism

Thus, we see that the functional derivatives of the truncated 2PI effective action with respect to the background fields, taken at the stationary point, define non-perturbative approximations to the self-energies and proper vertex functions which fulfill the usual WTIs. The basic mechanism, that made our approach successful, is simple. The Dyson equations (2.4.7) contain the s -channel ladder resummations and the Bethe-Salpeter equations (2.4.13) introduce t - and u -channels, and thus restore the crossing symmetry.

Let us now put it all together and show explicitly how the scheme works on the example of the lowest order modified effective action. It is given by

$$\begin{aligned} \Gamma[\psi, \bar{\psi}, A] = & S_{cl}[\psi, \bar{\psi}, A] + \frac{i}{2} \text{Tr} \text{Ln} \tilde{D}_{12}^{-1} + \frac{i}{2} \text{Tr} \left[(D_{12}^0)^{-1} (\tilde{D}_{21} - D_{21}^0) \right] - \\ & i \text{Tr} \text{Ln} \tilde{S}_{12}^{-1} - i \text{Tr} \left[(S_{12}^0)^{-1} (\tilde{S}_{21} - S_{21}^0) \right] + \Phi_{\text{approx}}[\tilde{S}, \tilde{D}], \end{aligned} \quad (2.4.31)$$

where $\Phi_{\text{approx}}[\tilde{S}, \tilde{D}]$ is the two-loop diagram with bare vertices and thick solid and



dashed lines corresponding to the fermion and photon propagators $\tilde{S}$ and $\tilde{D}$. The latter are the self-consistent solutions of the following Dyson equations:

$$\begin{aligned} \tilde{S}_{12}^{-1} &= (S_{12}^0)^{-1} + i \frac{\delta \Phi_{\text{approx}}[S, D]}{\delta S_{21}} \Big|_{\tilde{S}, \tilde{D}}; \\ \tilde{D}_{12}^{-1} &= (D_{12}^0)^{-1} - 2i \frac{\delta \Phi_{\text{approx}}[S, D]}{\delta D_{21}} \Big|_{\tilde{S}, \tilde{D}}. \end{aligned} \quad (2.4.32)$$

As we have seen earlier, the photon self-energy Π^{ext} in our construction is the bubble diagram with a resummed vertex and $\tilde{S}$ internal propagators (Fig.2.9). There are three types of vertices, a resummed three-photon one and the fermion-phonon ones, bare and dressed, respectively, subject to the system of Bethe-Salpeter equations, depicted in Fig.2.10.

Our goal is to prove the transversality of the self-energy Π^{ext} .

As usual, we will demonstrate this fact by the use of the following iterative process:

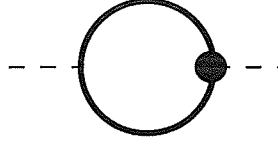


Figure 2.9: Photon self-energy Π^{ext} .

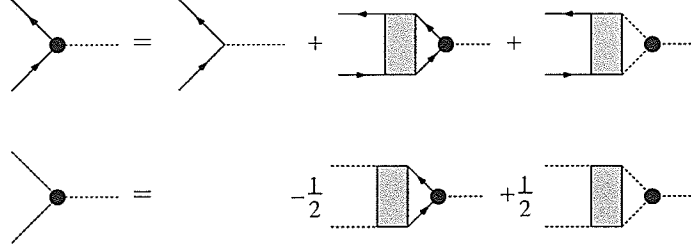
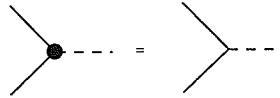


Figure 2.10: System of Bethe-Salpeter equations. Shaded boxes are the four-point vertex functions, defined in eq.(2.4.10).

1. solve the Dyson equations to find $\tilde{S}$ and $\tilde{D}$ in a given order of the loop expansion;
2. solve the Bethe-Salpeter equation to find the vertices in the same order of approximation;
3. substitute these back into the expression for Π^{ext} to make sure that the necessary minimal subset of diagrams is present.

Implementing this program, we find that in the lowest expansion order propagators $\tilde{S} = S^0$, $\tilde{D} = D^0$, as well as the vertices,



are undressed. Substituting these back into the self-energy expression, we find that the latter is nothing else but the familiar 1PI vacuum polarization diagram, which is obviously gauge invariant.

In the two-loop order, however, *both* propagators *and* vertices acquire corrections (Fig.2.11).

Compared to the truncated 2PI case, the vertex correction contributes the missing diagram to the expression for the self-energy, thus restoring its transversality (see Fig.2.12).

One may proceed the same way into the higher orders of approximation to make sure that the approach presented is free from gauge-dependence issues.

Selective resummations

One interesting thing about the approach developed is worth noting.

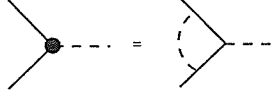


Figure 2.11: Vertex correction on the second iteration.

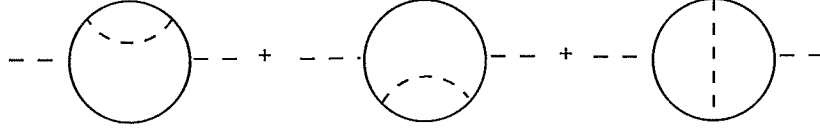


Figure 2.12: Vertex correction on the second iteration restores the gauge invariance.

As one may observe, the fact that the auxiliary functional $\Phi[S, D]$ is truncated to the leading order term, prevents us from obtaining the fermion self energies of the “cross” topology in the second order of approximation (see Fig.2.13). Despite



Figure 2.13: Topology missing in the lowest order truncated QED.

that, our theory remains perfectly gauge invariant, since the vertices with corresponding topologies (see Fig.2.14) are also not produced. This makes the approach very suitable for studying the problems where the selective resummations of special subsets of diagrams in all orders of approximation are required.

2.5 QED electrical conductivity using the 2PI effective action

Having discussed general properties of the modified 2PI effective action, we may apply it to a particular problem of interest. A good exercise is to calculate the QED electrical conductivity [60, 61].

The calculation will provide a field theoretic connection to the kinetic theory results of [62], which is useful in itself. In addition, it will show that it seems likely that quantum field theory provides a better framework than kinetic theory for calculations beyond leading order. The results will provide strong support for the use of n PI effective theories as a method to study the equilibration of quantum fields.

