Representative Ensembles in Statistical Mechanics

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Abstract

The notion of representative statistical ensembles, correctly representing statistical systems, is strictly formulated. This notion allows for a proper description of statistical systems, avoiding inconsistencies in theory. As an illustration, a Bose-condensed system is considered. It is shown that a self-consistent treatment of the latter, using a representative ensemble, always yields a conserving and gapless theory.

Key words: Statistical systems; representative statistical ensembles; Bose-condensed systems.

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1 Introduction

Statistical systems are characterized by statistical ensembles. It is crucially important that the given statistical system be correctly represented by a statistical ensemble. In other words, the chosen statistical ensemble must be representative for the considered statistical system. This necessitates a thorough definition of what, actually, a statistical system is, requiring an accurate enumeration of all its basic features. The usage of a nonrepresentative ensemble, incorrectly representing the considered statistical system, may lead, and often does lead, to inconsistencies in the theoretical description of the system.

The necessity of defining a statistical ensemble that would correctly represent the given statistical system was, first, emphasized already by Gibbs [1], who stressed that all additional conditions and constraints, imposed on the system, must be taken into account. The problem of a proper representation of equilibrium statistical systems by equilibrium statistical ensembles was discussed by ter Haar [2,3] and also analyzed in the review article [4].

The aim of the present paper is to formalize the notion of representative statistical ensembles by giving precise mathematical definitions and to generalize this notion for arbitrary systems, whether equilibrium or nonequilibrium. The application of the notion is illustrated by systems with Bose-Einstein condensate, when the global gauge symmetry is broken. It is shown that employing a representative ensemble for a Bose-condensed system results in the theory enjoying conservation laws and having no gap in the spectrum of collective excitations.

Throughout the paper, the system of units will be used with the Planck and Boltzmann constants set to unity, $\hbar = 1$, $k_B = 1$.

2 Representative Ensembles

Let us, first, recall several general preliminary definitions that are necessary for precisely defining the basic notion of a representative statistical ensemble.

*Physical system* is a collection of objects characterized by their typical features distinguishing this collection from other systems.

For example, a collection of particles can be characterized by their Hamiltonian, that is, by their energy operator.

*Statistical system* is a many-body physical system, whose typical features are complemented by all additional constraints and conditions which are necessary for uniquely describing the statistical properties of the system.

Statistical systems are characterized by statistical ensembles.

*Statistical ensemble* is a pair $\{\mathcal{F}, \hat{\rho}(t)\}$ composed by the space of microstates $\mathcal{F}$ and a statistical operator $\hat{\rho}(t)$ on that space.

The space of microstates can be the Fock space or its appropriate subspace. The statistical operator $\hat{\rho}(t)$, generally, is a function of time $t$. To give $\hat{\rho}(t)$ implies to define its form $\hat{\rho}(0)$ at the initial time $t = 0$ and to specify the evolution operator $\hat{U}(t)$ such that

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^+(t).$$

Therefore, a statistical ensemble can be defined as a triplet

$$\{\mathcal{F}, \hat{\rho}(0), \hat{U}(t)\} \longleftrightarrow \{\mathcal{F}, \hat{\rho}(t)\}.$$
The knowledge of a statistical ensemble allows one to find statistical averages. 

**Statistical average** for an operator $\hat{A}(t)$ on $\mathcal{F}$ is

$$
<\hat{A}(t)> = \text{Tr}_F \hat{\rho}(t) \hat{A}(0) = \text{Tr}_F \hat{\rho}(0) \hat{A}(t) .
$$

(2)

Here the Heisenberg representation of the operator $\hat{A}(t)$ is assumed, for which

$$
\hat{A}(t) = \hat{U}(t) \hat{A}(0) \hat{U}^+(t) .
$$

(3)

**Representative ensemble** is a statistical ensemble equipped with all additional constraints and conditions that are necessary for a unique representation of the given statistical system.

Additional constraints and conditions for statistical systems are usually formulated as conditions on statistical averages for some specified *condition operators* $\hat{C}_i(t)$, where $i = 1, 2, \ldots$. These operators do not need to be necessarily the integrals of motion, but they are supposed to be Hermitian.

**Statistical condition** is a prescribed equality for the statistical average of a condition operator,

$$
C_i(t) = <\hat{C}_i(t)> = \text{Tr}\hat{\rho}(0) \hat{C}_i(t) .
$$

(4)

Here and in what follows, the trace operation is assumed to be over the appropriate space of microstates $\mathcal{F}$.

Let us consider, first, an *equilibrium statistical system*, for which the statistical operator does not depend on time,

$$
\hat{\rho}(t) = \hat{\rho}(0) \equiv \hat{\rho} .
$$

(5)

The explicit form of the statistical operator follows from the principle of minimal information [5]. The latter presumes the conditional maximization of the Gibbs entropy

$$
S = -\text{Tr} \hat{\rho} \ln \hat{\rho}
$$

(6)

under the statistical conditions (4), among which one usually distinguishes the definition of the internal energy

$$
E = \text{Tr} \hat{\rho} \hat{H}
$$

(7)

and the normalization condition

$$
\text{Tr} \hat{\rho} = 1 .
$$

(8)

The **information functional** is

$$
I[\hat{\rho}] = -S + \lambda_0 (\text{Tr} \hat{\rho} - 1) + \beta \left( \text{Tr} \hat{\rho} \hat{H} - E \right) + \beta \sum_i \nu_i \left( \text{Tr} \hat{\rho} \hat{C}_i - C_i \right) ,
$$

(9)

where $\lambda_0 \equiv \ln Z - 1$ is the Lagrange multiplier preserving the normalization condition (8), $\beta$ is the inverse temperature, which is the Lagrange multiplier for condition (7), and $\beta \nu_i$ are the Lagrange multipliers related to statistical conditions (4).

