

Fluctuations of composite observables and stability of statistical systems

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Thermodynamic stability of statistical systems requires that susceptibilities be semipositive and finite. Susceptibilities are known to be related to the fluctuations of extensive observable quantities. This relation becomes nontrivial, when the operator of an observable quantity is represented as a sum of operators corresponding to the extensive system parts. The association of the dispersions of the partial operator terms with the total dispersion is analyzed. Special attention is paid to the dependence of dispersions on the total number of particles N in the thermodynamic limit. An operator dispersion is called thermodynamically normal if it is proportional to N at large values of the latter. While, if the dispersion is proportional to a higher power of N , it is termed thermodynamically anomalous. The following theorem is proved: The global dispersion of a composite operator, which is a sum of linearly independent self-adjoint terms, is thermodynamically anomalous if and only if at least one of the partial dispersions is anomalous, the power of N in the global dispersion being defined by the largest partial dispersion. Conversely, the global dispersion is thermodynamically normal if and only if all partial dispersions are normal. The application of the theorem is illustrated by several examples of statistical systems. The notion of representative ensembles is formulated. The relation between the stability and equivalence of statistical ensembles is discussed.

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I. INTRODUCTION

Stability of statistical systems and the fluctuations of observable quantities are known to be intimately related. The fluctuations can be characterized by the corresponding susceptibilities, such as specific heat, isothermal compressibility, or longitudinal magnetic susceptibility. The susceptibilities are connected with the dispersions of the operators representing observable quantities. In what follows, we shall deal with the so-called *extensive* observables, whose averages are proportional to the total number of particles N , when N is large [1,2]. The existence of the thermodynamic limit is assumed, when N is asymptotically large, such that $N \rightarrow \infty$.

Note that susceptibilities can also be connected with the fluctuations of intensive thermodynamic variables, such as pressure and temperature [3,4]. However, in this paper, we shall consider only the fluctuations of extensive observables.

For stable statistical systems in equilibrium, the susceptibilities are positive and finite, which follows from their relations to the dispersions of the corresponding operator observables [5] or, on the general thermodynamic level, stems from the second law of thermodynamics [6]. The susceptibilities may become divergent only at the points of second-order phase transitions, which, however, by definition, are the points of instability. Really, at the point of a phase transition, one phase becomes unstable, as a consequence, it transforms to another, stable, phase. After the phase transition has occurred, all susceptibilities in the stable phase go finite.

The fluctuations of extensive observables, related to the corresponding operator dispersions, can be classified onto two types, according to their dependence on the total number of particles N in the given statistical system, when the number N is large, such that $N \gg 1$. This implies that the thermodynamic limit is assumed. The fluctuations are called *thermodynamically normal*, when the related operator dispersion

is proportional to N . Conversely, if the operator dispersion is proportional to N^α , with $\alpha > 1$, then the related fluctuations are termed *thermodynamically anomalous*.

The finiteness of susceptibilities in stable equilibrium systems means that the corresponding fluctuations are thermodynamically normal. Oppositely, the divergence of susceptibilities at the critical points shows that the fluctuations of the related extensive observables are thermodynamically anomalous. In a stable system, outside phase transition points, all susceptibilities are finite, which tells us that the fluctuations of all extensive observables are thermodynamically normal.

It is worth warning the reader that thermodynamically normal or anomalous fluctuations have nothing to do with the normal, that is, Gaussian distributions. Thermodynamic normality or anomaly are the notions describing the thermodynamic behavior of the related operator dispersions with respect to the total number of particles. In calculating the corresponding averages, any quantum or classical probability measures, of arbitrary nature, can be employed.

In the present paper, general relations between the fluctuations of observables and the stability of statistical systems are studied. The emphasis is on the case, which is not a standard one, when the observable quantities are represented as sums of several terms, corresponding to macroscopic parts of the system. Then the relation between the fluctuations of the partial terms and the fluctuations of the global observables is not evident. A general theorem is rigorously proved, connecting the behavior of fluctuations of global and partial observables. This theorem is briefly formulated in the Abstract and its mathematically rigorous formulation is given in Sec. III. The direct interrelation between the thermodynamic behavior of fluctuations and stability is emphasized. It is also shown that the stability of statistical systems is intricately connected with the notions of symmetry breaking and ensemble equivalence.

II. FLUCTUATIONS OF OBSERVABLES AND STABILITY

In quantum statistical mechanics, observable quantities are represented by self-adjoint operators from the algebra of observables. As is explained in Sec. I, only extensive observables are considered in the paper. Fluctuations of the observable quantities are characterized by the related operator dispersions. Let \hat{A} be an operator representing an extensive observable quantity. Its dispersion is

$$\Delta^2(\hat{A}) \equiv \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2, \quad (1)$$

where the angle brackets, as usual, denote statistical averaging.