2.5.1 Keldysh representation of real time finite temperature field theory

We use the closed time path formulation of real time statistical field theory which consists of a contour with two branches: one runs from minus infinity to infinity



Figure 2.14: Vertex topologies missing in the lowest order truncated QED.

along the real axis, the other runs back from infinity to minus infinity just below the real axis. The closed time path contour results in a doubling of degrees of freedom. Physically, these extra contributions come from the additional processes that are present when the system interacts with a medium instead of sitting in a vacuum. As a result of these extra degrees of freedom, n -point functions have a tensor structure. Statistical field theory can be formulated in different bases, which produce different representations of these tensors. We will work in the Keldysh basis. Keldysh indices will be written c_i and are assigned the values $c_i = 1 := r$ and $c_i = 1 := a$.

For the 2-point green's functions and vertex functions in momentum space we use the notation

$$\begin{aligned} G_{ra}(P) &= G_{ret}(P); & G_{ar}(P) &= G_{adv}(P); \\ G_{rr}(P) &= G_{sym}(P) = N(P)(G_{ret}(P) - G_{adv}(P)); \\ \Pi_{ra}(P) &= \Pi_{ret}(P); & \Pi_{ar}(P) &= \Pi_{adv}(P); \\ \Pi_{rr}(P) &= \Pi_{sym}(P) = N(P)(\Pi_{ret}(P) - \Pi_{adv}(P)), \end{aligned} \quad (2.5.1)$$

where $N(P) = 1 - 2n(p_0)$ and $n(p_0) = 1/(e^{\beta p_0} - 1)$. The expression relating the symmetric function to the retarded and advanced functions is the KMS condition (see Appendix A).

Vertex functions are obtained from the n -point functions by truncating external legs:

$$G_{c_1 \dots c_n} = G_{c_1 \bar{c}_1} \dots G_{c_n \bar{c}_n} \Gamma^{\bar{c}_1 \dots \bar{c}_n}. \quad (2.5.2)$$

In order to simplify the notation for the vertices, we replace each combination of the indices $\{r, a\}$ by a single numerical index. In momentum space we write:

$$\Gamma^{\bar{c}_1 \dots \bar{c}_n}(p_1, \dots, p_n) = \Gamma(i, p_1, \dots, p_n). \quad (2.5.3)$$

We assign the choices of the variables $c_1, \dots, c_n$ to the variable i using the vector

$$V_n = \begin{pmatrix} r_n \\ a_n \end{pmatrix} \dots \otimes \begin{pmatrix} r_2 \\ a_2 \end{pmatrix} \otimes \begin{pmatrix} r_1 \\ a_1 \end{pmatrix}, \quad (2.5.4)$$

where the symbol $\otimes$ indicates the outer product. For each n , the i th component of the vector corresponds to a list of variables that is assigned the number i . To simplify the notation we drop the subscripts and write a list like $r_1 r_2 a_3$ as rra . For clarity, the results are listed below.

3-point functions: $rrr \rightarrow 1$, $arr \rightarrow 2$, $rar \rightarrow 3$, $aar \rightarrow 4$, $rra \rightarrow 5$, $ara \rightarrow 6$, $raa \rightarrow 7$, $aaa \rightarrow 1$.

4-point functions: $rrrr \rightarrow 1$, $arrr \rightarrow 2$, $rarr \rightarrow 3$, $aarr \rightarrow 4$, $rrar \rightarrow 5$, $arar \rightarrow 6$, $raar \rightarrow 7$, $aaar \rightarrow 8$, $rrra \rightarrow 9$, $arra \rightarrow 10$, $rara \rightarrow 11$, $aaaa \rightarrow 12$, $rraa \rightarrow 13$, $araa \rightarrow 14$, $raaa \rightarrow 15$, $aaaa \rightarrow 16$.

2.5.2 Propagators and vertices

We will need the fermion propagator, the photon propagator, the (two fermion-photon) 3-point vertex, the three photon 3-point vertex, and three different kinds of 4-point functions which couple four fermions, two fermions and two photons, and four photons. Of course, the three photon vertex and all 4-point vertices are zero at the tree level. We will work in the high temperature limit where the masses can be set to zero.

The concept of “pinch singularities” plays an important role in the calculation of transport coefficients. The basic idea is that there is an infinite number of terms that all contribute at the same order because of the low frequency limit in the Kubo formula (2.5.27). This limit produces pairs of retarded and advanced propagators which carry the same momenta. When integrating a term of the form $\int p_0 G^{ret}(P) G^{adv}(P)$, the integration contour is “pinched” between poles on each side of the real axis, and the integral contains a divergence known as a “pinch singularity”. These divergences are regulated by using resummed propagators which account for the finite width of thermal excitations. This procedure introduces extra factors of the coupling in the denominators which change the power counting. As a consequence, there is an infinite set of graphs which contain products of pinching pairs that all need to be resummed.

Propagators

In coordinate space the propagators are written:

$$S_{\alpha\beta}^{ab}(x_1, x_2); \quad D_{\mu\nu}^{ab}(x_1, x_2). \quad (2.5.5)$$

In momentum space we will use the same expressions (to simplify the notation we do not introduce tilde’s) with the coordinate variables $\{x_1, \dots, x_n\}$ replaced by the momentum variables $\{p_1, \dots, p_n\}$. Momenta are always taken to be incoming. Note that there is an overall delta function in momentum space so that, for example, the fermion propagator can be written:

$$S_{\alpha\beta}^{ab}(p_2) \equiv S_{\alpha\beta}^{ab}(-p_2, p_2). \quad (2.5.6)$$

For the fermion propagator we use the notation:

$$\begin{aligned} S^{-1}(P) - \gamma_\mu P^\mu - \Sigma(P); \quad \Sigma(P) &= \gamma_0 \Sigma_0(P) + \hat{p}^i \gamma^i \Sigma_s(P) \\ S(P) &= \frac{\gamma_\mu P^\mu - \Sigma(P)}{P^2 - \frac{1}{2} \hat{\Sigma}(P)}; \quad \hat{\Sigma}(P) \equiv \text{Tr}(\gamma_\mu P^\mu \Sigma(P)). \end{aligned} \quad (2.5.7)$$

We set Σ to zero except where it is needed to regulate a pinch singularity. We write:

$$S_{ret}(P) = \gamma_\mu P^\mu G_{ret}(P) \equiv \frac{\gamma_\mu P^\mu}{P^2 + i \text{Sign}(p_0)\epsilon - \frac{1}{2}\hat{\Sigma}_{ret}(P)}, \quad (2.5.8)$$

$$S_{adv}(P) = \gamma_\mu P^\mu G_{adv}(P) \equiv \frac{\gamma_\mu P^\mu}{P^2 - i \text{Sign}(p_0)\epsilon - \frac{1}{2}\hat{\Sigma}_{adv}(P)},$$

$$G_{ret}(P)G_{adv}(P) = -\frac{\rho(P)}{\text{Im}\hat{\Sigma}(P)}, \quad (2.5.9)$$

where we have defined

$$\rho(P) \equiv i d(P) \equiv i(G_{ret}(P) - G_{adv}(P)) \equiv \text{Sign}(p_0)\Delta(P). \quad (2.5.10)$$