The minimization of the information functional (9) yields the statistical operator

$$
\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}} ,
$$

(10)
corresponding to the grand canonical ensemble with the \textit{grand Hamiltonian}

\[ H \equiv \hat{H} + \sum_i \nu_i \hat{C}_i . \] (11)

The most customary expression for the grand Hamiltonian (11) is

\[ H = \hat{H} - \mu \hat{N} , \]

where \( \mu \) is the chemical potential and \( \hat{N} \) is the number-of-particle operator. However, the general form of the grand Hamiltonian is given by Eq. (11), in which any condition operators can be involved. Thus, an equilibrium representative ensemble is described by the statistical operator (10) with the grand Hamiltonian (11). The evolution operator for an equilibrium system is

\[ \hat{U}(t) = e^{-iHt} , \] (12)

which commutes with the statistical operator (10), because of which

\[ i \frac{d}{dt} \hat{\rho}(t) = [H, \hat{\rho}(t)] = 0 . \]

The general way of obtaining the evolution equations for arbitrary nonequilibrium systems is through the extremization of action functionals [6]. In our case, this extremization has to be accomplished under the prescribed statistical conditions (4).

Let the system Hamiltonian be a functional of the field operators \( \psi(x,t) \) and \( \psi^\dagger(x,t) \), that is, \( \hat{H} = \hat{H}[\psi] \), where \( \psi = \psi(x,t) \). The system Lagrangian is

\[ \hat{L}[\psi] \equiv \int \psi^\dagger(x,t) i \frac{\partial}{\partial t} \psi(x,t) \, dx - \hat{H}[\psi] . \] (13)

The \textit{action functional}, or effective action, under the prescribed statistical conditions (4), takes the form

\[ A[\psi] \equiv \int \{ \hat{L}[\psi] - \sum_i \nu_i \hat{C}_i(t) \} \, dt , \] (14)

where \( \nu_i \) are the Lagrange multipliers guaranteeing the validity of the given statistical conditions. The action functional is defined so that to be a self-adjoint operator,

\[ A^+[\psi] = A[\psi] . \] (15)

Similarly to Eq. (11), the grand Hamiltonian in the Heisenberg representation is

\[ H[\psi] = \hat{H}[\psi] + \sum_i \nu_i \hat{C}_i(t) . \] (16)

Then the effective action (14) can be rewritten as

\[ A[\psi] = \int \left\{ \int \psi^\dagger(x,t) i \frac{\partial}{\partial t} \psi(x,t) \, dx - H[\psi] \right\} \, dt . \] (17)

The extremization of the action functional, requiring that

\[ \delta A[\psi] = 0 , \]
with
\[ \delta A[\psi] = \frac{\delta A[\psi]}{\delta \psi(x, t)} \delta \psi(x, t) + \frac{\delta A[\psi]}{\delta \psi^\dagger(x, t)} \delta \psi^\dagger(x, t), \]
yields the evolution equations
\[ \frac{\delta A[\psi]}{\delta \psi^\dagger(x, t)} = 0, \quad \frac{\delta A[\psi]}{\delta \psi(x, t)} = 0. \]  
(18)

These equations are the Hermitian conjugated forms of each other.

From Eqs. (17) and (18), it is evident that the evolution equations for the field operators can be represented as
\[ i \frac{\partial}{\partial t} \psi(x, t) = \frac{\delta H[\psi]}{\delta \psi^\dagger(x, t)} \]  
and its Hermitian conjugated. This should be equivalent to the Heisenberg equation of motion
\[ i \frac{\partial}{\partial t} \psi(x, t) = [\psi(x, t), H[\psi]] , \]
that is, to the Heisenberg representation for the field operator
\[ \psi(x, t) = \hat{U}(t) \psi(x, 0) \hat{U}^+(t) . \]

Hence, the evolution operator satisfies the Schrödinger equation
\[ i \frac{d}{dt} \hat{U}(t) = H[\psi(x, 0)] \hat{U}(t) . \]  
(20)

In this way, a nonequilibrium representative ensemble is the set of the given space of microstates \( \mathcal{F} \), initial statistical operator \( \hat{\rho}(0) \), and of the evolution operator \( \hat{U}(t) \) defined by Eq. (20). An equilibrium representative ensemble is, of course, just a particular case of the general nonequilibrium ensemble.

## 3 Bose-Condensed Systems

To illustrate the explicit construction of a representative ensemble, let us consider a system with Bose-Einstein condensate. Such systems possess a variety of interesting properties, as can be inferred from review works [7–10]. Moreover, theoretical description of these systems is known to confront the notorious difficulty of defining a self-consistent approach. The theory of Bose-condensed systems is based on the Bogolubov idea [11-14] of breaking the global gauge symmetry by means of the famous Bogolubov shift for field operators. The condensate wave function, introduced in the course of this shift, has to satisfy the minimum of the related thermodynamic potential, which is the stability condition necessary for making the system stable and the theory conserving and self-consistent. At the same time, the spectrum of collective excitations, according to the Hugenholtz-Pines theorem [15], has to be gapless. The notorious problem is the appearance of the contradiction between the above two requirements, when the theory is either nonconserving or gapful. This contradiction does not arise only in the lowest orders with respect to particle interactions, when one uses...
the Bogolubov approximation at low temperatures [11,12] or the quasiclassical approximation at high temperatures [16]. However, this contradiction immediately arises as soon as the interaction strength is not asymptotically weak and one has to invoke a more elaborate approximation. This problem of conserving versus gapless approximations was first emphasized by Hohenberg and Martin [17] and recently covered comprehensively by Andersen [9].