There are no pinch terms involving photon propagators and therefore we can write the photon propagator (in the Feynman gauge) as:

$$D_{\mu\nu}^{ret}(P) = -g_{\mu\nu}G_{ret}(P) \equiv -\frac{g_{\mu\nu}}{p^2 + i \text{Sign}(p_0)\epsilon}, \quad (2.5.11)$$

$$D_{\mu\nu}^{adv}(P) = -g_{\mu\nu}G_{adv}(P) \equiv -\frac{g_{\mu\nu}}{p^2 - i \text{Sign}(p_0)\epsilon}.$$

We write cut fermion lines and cut photon lines as follows:

$$\begin{aligned} S_{\alpha\beta}^d &= S_{\alpha\beta}^{ret}(P) - S_{\alpha\beta}^{adv}(P) = \gamma_\mu P^\mu; \\ \gamma_\mu P^\mu &= \theta(p_0)u(P)\bar{u}(P) - \theta(-p_0)v(P)\bar{v}(P); \\ D_{\mu\nu}^d &= D_{\mu\nu}^{ret}(P) - D_{\mu\nu}^{adv}(P) = g_{\mu\nu}d(P); \\ g_{\mu\nu} &= (-1)\epsilon_\mu^\nu(P)\epsilon_\nu^{\star\lambda}(P). \end{aligned} \quad (2.5.12)$$

For the future use we also define the principle parts:

$$\begin{aligned} \text{Prin}(P) &= \frac{1}{2}(G_{ret}(P) + G_{adv}(P)), \\ S_{\alpha\beta}^{prin}(P) &= \frac{1}{2}(S_{\alpha\beta}^{ret}(P) + S_{\alpha\beta}^{adv}(P)) = \gamma_\mu P^\mu \text{Prin}(P), \\ D_{\mu\nu}^{prin}(P) &= \frac{1}{2}(D_{\mu\nu}^{ret}(P) + D_{\mu\nu}^{adv}(P)) = -g_{\mu\nu} \text{Prin}(P). \end{aligned} \quad (2.5.13)$$

Note that to simplify the notation we use the same expressions $G_{ret}(P)$, $G_{adv}(P)$, $d(P)$ and $\text{Prin}(P)$ in (2.5.8), (2.5.11), (2.5.12) and (2.5.13) for fermion and photon propagators. In any equation it will be clear if a given function refers to a photon or fermion propagator, depending on whether the momentum variable corresponds to a fermion or a photon line.

Vertices

In coordinate space the vertices are written:

$$\Lambda_{\alpha\mu\beta}^{acb}(x_1, x_2, x_3); \quad \Omega_{\mu\nu\tau}^{acb}(x_1, x_2, x_3); \quad (2.5.14)$$

$$\begin{aligned} (M^{SS})_{\alpha\beta;\gamma\delta}^{ab;cd}(x_1, x_2; x_3, x_4); \quad (M^{SD})_{\alpha\beta;\mu\nu}^{ab;cd}(x_1, x_2; x_3, x_4); \\ (M^{DD})_{\mu\nu;\lambda\tau}^{ab;cd}(x_1, x_2; x_3, x_4); \end{aligned} \quad (2.5.15)$$

The two terms in the first line indicate that the two fermion - photon 3-point vertex and the three photon 3-point vertex, respectively. The three terms in the second line are the four fermion 4-point vertex, the two-fermion - two-photon 4-point vertex, and the four photon 4-point vertex. The variables on each side of the semicolon indicate the legs that will join with a pinching pair of propagators. The pinch terms involve two kinds of vertices: 3-point functions in which the momentum on one leg (which we take to be the middle leg) goes to zero, and 4-point functions which connect to two pairs of propagators with the same momenta. We write these vertices:

$$\begin{aligned}\Lambda_{\alpha\mu\beta}(j, P) &\equiv \lim_{Q \rightarrow 0} \Lambda_{\alpha\mu\beta}(j, -P - Q, Q, P) = \Lambda_{\alpha\mu\beta}(j, -P, 0, P), \quad (2.5.16) \\ (M^{SS})_{\alpha\beta;\gamma\delta}(j, P, K) &\equiv \lim_{Q \rightarrow 0} (M^{SS})_{\alpha\beta;\gamma\delta}(j, -P, P + Q, -K - Q, K) \\ &= (M^{SS})_{\alpha\beta;\gamma\delta}(j, -P, P, -K, K)\end{aligned}$$

with similar expressions for the vertices Ω , M^{SD} and M^{DD} . In these expressions the index j refers to the Keldysh component of the vertex, as defined earlier.

In the pinch limit, the spatial part (using $\mu = (0, z)$) of the 2 fermion - photon vertex can be decomposed as:

$$\Lambda^z(j, P) = (A(j)\gamma_0 p_0 + B(j)\gamma^i p^i)\hat{p}^z + E(j)\gamma^z. \quad (2.5.17)$$

It is easy to show that:

$$\begin{aligned}\gamma_\mu K^\mu \Lambda^z(j, K) \gamma_\nu K^\nu &= \frac{1}{2} \gamma_\mu K^\mu \hat{\Lambda}^z(j, K) - K^2 \Lambda^z(j, K); \quad (2.5.18) \\ \hat{\Lambda}^z(j, K) &\equiv \text{Tr}(\gamma_\mu K^\mu \Lambda^z(j, K)).\end{aligned}$$

For the conductivity we will need only the quantity $\hat{\Lambda}^z(j, K)$. In addition, we will show that we only need the trace of a pinched 4-point vertex:

$$\hat{M}(P, K) \equiv \text{Tr}(\gamma_\mu P^\mu [-i\mathbf{M}(P, K)] \gamma_\nu P^\nu), \quad (2.5.19)$$

where the quantity $\mathbf{M}(P, K)$ is a particular combination of Keldysh components and is defined below.