The problem is caused by the usage of nonrepresentative ensembles, which renders the system unstable [18]. Here we show that employing a representative ensemble never yields the above contradiction, always resulting in a self-consistent theory, being both conserving and gapless.

We consider a system with the Hamiltonian

\[ \hat{H} = \int \psi^\dagger(r) \left( -\frac{\nabla^2}{2m} + U \right) \psi(r) \, dr + \frac{1}{2} \int \psi^\dagger(r) \psi^\dagger(r') \Phi(r - r') \psi(r') \psi(r) \, dr \, dr' , \]  

in which the field operators \( \psi(r) = \psi(r,t) \) satisfy the Bose commutation relations, \( U = U(r,t) \) is an external field, and \( \Phi(r) = \Phi(-r) \) is an interaction potential. For describing a Bose-condensed system with broken global gauge symmetry, the Bogolubov shift [13,14] has to be done through the replacement

\[ \psi(r,t) \rightarrow \hat{\psi}(r,t) \equiv \eta(r,t) + \psi_1(r,t) , \]  

where \( \eta(r,t) \) is the condensate wave function and \( \psi_1(r,t) \) is the field operator of noncondensed particles. The latter field variables are assumed to be orthogonal to each other,

\[ \int \eta^*(r,t) \psi_1(r,t) \, dr = 0 . \]

It is necessary to emphasize that the Bogolubov shift (22) realizes unitary nonequivalent operator representations [18,19]. Accomplishing the Bogolubov shift (22) in Hamiltonian (21), as well as in all operators of observables, we get the algebra of observables defined on the Fock space \( \mathcal{F}(\psi_1) \) generated by the field operators \( \psi_1^\dagger(r) \) (see details in Refs. [5,18,19]).

The condensate function is normalized to the number of condensed particles

\[ N_0 = \int |\eta(r,t)|^2 \, dr . \]  

The Bogolubov shift (22) is only rational when the number of condensed particles (24) is macroscopic, which means that the limit

\[ \lim_{N \to \infty} \frac{N_0}{N} > 0 \]

is not zero, where \( N \) is the total number of particles. The latter is given by the average

\[ N = \langle \hat{N} \rangle \]

for the number-of-particle operator

\[ \hat{N} = \int \hat{\psi}^\dagger(r) \hat{\psi}(r) \, dr , \]
in which the Bogolubov shift (22) is again assumed. The statistical averaging in Eq. (25) and everywhere below is over the Fock space $\mathcal{F}(\psi_1)$.

Substituting the Bogolubov shift (22) into Hamiltonian (21) gives in the latter the terms linear in $\psi_1$, because of which the average $\langle \psi_1 \rangle$ can be nonzero. This, however, would result in the nonconservation of quantum numbers, e.g., of spin or momentum. Therefore, one has to impose the constraint for the conservation of quantum numbers,

$$\langle \psi_1(\mathbf{r},t) \rangle = 0 .$$

(27)

Defining the self-adjoint condition operator

$$\hat{\Lambda}(t) \equiv \int \left[ \lambda(\mathbf{r},t) \psi_1^\dagger(\mathbf{r},t) + \lambda^*(\mathbf{r},t) \psi_1(\mathbf{r},t) \right] d\mathbf{r} ,$$

(28)

in which $\lambda(\mathbf{r},t)$ is a complex function, we may represent constraint (27) as the *quantum conservation condition*

$$\langle \hat{\Lambda}(t) \rangle = 0 .$$

(29)

In this way, there are three statistical conditions. The first condition is the normalization (24) for the number of condensed particles. Condition (24) can be represented in the standard form (4) by defining the operator

$$\hat{N}_0 \equiv \hat{1} \int |\eta(\mathbf{r},t)|^2 d\mathbf{r} ,$$

(30)

in which $\hat{1}$ is the unity operator in the Fock space $\mathcal{F}(\psi_1)$. Then Eq. (24) reduces to the statistical condition

$$N_0 = \langle \hat{N}_0 \rangle .$$

(31)

The second condition is the normalization (25) for the total number of particles. Equivalently, instead of normalization (25), we may consider the normalization condition

$$N_1 = \langle \hat{N}_1 \rangle , \quad \hat{N}_1 \equiv \int \psi_1^\dagger(\mathbf{r}) \psi_1(\mathbf{r}) d\mathbf{r}$$

(32)

for the number of uncondensed particles $N_1 = N - N_0$. And the third condition is the conservation condition (29). Respectively, the effective action, which is now a functional of the two field variables, $\eta(\mathbf{r},t)$ and $\psi_1(\mathbf{r},t)$, with taking account of the statistical conditions (29), (31), and (32), becomes

$$A[\eta, \psi_1] = \int \left( \hat{\Lambda} + \mu_0 \hat{N}_0 + \mu_1 \hat{N}_1 + \hat{\Lambda} \right) dt .$$

(33)

Here $\hat{\Lambda} = \hat{\Lambda}(\hat{\psi})$ is the Lagrangian (13) under the Bogolubov shift (22) and $\hat{\Lambda} = \hat{\Lambda}(t)$ from Eq. (28). The quantities $\mu_0$, $\mu_1$, and $\Lambda(\mathbf{r},t)$ are the Lagrange multipliers guaranteeing the validity of the corresponding statistical conditions. Introducing the grand Hamiltonian

$$H[\eta, \psi_1] \equiv \hat{H} - \mu_0 \hat{N}_0 - \mu_1 \hat{N}_1 - \hat{\Lambda} ,$$