Bethe-Salpeter equation

We obtain a Bethe-Salpeter type integral equation for the two-fermion - photon 3-point vertex by substituting the second equation in (2.4.13) into the first and iterating. We show the result in Fig.2.15. The corresponding equation can be written:

$$\Lambda_{132} = \Lambda_{132}^0 + i\mathcal{M}_{12;45}^{SS} \tilde{S}_{55'} \Lambda_{5'34'} \tilde{S}_{4'4}, \quad (2.5.20)$$

where we have defined the composite vertex:

$$\mathcal{M}_{12;45}^{SS} = M_{12;45}^{SS} - \frac{i}{2} M_{12;2'1'}^{SD} \tilde{D}_{1'6} \tilde{D}_{72'} M_{67;45}^{DS}. \quad (2.5.21)$$

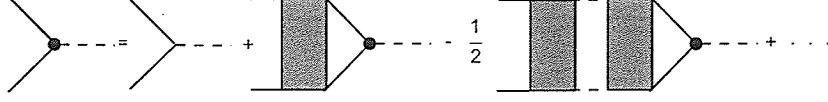


Figure 2.15: Graphical representation of eqn. (2.5.21).

To reduce the number of indices, we introduce a type of matrix notation. The indices that correspond to legs that are joined in a closed loop are summed over, and are not written explicitly. Using this notation, eqn. (2.5.21) is written:

$$\mathcal{M}_{12;45}^{SS} = M_{12;45}^{SS} - \frac{i}{2} \left(M^{SD} \tilde{D} \tilde{D} M^{DS} \right)_{12;45} \quad (2.5.22)$$

and eqn. (2.5.20):

$$\Lambda_{132} = \Lambda_{132}^0 + i \left(\mathcal{M}^{SS} \tilde{S} \tilde{S} \Lambda \right)_{132}. \quad (2.5.23)$$

Equation (2.5.23) is illustrated in Fig.2.16. The dark box indicated the composite vertex $\mathcal{M}$ defined in (2.5.22). For clarity, the indices that are not summed over are shown explicitly on the diagram. We note that this notation does not really

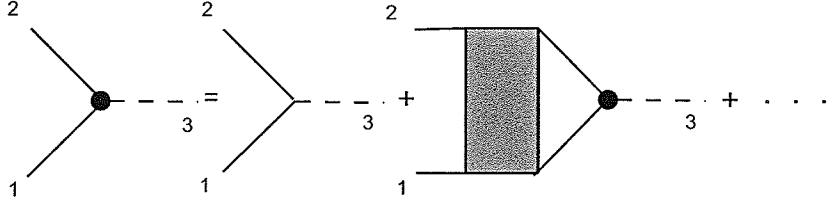


Figure 2.16: Graphical representation of eqn. (2.5.23).

represent matrix multiplication because of the fact that the indices which are summed over cannot always be written next to each other. However, the meaning of the notation is immediately clear from the corresponding diagram.

The vertex $\mathcal{M}$ is obtained from (2.4.10) and (2.5.22). In order to include all contributions that correspond to binary scattering and production process within the 2PI formalism, we need to work to 3-loop order in the Φ functional. The two diagrams we need are shown in Fig.2.17. The first graph in Fig.2.17 produces the leading order contributions to the vertices and the second graph gives next-to-leading order terms. There are no next-to-leading order contributions to the vertices M^{SD} and M^{DS} . We write

$$M^{SS} = M_{lo}^{SS} + M_{nlo}^{SS}; \quad M^{SD} = M_{lo}^{SD} \quad M^{DS} = M_{lo}^{DS}. \quad (2.5.24)$$

The results are shown in Fig.2.18. Substituting (2.5.22) and (2.5.24) into (2.5.23)

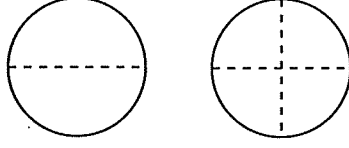


Figure 2.17: 2PI contributions to the Φ functional.

$$\begin{aligned}
 -i M^{ss} &= \text{[Diagram 1]} + \text{[Diagram 2]} + \text{[Diagram 3]} + \text{[Diagram 4]} \\
 -i M^{sd} &= \text{[Diagram 5]} + \text{[Diagram 6]}
 \end{aligned}$$

Figure 2.18: Contributions to the 4-point functions.

we iterate and keep terms that correspond to binary scattering and production processes. We obtain:

$$\begin{aligned}
 \Lambda_{132} &= \Lambda_{132}^0 \\
 &+ \left(\underbrace{iM_{lo}^{ss}}_a + \underbrace{iM_{nlo}^{ss}}_{\{c,d,e\}} - \underbrace{M_{lo}^{ss} \tilde{S} \tilde{S} M_{lo}^{ss}}_b + \frac{1}{2} \underbrace{M_{lo}^{sd} \tilde{D} \tilde{D} M_{lo}^{ds}}_{\{f,g\}} \right)_{12;45} \tilde{S}_{55'} \tilde{S}_{4'4} \Lambda_{5'3'4'}.
 \end{aligned} \tag{2.5.25}$$

Equation (2.5.25) is shown in Fig.2.19. We write the final result:

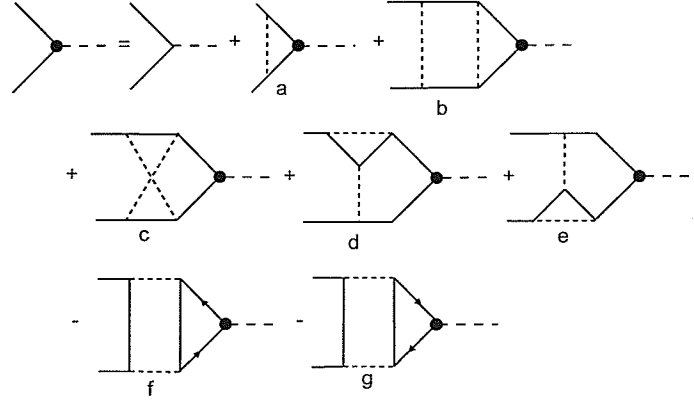


Figure 2.19: Binary contributions to the Bethe-Salpeter equation.

$$\Lambda_{132} = \Lambda_{132}^0 + \sum_{j=\{a,b,c,d,e,f,g\}} iM_{12;45}^{(j)} \tilde{S}_{55'} \tilde{S}_{4'4} \Lambda_{5'3'4'}, \tag{2.5.26}$$

where the superscript $j = \{a, b, c, d, e, f, g\}$ indicates the 4-point function shown in part (j) in Fig.2.19.

Kubo formula

We introduce several notational changes in this section. Keldysh components and momentum variables are written explicitly, and traces are over dirac indices only. All tilde's on propagators are suppressed. We also introduce a slightly different notation for the vertices. No factors of the coupling have been extracted from the vertices as defined in (2.4.10). For example, using (2.3.2) and (2.4.10) gives Λ_μ^0 and Λ_μ to obtain expressions with conventional form. To simplify the notation, we do not introduce additional primes on the new vertices.

The electrical conductivity can be obtained from the Kubo formula:

$$\sigma = \frac{1}{6} \left(\frac{\partial}{\partial q_0} 2\text{Im}\rho^{ii}(q_0, 0) \right) \Big|_{q_0 \rightarrow 0}, \quad (2.5.27)$$

$$\rho^{ii}(x, y) = \langle j^i(x) j^i(y) \rangle; \quad j^i(x) = \bar{\psi}(x) \gamma^i \psi(x). \quad (2.5.28)$$

We can write the conductivity in terms of the polarization tensor using:

$$\rho^{ii}(q_0, 0) = -\frac{1}{e^2} \Pi_{ret}^{ii}(q_0, 0). \quad (2.5.29)$$

The polarization tensor is given in (2.4.17). Summing over Keldysh indices we obtain:

$$\begin{aligned} \Pi_{\mu\nu}^{ret}(Q) &= \frac{i}{2} e^2 \int dP \text{Tr}(\Lambda_\mu^0 [S^{sym}(P) \Lambda_\nu(5, -P, -Q, P+Q) S^{ret}(P+Q) \\ &+ S^{adv}(P) \Lambda_\nu(2, -P, Q, Q+P) S^{sym}(P+Q) \\ &+ S^{adv}(P) \Lambda_\nu(6, -P, Q, Q+P) S^{ret}(P+Q)]). \end{aligned} \quad (2.5.30)$$

Note that the surviving indices on the 3-point functions correspond to the middle legs of the 3-point vertices. Eqn. (2.5.30) can be rewritten using the KMS condition. The KMS condition for the 2-point function is given in (2.5.1). Similar KMS conditions exist for the 3-point functions. A complete list is given in [63]. The expression we need in this case is:

$$\begin{aligned} \Gamma(6, P_1, P_2, P_3) &= N_F(p_3^0) (\Gamma^*(3, P_1, P_2, P_3) - \Gamma(2, P_1, P_2, P_3)) \\ &+ N_F(p_1^0) (\Gamma^*(3, P_1, P_2, P_3) - \Gamma(5, P_1, P_2, P_3)). \end{aligned} \quad (2.5.31)$$

Substituting (2.5.1) and (2.5.31) into (2.5.30) and only including terms which contain pinch singularities gives:

$$\begin{aligned} \Pi_{\mu\nu}^{ret}(Q) &= -\frac{i}{2} e^2 \int dP (N_F(p_0) - N_F(p_0 + q_0)) \\ &\text{Tr}(\Lambda_\mu^0 S^{adv}(P) \Lambda_\nu^*(3, -P, -Q, P+Q) S^{ret}(P+Q)). \end{aligned} \quad (2.5.32)$$

Substituting (2.5.32) into (2.5.27) we obtain:

$$\sigma = \frac{1}{3} \beta \int dP (1 - n_f(p_0)) n_f(p_0) \text{Tr}(\Lambda_0^i S^{ret}(P) \text{Re}\lambda^i(3, P) S^{adv}(P)). \quad (2.5.33)$$

As explained earlier, the index "3" indicated the Keldysh component that is retarded with respect to the middle leg. We substitute (2.5.8) and (2.5.18) into (2.5.33) and obtain:

$$\sigma = \frac{4}{3} \beta \int dP (1 - n_f(p_0)) n_f(p_0) \rho(P) p^i B^i(P); \quad B^i(P) \equiv \frac{\text{Re}\hat{\Lambda}^i(3, P)}{2\text{Im}\hat{\Sigma}(P)}. \quad (2.5.34)$$

From (2.5.34) we only need to calculate the third Keldysh component of the 3-point vertex in (2.5.26). We do the sums over Keldysh indices and only include terms which contain pinch singularities. Eqn. (2.5.26) becomes:

$$\Lambda_{\alpha\mu\beta}(3, P) = \Lambda_{\alpha\mu\beta}^0(3, P) + \sum_{j=\{a,b,c,d,e,f,g\}} \frac{i}{2} \int dK M_{\alpha\beta;\gamma\delta}^{(j)}(P, K) S_{\delta\delta'}^{ret}(K) \Lambda_{\delta'\mu\gamma'}(3, K) S_{\gamma'\gamma}^{adv}(K), \quad (2.5.35)$$

where the 4-point function that appears in this equation is a combination of Keldysh components and thermal functions:

$$\mathbf{M}^{(j)}(P, K) = M^{(j)}(13, P, K) + N_F(K) (M^{(j)}(5, P, K) - M^{(j)}(9, P, K)).$$

The superscript $j = \{a, b, c, d, e, f, g\}$ indicated the 4-point function shown in part (j) of Fig.2.19. From (2.5.34) we need to find an integral equation for $\hat{\Lambda}^i(P) = \text{Tr}(\gamma_\mu P^\mu \Lambda^i(P))$. We multiple both sides of (2.5.35) by $\gamma_\mu P^\mu$ and take the trace. Using (2.5.8), (2.5.18) and (2.5.19) we obtain:

$$\hat{\Lambda}^i(3, P) = \hat{\Lambda}_0^i(3, P) + \sum_{j=\{a,b,c,d,e,f,g\}} \frac{i}{2} \int dK \hat{M}^{(j)}(P, K) \rho(K) B^i(P). \quad (2.5.36)$$

Taking the real part of both sides and using the definition of $B^i(P)$ in (2.5.34) we obtain:

$$2\text{Im}\hat{\Sigma}(P) \cdot B^i(P) = \text{Re}\hat{\Lambda}_0^i(3, P) + \sum_{j=\{a,b,c,d,e,f,g\}} \frac{i}{2} \int dK \text{Re}[\hat{M}^{(j)}(P, K)] \rho(K) B^i(K). \quad (2.5.37)$$

Further progress requires technically tedious exploration of each of the factors contributing to $\text{Re}[\hat{M}^{(j)}(P, K)]$ and $\text{Im}\hat{\Sigma}(P)$. It was shown (see [60]), that the complete set of diagrams produces all of the amplitudes that correspond to binary scattering and production processes. As a result, eqn. (2.5.37) takes the form:

$$\begin{aligned} -(1 - n_f(p^0)) \cdot \text{Re}\hat{\Lambda}_0^i(3, P) &= \frac{1}{2} \int dP_2 \int dL_1 \int dL_2 |M|^2 \delta_{P+P_2-L_1-L_2} \\ &\quad \Delta(P_2) \Delta(L_1) \Delta(L_2) [B^i(P) + B^i(P_2) - B^i(L_1) - B^i(L_2)], \end{aligned} \quad (2.5.38)$$

where $|M|^2$ corresponds to the sum of the squared amplitudes of the leading-order binary QED processes in a grand canonical ensemble. This equation is exactly the same as that obtained in [62] using kinetic theory.