(34)

in which $\hat{H} = \hat{H}[\hat{\psi}]$, with shift (22), and the effective Lagrangian

$$L[\eta, \psi_1] \equiv \int \left[ \eta^\dagger(\mathbf{r},t) i \frac{\partial}{\partial t} \eta(\mathbf{r},t) + \psi_1^\dagger(\mathbf{r},t) i \frac{\partial}{\partial t} \psi_1(\mathbf{r},t) \right] d\mathbf{r} - H[\eta, \psi_1] ,$$

(35)
for the action functional (33), we get

\[ A[\eta, \psi_1] = \int L[\eta, \psi_1] \, dt. \]  

(36)

The evolution equations follow from the extremization of the action functional (36), that is, from the variations

\[ \frac{\delta A[\eta, \psi_1]}{\delta \eta^*(\mathbf{r}, t)} = 0 \]  

(37)

and

\[ \frac{\delta A[\eta, \psi_1]}{\delta \psi_1^*(\mathbf{r}, t)} = 0. \]  

(38)

These equations, as is clear from Eqs. (35) and (36), are equivalent to the equations of motion

\[ i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \frac{\delta H[\eta, \psi_1]}{\delta \eta^*(\mathbf{r}, t)} \]  

(39)

and

\[ i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \frac{\delta H[\eta, \psi_1]}{\delta \psi_1^*(\mathbf{r}, t)}. \]  

(40)

One has to substitute here Hamiltonian (34) under the Bogolubov shift (22). Accomplishing the variation in Eq. (39), we get

\[ i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left( -\frac{\nabla^2}{2m} + U - \mu \right) \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ \eta(\mathbf{r})^2 \eta(\mathbf{r}) + \tilde{X}(\mathbf{r}, \mathbf{r}') \right] \, d\mathbf{r}', \]  

(41)

where the time dependence in the right-hand side, for short, is not explicitly shown, \( U = U(\mathbf{r}, t) \), and the notation for the correlation operator

\[ \tilde{X}(\mathbf{r}, \mathbf{r}') \equiv \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}) \eta(\mathbf{r}) + \psi_1(\mathbf{r}') \psi_1^*(\mathbf{r}) \eta(\mathbf{r}) + \eta(\mathbf{r})^* \eta(\mathbf{r})^* \psi_1(\mathbf{r}') \psi_1^*(\mathbf{r}) + \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}) \eta(\mathbf{r}) \eta(\mathbf{r}) \psi_1^*(\mathbf{r}') + \tilde{X}(\mathbf{r}, \mathbf{r}') \]  

(42)

is used. The variation in Eq. (40) gives

\[ i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \left( -\frac{\nabla^2}{2m} + U - \mu_1 \right) \psi_1(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ |\eta(\mathbf{r}')|^2 \psi_1(\mathbf{r}) + |\psi_1(\mathbf{r}')|^2 \eta(\mathbf{r}) \psi_1(\mathbf{r}) + \eta^*(\mathbf{r})^* \eta(\mathbf{r}) \psi_1(\mathbf{r}) + \eta(\mathbf{r})^* \eta(\mathbf{r}) \psi_1^*(\mathbf{r}') + \tilde{X}(\mathbf{r}, \mathbf{r}') \right] \, d\mathbf{r}'. \]  

(43)

To get an equation for the condensate wave function, we have to take the statistical average of Eq. (41). For this purpose, we introduce the normal density matrix

\[ \rho_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1^*(\mathbf{r}') \psi_1(\mathbf{r}) \rangle, \]  

(44)

the anomalous density matrix

\[ \sigma_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle, \]  

(45)
and their diagonal elements, giving the density of noncondensed particles

\[ \rho_1(\mathbf{r}) \equiv \rho_1(\mathbf{r}, \mathbf{r}) = \langle \psi_1^\dagger(\mathbf{r}) \psi_1(\mathbf{r}) \rangle \quad (46) \]

and the anomalous average

\[ \sigma_1(\mathbf{r}) \equiv \sigma_1(\mathbf{r}, \mathbf{r}) = \langle \psi_1(\mathbf{r}) \psi_1(\mathbf{r}) \rangle . \quad (47) \]

The quantity \( |\sigma_1(\mathbf{r})| \) can be interpreted as the density of paired particles [19]. The total density of particles

\[ \rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \rho_1(\mathbf{r}) \quad (48) \]

consists of the condensate density

\[ \rho_0(\mathbf{r}) \equiv |\eta(\mathbf{r})|^2 \quad (49) \]

and the density of noncondensed particles \((46)\). Averaging Eq. \((41)\), we find the equation for the condensate wave function

\[
i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ \rho(\mathbf{r}') \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') + \langle \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}) \psi_1(\mathbf{r}) \rangle \right] d\mathbf{r}' . \quad (50)\]

Equations \((43)\) and \((50)\) are the basic equations of motion for the field variables \(\eta(\mathbf{r}, t)\) and \(\psi_1(\mathbf{r}, t)\). These equations, according to Eqs. \((39)\) and \((40)\), are generated by the variation of the grand Hamiltonian \((34)\). The latter, in agreement with Eq. \((20)\), also defines the evolution operator \(\hat{U}(t)\), which satisfies the Schrödinger equation

\[ i \frac{d}{dt} \hat{U}(t) = H[\eta(\mathbf{r}, 0), \psi_1(\mathbf{r}, 0)]\hat{U}(t) . \]

Thus, the representative ensemble for a Bose-condensed system is the triplet

\[ \{ \mathcal{F}(\psi_1), \hat{\rho}(0), \hat{U}(t) \} . \]