However, the result obtained is not complete at the leading order. In gauge theories in addition to pinch singularities, the presence of collinear singularities makes the $1 \rightarrow 2$ scatterings as important as the $2 \rightarrow 2$ scatterings. These collinear terms must also be resummed by solving an integral equation. The complete leading order result then obtained by solving these two coupled integral equations. As it was shown in [61], both of these integral equations can be derived directly from the 3-loop resummed 3PI effective action. Thus it was shown that the full leading order contribution to the QED electrical conductivity can be obtained directly from the 3PI formalism.

2.6 Conclusion

Thus, we have performed a major cleanup in n PI effective action approach, which enables us to safely apply it to a variety of problems in particle physics without being worried about the gauge-dependence issues. Introduction of the modified effective theory defined on the physical propagators of the original functional solved the problem. Same strategy has already proved to be fruitful in non-gauge $O(N)$ scalar ϕ^4 theory, where the failure of Goldstone's theorem for the internal propagators was successfully cured with its help [59]. Looks like any other choice of the resummed propagators than those which satisfy the equations of motion will lead to a failure. Probably, that was the reason why previous attempts (see, for example, [56]) did not give a complete resolution of the problem.

The approach developed has already proved its usefulness in electrical conductivity calculations of QED plasma by providing a convenient framework to treat the kinetic theory tasks [60, 61]. Current and upcoming heavy ion collision experiments are an important motivation to extend the consideration to non-equilibrium domain. In contrast to a thermally equilibrated state, which keeps no information about the details of the initial conditions, non-equilibrium phenomena may help to understand in particular the earlier stages of a collision.

A successful description of the dynamics of quantum fields away from equilibrium is tightly related to the basic problem of how macroscopic “dissipative” behavior arises from time-reversal invariant quantum dynamics. This is a fundamental question with most diverse applications. The technique developed may become useful to understand the physics of heavy ion collision experiments, will be of relevance to the inflationary dynamics in the early universe or even to non-equilibrium aspects of mesoscopic quantum devices.

Appendix A

A.1 Real-time finite temperature field theory. Path integral formulation

In the first part of this work we have used the TFD framework to calculate the interaction correction to the thermodynamic properties of a Bose gas. This approach is an extension of the conventional operator formalism and allows, as we have seen, to consistently calculate all physical parameters of interest. However, methods, based on the secondary quantization formulation of the quantum field theory, are slowly losing ground in favor of the much more versatile path integral techniques.

Therefore, we find it reasonable to demonstrate, how results obtained within the operator approach, could have been equally derived with the use of functional methods. In other words, we will give the path-integral representation of the TFD formalism.

A.1.1 Generating functional

In order to be specific, let us suppose that we are considering a local quantum field theory that describes particles with momenta much lower than the inverse of the range of the interatomic potential. The many-body quantum mechanics for the atoms, described by a single complex field $\phi(x)$, can therefore be formulated in terms of a quantum field theory whose Hamiltonian density is a local function of the field:

$$H = \frac{\hbar^2}{2m} \nabla \phi(t, \vec{x})^\dagger \cdot \nabla \phi(t, \vec{x}) + V(\phi). \quad (\text{A.1.1})$$

where $V(\phi)$ is the interacting part.

Then the thermal Green's functions $G_\beta(x_1, \dots, x_n)$ are defined by the Gibbs ensemble averages of the products of fields $\phi(x)$:

$$G_\beta(x_1, \dots, x_n) = \frac{1}{\text{Tr} \exp(-\beta H)} \text{Tr} (\exp(-\beta H) P[\phi(x_1), \dots, \phi(x_n)]), \quad (\text{A.1.2})$$

where P represents ordering along a time path, shown in Fig.A.1, and where β is an inverse temperature.

Invariance of the thermal trace of a product of operators under cyclic permutations imposes restrictions on a possible form of many-point functions. In the

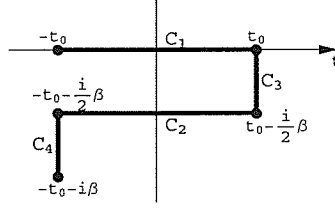


Figure A.1: The contour $C = C_1 + C_2 + C_3 + C_4$ used in defining the generating functional for the real-time finite-temperature Green's functions. The horizontal legs are presumed to have an infinitesimal downward slope.

case of one- and two-point functions these are periodicity and the Kubo-Martin-Schwinger (KMS) conditions [64]

$$\phi(t, \vec{x}) = \phi(t - i\beta, \vec{x}) \quad (\text{A.1.3})$$

$$G_\beta^>(t - t' - i\beta, \vec{x} - \vec{x}') = G_\beta^<(t - t', \vec{x} - \vec{x}') \quad (\text{A.1.4})$$

Then the generating functional for the thermal Green's functions has the following path-integral representation [65, 66]:

$$Z_\beta[J] = \int D_c[\phi] \exp \left(i \int_C d\tau \int d^3x [L(\phi) + J(\tau, \vec{x})\phi(\tau, \vec{x})] \right), \quad (\text{A.1.5})$$

where $J(\tau, \vec{x})$ is the classical source and $L(\phi)$ is the conventional contour Lagrangian

$$L(\phi) = \frac{1}{2} \phi(\tau, \vec{x})^\dagger \left(i \frac{\partial}{\partial \tau_C} - \frac{\Delta}{2m} + \mu_0 \right) \phi(\tau, \vec{x}) - V(\phi), \quad (\text{A.1.6})$$

with μ_0 being the chemical potential of the ideal Bose gas. The path integration is over all fields satisfying the periodicity condition

$$\phi(-t_0 - i\beta, \vec{x}) = \phi(-t_0, \vec{x}), \quad (\text{A.1.7})$$

corresponding to the end points of the contour C (Fig.A.1) that are specified by the earliest time $-t_0$ and an inverse temperature β . The contour end points are allowed to move off indefinitely to the left in order to accommodate the possibility of Green's functions defined with respect to arbitrarily set times.