It is important to stress that the so defined representative ensemble possesses a principal feature making it different from the standardly used ensemble having the sole Lagrange multiplier \(\mu_0 \equiv \mu_1\). But then the normalization condition \((24)\) cannot be guaranteed. Then the evolution equation for the condensate wave function is not a result of a variational procedure. For an equilibrium system, this means that the number of condensed particles \(N_0\) does not provide the minimum of a thermodynamic potential, which implies the system instability. All notorious inconsistencies in theory, manifesting themselves in the lack of conservation laws or in the appearance of an unphysical gap in the spectrum, are caused by the usage of nonrepresentative ensembles.
4 Green Functions

The equations of motion (43) and (50) allow us to derive the evolutional equations for the Green functions. To this end, we shall use the compact notation denoting the set \( \{ r_j, t_j \} \) by the sole letter \( j \), so that the dependence of functions on the spatial and temporal variables looks like

\[
 f(12\ldots n) \equiv f(r_1, t_1, r_2, t_2, \ldots, r_n, t_n) .
\]

The product of the differentials \( dr_j dt_j \) will be denoted as \( d(j) \), so that

\[
 d(12\ldots n) \equiv \prod_{j=1}^{n} dr_j dt_j .
\]

We shall employ the Dirac delta function

\[
 \delta(12) \equiv \delta(r_1 - r_2) \delta(t_1 - t_2) .
\]

For the interaction potential, we shall use the retarded form

\[
 \Phi(12) \equiv \Phi(r_1 - r_2) \delta(t_1 - t_2 + 0) .
\]

The matrix Green function \( G(12) = [G_{\alpha\beta}(12)] \) is a \( 2 \times 2 \) matrix, with \( \alpha, \beta = 1, 2 \), and with the following elements:

\[
 G_{11}(12) \equiv -i < \hat{T} \psi_1(1) \psi_1^\dagger(2) > , \quad G_{12}(12) \equiv -i < \hat{T} \psi_1(1) \psi_1(2) > , \\
 G_{21}(12) \equiv -i < \hat{T} \psi_1^\dagger(1) \psi_1^\dagger(2) > , \quad G_{22}(12) \equiv -i < \hat{T} \psi_1^\dagger(1) \psi_1(2) > ,
\]

where \( \hat{T} \) is the time-ordering operator.

Let us introduce the operator

\[
 \hat{K}_j \equiv - \frac{\nabla_j^2}{2m} + U(j) - \mu_1 ,
\]

the condensate effective potential

\[
 V(12) \equiv \delta(12) \int \Phi(13)|\eta(3)|^2 d(3) + \Phi(12)\eta(1)\eta^*(2) ,
\]

and let us rewrite the correlation operator (42) in the form

\[
 \hat{X}(12) = \psi_1^\dagger(2) \psi_1(2) \eta(1) + \psi_1^\dagger(2) \eta(2) \psi_1(1) + \eta^*(2) \psi_1(2) \psi_1(1) + \psi_1^\dagger(2) \psi_1(2) \psi_1(1) .
\]

We also define the matrix correlation function \( X(123) = [X_{\alpha\beta}(123)] \) with the elements:

\[
 X_{11}(123) \equiv - < \hat{T} \hat{X}(12) \psi_1^\dagger(3) > , \quad X_{12}(123) \equiv - < \hat{T} \hat{X}(12) \psi_1(3) > , \\
 X_{21}(123) \equiv - < \hat{T} \hat{X}^+(12) \psi_1^\dagger(3) > , \quad X_{22}(123) \equiv - < \hat{T} \hat{X}^+(12) \psi_1(3) > .
\]

From the equations of motion (43) and (50), we find the equations

\[
 \left( i \frac{\partial}{\partial t_1} - \hat{K}_1 \right) G_{11}(12) - \int V(13) G_{11}(32) d(3) =
\]

\[
 - \frac{\partial}{\partial t_1} \int \Phi(13)|\eta(3)|^2 d(3) - \Phi(12)\eta(1)\eta^*(2) .
\]
\[-\int \Phi(13) \left[ \eta(1)\eta(3)G_{21}(32) + iX_{11}(132) \right] d(3) = \delta(12) ,
\begin{align*}
&\left( i \frac{\partial}{\partial t_1} - \hat{K}_1 \right) G_{12}(12) - \int V(13)G_{12}(32) d(3) - \\
&- \int \Phi(13) \left[ \eta(1)\eta(3)G_{22}(32) + iX_{12}(132) \right] d(3) = 0 ,
\end{align*}
\begin{align*}
&\left( -i \frac{\partial}{\partial t_1} - \hat{K}_1 \right) G_{21}(12) - \int V^*(13)G_{21}(32) d(3) - \\
&- \int \Phi(13) \left[ \eta^*(1)\eta^*(3)G_{11}(32) + iX_{21}(132) \right] d(3) = 0 ,
\end{align*}
\begin{align*}
&\left( -i \frac{\partial}{\partial t_1} - \hat{K}_1 \right) G_{22}(12) - \int V^*(13)G_{22}(32) d(3) - \\
&- \int \Phi(13) \left[ \eta^*(1)\eta^*(3)G_{12}(32) + iX_{22}(132) \right] d(3) = \delta(12) . \tag{57}
\end{align*}

The self-energy $\Sigma(12) = [\Sigma_{\alpha\beta}(12)]$ is a matrix whose elements are defined by the relations
\begin{align*}
\int \left[ \Sigma_{11}(13)G_{11}(32) + \Sigma_{12}(13)G_{21}(32) \right] d(3) = \\
= \int V(13)G_{11}(32) d(3) + \int \Phi(13) \left[ \eta(1)\eta(3)G_{21}(32) + iX_{11}(132) \right] d(3) ,
\end{align*}
\begin{align*}
\int \left[ \Sigma_{11}(13)G_{12}(32) + \Sigma_{12}(13)G_{22}(32) \right] d(3) = \\
= \int V(13)G_{12}(32) d(3) + \int \Phi(13) \left[ \eta(1)\eta(3)G_{22}(32) + iX_{12}(132) \right] d(3) ,
\end{align*}
\begin{align*}
\int \left[ \Sigma_{21}(13)G_{11}(32) + \Sigma_{22}(13)G_{21}(32) \right] d(3) = \\
= \int V^*(13)G_{21}(32) d(3) + \int \Phi(13) \left[ \eta^*(1)\eta^*(3)G_{11}(32) + iX_{21}(132) \right] d(3) ,
\end{align*}
\begin{align*}
\int \left[ \Sigma_{21}(13)G_{12}(32) + \Sigma_{22}(13)G_{22}(32) \right] d(3) = \\
= \int V^*(13)G_{22}(32) d(3) + \int \Phi(13) \left[ \eta^*(1)\eta^*(3)G_{12}(32) + iX_{22}(132) \right] d(3) . \tag{58}
\end{align*}

Let us introduce the matrix condensate propagator $C(12) = [C_{\alpha\beta}(12)]$, with the elements
\begin{align*}
C_{11}(12) &\equiv -i\eta(1)\eta^*(2) , & C_{12}(12) &\equiv -i\eta(1)\eta(2) , \\
C_{21}(12) &\equiv -i\eta^*(1)\eta^*(2) , & C_{22}(12) &\equiv -i\eta^*(1)\eta(2) , \tag{59}
\end{align*}

The latter have the properties
\begin{align*}
C_{11}(21) & = C_{22}(12) , & C_{11}(11) & = C_{22}(11) , & C_{12}(21) & = C_{12}(12) , \\
C_{21}(21) & = C_{21}(12) , & C^*_{11}(12) & = -C_{22}(12) , & C^*_{12}(12) & = -C_{21}(12) . \tag{60}
\end{align*}
The binary Green function is a matrix \( B(123) = [B_{\alpha\beta}(123)] \),

\[
B(123) = C(12)G(23) - i\rho_0(2)G(13) + X(123) ,
\]

which is defined by the following relations:

\[
\begin{align*}
B_{11}(123) &\equiv C_{11}(12)G_{11}(23) + C_{11}(12)G_{11}(13) + C_{12}(12)G_{21}(23) + X_{11}(123) , \\
B_{12}(123) &\equiv C_{11}(12)G_{12}(23) + C_{11}(12)G_{12}(13) + C_{12}(12)G_{22}(23) + X_{12}(123) , \\
B_{21}(123) &\equiv C_{22}(12)G_{21}(23) + C_{22}(12)G_{21}(13) + C_{21}(12)G_{11}(23) + X_{21}(123) , \\
B_{22}(123) &\equiv C_{22}(12)G_{22}(23) + C_{22}(12)G_{22}(13) + C_{21}(12)G_{12}(23) + X_{22}(123) ,
\end{align*}
\]

and where \( \rho_0(1) \equiv |\eta(1)|^2 \).

With Eqs. (59) and (61), relations (58), defining the self-energy, can be rewritten in the matrix form

\[
\int \Sigma(13)G(32) \, d(3) = i \int \Phi(13)B(132) \, d(3) .
\]

Then the equations of motion (57) acquire the matrix representation

\[
\left( \hat{\tau}_3 i \frac{\partial}{\partial t_1} - \hat{K}_1 \right) G(12) - \int \Sigma(13)G(32) \, d(3) = \delta(12) ,
\]

in which the delta function \( \delta(12) \) in the right-hand side is assumed to be factored with the unity matrix \( \hat{1} = [\delta_{\alpha\beta}] \) and

\[
\hat{\tau}_3 \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}
\]

is a Pauli matrix.

Introducing the inverse propagator

\[
G^{-1}(12) \equiv \left( \hat{\tau}_3 i \frac{\partial}{\partial t_1} - \hat{K}_1 \right) \delta(12) - \Sigma(12)
\]

allows us to transform Eq. (64) into

\[
\int G^{-1}(13)G(32) \, d(3) = \delta(12) .
\]

An equivalent representation, following from Eq. (66), is

\[
\int G(13)G^{-1}(32) \, d(3) = \delta(12) .
\]

For the self-energy, using Eq. (63), we have

\[
\Sigma(12) = i \int \Phi(13)B(134)G^{-1}(42) \, d(34) .
\]
The equations for the Green functions are to be complimented by the equation for the condensate wave function (50), which, introducing one more anomalous average

\[ \xi(12) \equiv \langle \psi^\dagger_1(2)\psi_1(2)\psi(1) \rangle , \]  

(69)
can be represented as

\[ i \frac{\partial}{\partial t_1} \eta(1) = \left[ -\frac{\nabla_1^2}{2m} + U(1) - \mu_0 \right] \eta(1) + \]

\[ + \int \Phi(12) \left[ \rho(2)\eta(1) + \rho_1(12)\eta(2) + \sigma_1(12)\eta^*(2) + \xi(12) \right] d(2) . \]

(70)

It is the equations for the Green functions and the equation for the condensate function, which become mutually incompatible in the standard approach, while employing the representative ensemble renders the theory self-consistent in any approximation.

5 Theory Self-Consistency

One usually confronts inconsistencies in theory considering a uniform equilibrium Bose-condensed system. Then, in any given approximation, one gets either a nonconserving theory, that is, an unstable system, or one finds an unphysical gap in the spectrum, which, actually, again corresponds to an unstable system [9,18]. To analyze this problem, we pass now to the case of an equilibrium uniform system, when \( U = 0 \).