Functional operations involving quantities defined in terms of the contour time τ can be handled in terms of the contour-ordering function $\theta_c(\tau - \tau')$ and the associated contour Dirac delta function

$$\delta_c(\tau - \tau') = \frac{d}{d\tau} \theta_c(\tau - \tau'), \quad (\text{A.1.8})$$

so, e.g.,

$$\frac{\delta J(\tau', \vec{x}')}{J(\tau, \vec{x})} = \delta_c(\tau - \tau') \delta^3(\vec{x}' - \vec{x}) \equiv \delta_c(x' - x). \quad (\text{A.1.9})$$

Now, making use of the identity

$$\exp(iJ \cdot \phi) F(\phi) = F \left(\frac{\delta}{i\delta J} \right) \exp(iJ \cdot \phi), \quad (\text{A.1.10})$$

where

$$J \cdot \phi \equiv \int_C d\tau \int d^3x J(\tau, \vec{x}) \phi(\tau, \vec{x}), \quad (\text{A.1.11})$$

$$F[\phi] = \exp \left(-i \int_C d\tau \int d^3x V[\phi] \right), \quad (\text{A.1.12})$$

we can rewrite (A.1.5) in the following form:

$$Z_\beta[J] = F \left(\frac{\delta}{i\delta J} \right) \int D_c[\phi] \exp \left[i \left(\frac{1}{2} \phi \cdot D_\beta^{-1} \cdot \phi \right) + J \cdot \phi \right]. \quad (\text{A.1.13})$$

Here we have used an obvious extension of the dot notation to express the unperturbed contour-integrated action in terms of the inverse thermal propagator $D_\beta(\tau - \tau', \vec{x} - \vec{x}') = D_\beta(x - x')$:

$$\int_C d\tau \int d^3x L_0(\phi) = \frac{1}{2} \phi \cdot D_\beta^{-1} \cdot \phi, \quad (\text{A.1.14})$$

where

$$\left(i\partial_c - \frac{\Delta}{2m} + \mu_0 \right) D_\beta(x - x') = -\delta_c(\tau - \tau') \delta(\vec{x} - \vec{x}'). \quad (\text{A.1.15})$$

We expect that

$$D_\beta(x - y) = D_\beta^>(x - y) \theta_c(\tau_x - \tau_y) + D_\beta^<(x - y) \theta_c(\tau_y - \tau_x). \quad (\text{A.1.16})$$

Due to the KMS condition, the path integral is translationally invariant with respect to shifts in the variable of path integration that preserve (A.1.7). Then upon making a variable change

$$\phi' = \phi + J \cdot D_\beta = \phi + D_\beta \cdot J \quad (\text{A.1.17})$$

we find that (A.1.13) becomes

$$Z_\beta[J] = F \left(\frac{1}{i} \frac{\delta}{\delta J} \right) \exp \left(-\frac{1}{2} J \cdot D_\beta \cdot J \right), \quad (\text{A.1.18})$$

where we have dropped a J -dependent normalization factor.

It is shown in [65] that as $|t_0| \rightarrow \infty$ the asymptotic properties of the D_β function that satisfies (A.1.15) imply the factorization

$$Z_\beta[J] = Z_\beta[J; C_1, C_2] Z_\beta[J; C_3, C_4], \quad (\text{A.1.19})$$

where each of the factors on the right side of (A.1.19) has the form of (A.1.18), but with the implicit τ integrations limited only to their respective disjoint portions of the contour. Evidently, $Z_\beta[J; C_3, C_4]$ serves as a normalization factor in $Z_\beta[J]$ in the determination of the real-time thermal Green's functions.

Next we note, that

$$(J \cdot D \cdot J)_{C_1, C_2} = \int_{-\infty}^{+\infty} dt \int d^3x \int_{-\infty}^{+\infty} dt' \int d^3x' J_a(t, \vec{x}) D_\beta^{ab}(t - t', \vec{x} - \vec{x}') J_b(t', \vec{x}'), \quad (\text{A.1.20})$$

where $a, b = \{1, 2\}$ are the thermal indices and the Fourier transforms of the unique free thermal propagators $D_\beta^{ab}(x - y)$ read

$$iD_\beta^{11}(p) = \frac{i}{p_0 - \frac{\vec{p}^2}{2m} + \mu_0 + i\epsilon} + 2\pi\delta\left(p_0 - \frac{\vec{p}^2}{2m} + \mu_0\right) f(|p_0|), \quad (\text{A.1.21})$$

$$iD_\beta^{22}(p) = \frac{-i}{p_0 - \frac{\vec{p}^2}{2m} + \mu_0 + i\epsilon} + 2\pi\delta\left(p_0 - \frac{\vec{p}^2}{2m} + \mu_0\right) f(|p_0|), \quad (\text{A.1.22})$$

$$iD_\beta^{12}(p) = -2\pi\delta\left(p_0 - \frac{\vec{p}^2}{2m} + \mu_0\right) \sqrt{f(|p_0|)(1 + f(|p_0|))}, \quad (\text{A.1.23})$$

$$iD_\beta^{21}(p) = iD_\beta^{12}(p), \quad (\text{A.1.24})$$

where

$$f(p_0) = \frac{1}{\exp(p_0\beta) - 1}. \quad (\text{A.1.25})$$

The correct form of $F\left(\frac{\delta}{i\delta J}\right)$, when restricted to C_1 and C_2 , can be deduced when referring back to (A.1.18). First we note that

$$\frac{\delta(J \cdot \phi)}{\delta J(\tau)} = \phi(\tau) \quad (\text{A.1.26})$$

for all τ , where we have ignored the dependence of the spatial variables for simplicity. However,

$$J \cdot \phi = \int_{-\infty}^{+\infty} dt J_1(t) \phi_1(t) - \int_{-\infty}^{+\infty} dt J_2(t) \phi_2(t) + \dots, \quad (\text{A.1.27})$$

where the ellipsis represents the contributions of C_3 and C_4 and

$$\phi_1(t, \vec{x}) \equiv \phi(t, \vec{x}), \quad (\text{A.1.28})$$

$$\phi_2(t, \vec{x}) \equiv \phi\left(t - i\frac{\beta}{2}, \vec{x}\right). \quad (\text{A.1.29})$$

Thus we infer that

$$\frac{\delta}{\delta J(\tau)} = \frac{\delta}{\delta J_1(\tau)}, \tau = t \in C_1, \quad (\text{A.1.30})$$

$$\frac{\delta}{\delta J(\tau)} = -\frac{\delta}{\delta J_2(\tau)}, \tau = t - i\frac{\beta}{2} \in C_2. \quad (\text{A.1.31})$$

If we denote

$$Z_\beta[J_1, J_2] = Z_\beta[J; C_1, C_2], \quad (\text{A.1.32})$$

we obtain from (A.1.18):

$$Z_\beta[J_1, J_2] = \exp\left(-i \int d^4x \left[V\left(\frac{1}{i} \frac{\delta}{\delta J_1}\right) - V\left(\frac{1}{i} \frac{\delta}{\delta J_2}\right) \right]\right) Z_\beta^0[J_1, J_2]. \quad (\text{A.1.33})$$

Here

$$Z_\beta^0[J_1, J_2] = \exp \left(-i \int d^4x \int d^4y J_a(x) D_\beta^{ab}(x-y) J_b(y) \right) \quad (\text{A.1.34})$$

is the generating functional for the free thermal Green's function.