Then we use the Fourier transform for the Green function

\[ G(21) = \int G(k,\omega)e^{i(k \cdot r_{12} - \omega t_{12})} \frac{dk d\omega}{(2\pi)^3} , \]

in which

\[ r_{12} \equiv r_1 - r_2 , \quad t_{12} \equiv t_1 - t_2 . \]

By their definition in Eq. (52), the Green function elements possess the properties

\[ G_{11}(21) = G_{22}(12) , \quad G_{12}(21) = G_{12}(12) , \quad G_{21}(21) = G_{21}(12) . \]

(71)

Therefore the corresponding Fourier transforms satisfy the relations

\[ G_{11}(-k, -\omega) = G_{22}(k, \omega) , \quad G_{12}(-k, -\omega) = G_{12}(k, \omega) , \]

\[ G_{21}(-k, -\omega) = G_{21}(k, \omega) . \]

(72)

Assuming that the system is isotropic, one has

\[ G_{\alpha\beta}(-k, \omega) = G_{\alpha\beta}(k, \omega) \]

(73)

for all \( \alpha, \beta \). Combining Eqs. (72) and (73), we find

\[ G_{11}(k, -\omega) = G_{22}(k, \omega) , \quad G_{12}(k, -\omega) = G_{12}(k, \omega) , \]

\[ G_{12}(k, \omega) = G_{21}(k, \omega) . \]
\[ G_{21}(k, -\omega) = G_{21}(k, \omega) . \] (74)

Also, for a uniform equilibrium system, one has [14] the equality
\[ G_{21}(k, \omega) = G_{12}(k, \omega) . \] (75)

Fourier-transforming the self-energy
\[
\Sigma(12) = \int \Sigma(k, \omega) e^{i(k \cdot r_{12} - \omega t_{12})} dk d\omega \left(2\pi\right)^4
\]
and, similarly, the inverse propagator (65), we have for the latter
\[ G^{-1}(k, \omega) = \hat{\tau}_3 \omega - \frac{k^2}{2m} + \mu - \Sigma(k, \omega) . \] (76)

Then Eq. (67) reduces to
\[ G^{-1}(k, \omega) G(k, \omega) = \hat{1} , \] (77)

where \( \hat{1} = [\delta_{\alpha \beta}] \).

From Eqs. (76) and (77), it follows that \( G^{-1}(k, \omega) \), hense, also \( \Sigma(k, \omega) \), have the same symmetry properties as \( G(k, \omega) \). In particular,
\[
\Sigma_{\alpha \beta}(-k, \omega) = \Sigma_{\alpha \beta}(k, \omega) , \quad \Sigma_{12}(k, -\omega) = \Sigma_{12}(k, \omega) , \quad \Sigma_{21}(k, -\omega) = \Sigma_{21}(k, \omega) ,
\]
\[ \Sigma_{21}(k, \omega) = \Sigma_{12}(k, \omega) , \quad \Sigma_{11}(k, -\omega) = \Sigma_{22}(k, \omega) . \] (78)

The matrix equation (77), explicitly, is the system of equations
\[
\begin{align*}
\left( \omega - \frac{k^2}{2m} + \mu_1 - \Sigma_{11} \right) G_{11} - \Sigma_{12} G_{21} &= 1 , \\
\left( \omega - \frac{k^2}{2m} + \mu_1 - \Sigma_{11} \right) G_{12} - \Sigma_{12} G_{22} &= 0 , \\
\left( -\omega - \frac{k^2}{2m} + \mu_1 - \Sigma_{22} \right) G_{21} - \Sigma_{21} G_{11} &= 0 , \\
\left( -\omega - \frac{k^2}{2m} + \mu_1 - \Sigma_{22} \right) G_{22} - \Sigma_{21} G_{12} &= 1 ,
\end{align*}
\] (79)

where, for short, \( G_{\alpha \beta} = G_{\alpha \beta}(k, \omega) \) and \( \Sigma_{\alpha \beta} = \Sigma_{\alpha \beta}(k, \omega) \). The solutions to these equations are
\[
\begin{align*}
G_{11}(k, \omega) &= \frac{\omega + k^2/2m + \Sigma_{11}(k, \omega) - \mu_1}{D(k, \omega)} , \\
G_{12}(k, \omega) &= -\frac{\Sigma_{12}(k, \omega)}{D(k, \omega)} ,
\end{align*}
\] (80)

with the denominator
\[
D(k, \omega) \equiv \left[ \omega - \frac{k^2}{2m} - \Sigma_{11}(k, \omega) + \mu_1 \right] \times
\]
\[ \times \left[ \omega + \frac{k^2}{2m} + \Sigma_{22}(\mathbf{k}, \omega) - \mu_1 \right] + \Sigma_{12}^2(\mathbf{k}, \omega) . \] (81)

The solutions for \( \Sigma_{21}(\mathbf{k}, \omega) \) and \( G_{22}(\mathbf{k}, \omega) \) are defined by the symmetry properties (72) to (75).

The excitation spectrum is given by the poles of the Green functions, that is, by the zero of denominator (81),

\[ D(\mathbf{k}, \varepsilon_k) = 0 . \] (82)

Equation (82) can be represented as

\[ \varepsilon_k = \frac{1}{2} \left[ \Sigma_{11}(\mathbf{k}, \varepsilon_k) - \Sigma_{22}(\mathbf{k}, \varepsilon_k) \right] \pm \sqrt{\omega_k^2 - \Sigma_{12}^2(\mathbf{k}, \varepsilon_k)} , \] (83)

with the notation

\[ \omega_k \equiv \frac{k^2}{2m} + \frac{1}{2} \left[ \Sigma_{11}(\mathbf{k}, \varepsilon_k) + \Sigma_{22}(\mathbf{k}, \varepsilon_k) \right] - \mu_1 . \] (84)

Denominator (81) enjoys the property

\[ D(\mathbf{k}, -\omega) = D(\mathbf{k}, \omega) . \]

Consequently, if \( \varepsilon_k \) is a solution of Eq. (82), then \( -\varepsilon_k \) is also its solution, which is in agreement with the form of Eq. (83).

For an equilibrium uniform system, the Bogolubov shift (22) is equivalent to the separation of the zero-momentum term in the expansion of the field operator over plane waves. The shift itself has meaning only under the normalization condition (24), in which \( N_0 \sim N \), that is, the zero-momentum state is macroscopically occupied. The latter becomes possible when the single particle spectrum touches zero. Therefore, the necessary condition for the existence of Bose-Einstein condensate is

\[ \lim_{k \to 0} \varepsilon_k = 0 . \] (85)

This is to be complimented by the stability condition

\[ \text{Re} \ \varepsilon_k \geq 0 ; \quad \text{Im} \ \varepsilon_k \leq 0 . \] (86)

This condition should be kept in mind when choosing the sign plus in front of the square root in spectrum (83).

Taking limit (85) for spectrum (83), we notice that, according to properties (78),

\[ \Sigma_{11}(\mathbf{k}, 0) = \Sigma_{22}(\mathbf{k}, 0) . \] (87)

By using perturbation theory for a stable system, one can show [15] that in all orders of the theory

\[ \Sigma_{\alpha\beta}(0, 0) \geq 0 . \] (88)

Then the necessary condition (85) yields the expression for the chemical potential

\[ \mu_1 = \Sigma_{11}(0, 0) - \Sigma_{12}(0, 0) , \] (89)
which is the Hugenholtz-Pines relation [15].

On the other hand, we have Eq. (70) for the condensate wave function. For an equilibrium uniform system, with no external potential $U$, all densities do not depend on the spatial and temporal variables,

$$\rho_0(r) = \rho_0, \quad \rho_1(r) = \rho_1, \quad \sigma_1(r) = \sigma_1, \quad \rho(r) = \rho.$$  \(90\)

The condensate wave function reduces to the constant

$$\eta(r,t) = \eta = \sqrt{\rho_0}.$$  \(91\)

Then we substitute into Eq. (70) the Fourier transforms for the interaction potential

$$\Phi(r) = \int \Phi_k e^{i k \cdot r} \frac{dk}{(2\pi)^3},$$

for the normal density matrix (44),

$$\rho_1(r_1, r_2) = \int n_k e^{i k \cdot r_{12}} \frac{dk}{(2\pi)^3},$$

and for the anomalous density matrix (45),

$$\sigma_1(r_1, r_2) = \int \sigma_k e^{i k \cdot r_{12}} \frac{dk}{(2\pi)^3}.$$

Similarly, the Fourier transform for the anomalous average (69) is

$$\xi_1(r_1, r_2) = \int \xi_k e^{i k \cdot r_{12}} \frac{dk}{(2\pi)^3}.$$

As a result, Eq. (70) gives

$$\mu_0 = \rho \Phi_0 + \int \left( n_k + \sigma_k + \frac{\xi_k}{\sqrt{\rho_0}} \right) \Phi_k \frac{dk}{(2\pi)^3}.$$  \(92\)

Generally, expressions (92) and (89) do not coincide with each other, their difference being

$$\mu_0 - \mu_1 = \rho \Phi_0 + \int \left( n_k + \sigma_k + \frac{\xi_k}{\sqrt{\rho_0}} \right) \Phi_k \frac{dk}{(2\pi)^3} - \Sigma_{11}(0,0) + \Sigma_{12}(0,0).$$  \(93\)

This is the general expression for the difference between the Lagrange multipliers $\mu_0$ and $\mu_1$ for an arbitrary equilibrium uniform Bose-condensed system.

Usually, one does not distinguish between the Lagrange multipliers $\mu_0$ and $\mu_1$, which implies setting $\mu_0 - \mu_1 \to 0$. However, as is evident from Eq. (93), there is no any reason for requiring that this quantity be zero. As an illustration, we may resort to the Hartree-Fock-Bogolubov approximation, in which $\xi_k = 0$ and

$$\Sigma_{11}(0,0) = (\rho + \rho_0) \Phi_0 + \int n_k \Phi_k \frac{dk}{(2\pi)^3}, \quad \Sigma_{12}(0,0) = \rho_0 \Phi_0 + \int \sigma_k \Phi_k \frac{dk}{(2\pi)^3}.$$
Relation (89) then yields
\[ \mu_1 = \rho \Phi_0 + \int (n_k - \sigma_k) \Phi_k \frac{d\mathbf{k}}{(2\pi)^3}. \]  
(94)

The difference of the chemical potentials (93) becomes
\[ \mu_0 - \mu_1 = 2 \int \sigma_k \Phi_k \frac{d\mathbf{k}}{(2\pi)^3}, \]  
(95)

which, certainly, is nonzero [20].

In this way, the introduction of the additional Lagrange multiplier makes the theory completely self-consistent. All inconsistencies that often arise in other works, such as the appearance of a gap in the spectrum, system instability or a distortion of the phase transition order, are caused by neglecting the difference between the multiplier \( \mu_1 \) and the multiplier \( \mu_0 \). It is worth emphasizing that the introduction of the Lagrange multiplier \( \mu_0 \) for preserving the normalization condition (24), from the mathematical point of view is strictly necessary. In other case, the employed ensemble would not be representative, hence, could not correctly describe the Bose-condensed system with broken gauge symmetry.

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