The functional $Z_\beta[J_1, J_2]$ can be expressed in terms of path integrals over the physical and auxiliary fields $\phi_1(x)$ and $\phi_2(x)$, respectively. One finds that

$$Z_\beta[J_1, J_2] = \int D[\phi_1] \int D[\phi_2] \exp \left(i \int \left[\frac{1}{2} \phi_a (D_{\beta^{-1}})^{ab} \phi_b - V(\phi_1) + V(-\phi_2) + J_a \phi_a \right] \right). \quad (\text{A.1.35})$$

We observe that in the loop expansion of this generating functional two types of vertices occur, one type describing the interactions of the original real-time field ϕ_1 and the other the interactions of the auxiliary field ϕ_2 . The Feynman rules for these two types of vertices differ by sign only in case of even interactions [67]. There is no direct coupling between the two types of fields but they may interact with each other through the temperature-dependent off-diagonal parts of the matrix propagator D_β^{ab} . Only type-1 fields can appear on external lines. The topological and combinatorial structure of the diagrams remains the same as in zero temperature field theory.

A.1.2 Thermal propagator

The real-time thermal Green's functions are generated by differentiating (A.1.33) with respect to J_1 and setting both J_1 and J_2 equal to zero

$$G_\beta^{ab}(x_1, x_2) = \frac{1}{i^2} \frac{1}{Z[0, 0]} \frac{\delta}{\delta J_a(x_1)} \frac{\delta}{\delta J_b(x_2)} Z[J_1, J_2] \Big|_{J_1=J_2=0} \quad (\text{A.1.36})$$

The full matrix propagator G_β^{ab} satisfies the Dyson equation

$$G_\beta^{ab} = i D_\beta^{ab} - (D_\beta \Sigma_\beta G_\beta)^{ab}. \quad (\text{A.1.37})$$

This equation defines the self-energy matrix $-i \Sigma_\beta^{ab}$ as the sum of one-particle irreducible diagrams with one external vertex of type a and the other of type b . The formal solution of (A.1.37) is

$$(G_\beta^{-1})^{ab} = -i (D_\beta^{-1})^{ab} - i \Sigma_\beta^{ab}. \quad (\text{A.1.38})$$

Therefore, the calculation of G_β^{ab} is reduced to the calculation of Σ_β^{ab} which contains a limited number of topologically distinct diagrams.

Thus, as we observe, the operator TFD technique is represented in the functional formalism by a special choice of the contour, depicted in Fig.A.1. Depending on the problem, different forms of paths are possible. Basically, they modify the boundary conditions for the propagator equations (A.1.15), which in turn influence the explicit forms of the propagators themselves. In a number of cases this results in a significant reduction of the technical complexity of calculations.

Appendix B

B.1 Dimensional regularization

In this appendix we evaluate the ultraviolet integrals met in formula (1.10.104).

A particularly convenient regularization method is *dimensional regularization*. In this method, the number of spatial dimensions D is taken to be a complex variable. The integral is calculated as a function of D in a region of the complex D -plane where it converges. This defines an analytic function of D which can be analytically continued to $D = 3$.

The momentum integrals one generally has to deal with have the following form:

$$I_{m,n} = \int \frac{d^D p}{(2\pi)^D} \frac{p^{2m-n}}{(p^2 + \Lambda^2)^{n/2}}. \quad (\text{B.1.1})$$

The integrals (B.1.1) satisfy the identities

$$\frac{d^2}{d\Lambda^2} I_{m,n} = -\frac{n}{2} I_{m+1,n+2}, \quad (\text{B.1.2})$$

$$\Lambda^2 I_{m,n} = I_{m-1,n-2} - I_{m+1,n}. \quad (\text{B.1.3})$$

After integrating over angles, the integral is

$$I_{m,n} = \frac{1}{(4\pi)^{D/2} \Gamma(\frac{D}{2})} \int_0^\infty dp^2 \frac{(p^2)^{m+(D-n-2)/2}}{(p^2 + \Lambda^2)^{n/2}}. \quad (\text{B.1.4})$$

If the integral is convergent, we can use integration by parts to derive the identity

$$(D + 2m - n) I_{m,n} = n I_{m+2,n+2}. \quad (\text{B.1.5})$$

The integral (B.1.4) is ultraviolet divergent if $D \geq 2(n-m)$ and infrared divergent if $D \leq n - 2m$. If the integral converges, its value is

$$I_{m,n} = \frac{1}{(4\pi)^{D/2}} \frac{\Gamma(\frac{2n-2m-D}{2}) \Gamma(\frac{D+2m-n}{2})}{\Gamma(\frac{n}{2}) \Gamma(\frac{D}{2})} \Lambda^{D+2(m-n)}. \quad (\text{B.1.6})$$

If the integral (B.1.4) is ultraviolet or infrared divergent, it can be regularized using dimensional regularization. The regularized integral is obtained by analytically continuing the expression (B.1.6) to $D = 3$. The result is

$$I_{m,n} = \frac{1}{4\pi^2} \frac{\Gamma(\frac{2n-2m-3}{2}) \Gamma(\frac{3+2m-n}{2})}{\Gamma(\frac{n}{2})} \Lambda^{3+2(m-n)}. \quad (\text{B.1.7})$$

The integrals that appear in the equation (1.10.104) for the density are $I_{0,1}$ and $I_{1,1}$. In three dimensions these integrals have power ultraviolet divergencies. With dimensional regularization, they are given by the finite expressions:

$$I_{0,1} = -\frac{1}{2\pi^2}\Lambda, \quad (\text{B.1.8})$$

$$I_{1,1} = \frac{1}{3\pi^2}\Lambda^3. \quad (\text{B.1.9})$$

Also, one of the great advantages of dimensional regularization is that integrals that contain no scale disappear:

$$\int \frac{d^D p}{(2\pi)^D} p^\alpha = 0. \quad (\text{B.1.10})$$

Because of the identity (B.1.10), dimensional regularization sets pure power ultraviolet divergencies to zero.

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