The dispersions of the operators, representing extensive observables, are directly connected with the associated susceptibilities, which can be measured. Thus, the fluctuations of the Hamiltonian H , quantified by its dispersion $\Delta^2(H)$, define the specific heat

$$C_V \equiv \frac{1}{N} \left(\frac{\partial E}{\partial T} \right)_V = \frac{\Delta^2(\hat{H})}{NT^2}, \quad (2)$$

where $E \equiv \langle H \rangle$ is internal energy, N is the total number of particles in the system of volume V , and T is temperature. Here and in what follows, the Boltzmann constant is set to unity, $k_B \equiv 1$. The fluctuations of the number of particles are described by the dispersion $\Delta^2(\hat{N})$ of the number-of-particle operator \hat{N} , yielding the isothermal compressibility

$$\kappa_T \equiv - \frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T = \frac{\Delta^2(\hat{N})}{N\rho T}, \quad (3)$$

in which P is pressure, $N \equiv \langle \hat{N} \rangle$, and $\rho \equiv N/V$ is the average particle density. In magnetic systems, with the Zeeman interaction $-\mu_0 \sum_i \mathbf{B} \cdot \mathbf{S}_i$ of the operator spins \mathbf{S}_i with an external magnetic field \mathbf{B} , the fluctuations of the magnetization $M_\alpha \equiv \langle \hat{M}_\alpha \rangle$ are described by the dispersion $\Delta^2(\hat{M}_\alpha)$ of the magnetization operator $\hat{M}_\alpha \equiv \mu_0 \sum_{i=1}^N S_i^\alpha$, which results in the longitudinal magnetic susceptibility

$$\chi_\alpha \equiv \frac{1}{N} \left(\frac{\partial M_\alpha}{\partial B_\alpha} \right) = \frac{\Delta^2(\hat{M}_\alpha)}{NT}. \quad (4)$$

In the notation used above, $\mu_0 = \hbar \gamma_S$ with γ_S being the gyromagnetic ratio for a particle of spin S . In what follows, we shall use the system of units setting to unity the Planck constant $\hbar \equiv 1$.

The specific heat (2), isothermal compressibility (3), or magnetic susceptibility (4) are the examples of the susceptibilities associated with the fluctuations of observables. These thermodynamic characteristics are readily measured in experiments. At the points of phase transitions, the susceptibilities can diverge, since such points are the points of instability. But for the stable equilibrium system, the susceptibilities are always positive and finite for all N , including the thermodynamic limit, when $N \rightarrow \infty$, $V \rightarrow \infty$, so that $\rho \equiv N/V \rightarrow \text{const}$. In principle, it is admissible to imagine the situation, when a phase transition occurs not merely at a point but in a finite region of a thermodynamic variable [7], inside

which region the system remains unstable and displays a divergent susceptibility. Such a case, however, is quite marginal, and rarely, if ever, happens for real statistical systems. In any event, as soon as the phase transition is over, so that the system becomes stable, all susceptibilities go finite.

The following picture summarizes the above consideration. The extensive observables of a statistical system are represented by Hermitian operators. The fluctuations of an observable, represented by an operator \hat{A} , are quantified by the operator dispersion $\Delta^2(\hat{A})$, whose ratio $\Delta^2(\hat{A})/N$ to the total number of particles characterizes the associated susceptibility. For a stable system, the latter must be semipositive and finite, while if it is divergent or negative, the system is unstable. This can be formulated as a *necessary stability condition*

$$0 \leq \frac{\Delta^2(\hat{A})}{N} < \infty. \quad (5)$$

The ratio $\Delta^2(\hat{A})/N$ plays the role of a generalized susceptibility, related to the operator \hat{A} . Examples of condition (5) are the stability conditions on the specific heat (2), isothermal compressibility (3), and magnetic susceptibility (4), according to which

$$0 \leq C_V < \infty, \quad 0 \leq \kappa_T < \infty, \quad 0 \leq \chi_\alpha < \infty. \quad (6)$$

These thermodynamic characteristics are usually strictly positive at finite temperature, becoming zero only at zero temperature.

In this way, the dispersion of the operator \hat{A} , representing an extensive observable, has to be proportional to the number of particles

$$\Delta^2(\hat{A}) \propto N. \quad (7)$$

Then the dispersion is called *thermodynamically normal*. The thermodynamic limit is assumed here, so that $N \gg 1$. When Eq. (7) is not satisfied, so that $\Delta^2(\hat{A}) \propto N^\alpha$ with $\alpha > 1$, the dispersion is called *thermodynamically anomalous*. Respectively, the fluctuations of the related observable, characterized by the dispersion $\Delta^2(\hat{A})$, are termed thermodynamically normal, provided Eq. (7) is valid, and they are named thermodynamically anomalous if Eq. (7) does not hold.

In stable systems, the fluctuations of observables are always normal, and the corresponding susceptibilities are finite. These susceptibilities can be measured in experiment, either directly or through other measurable quantities. For example, the isothermal compressibility can be measured through the sound velocity

$$s^2 \equiv \frac{1}{m} \left(\frac{\partial P}{\partial \rho} \right)_T = \frac{1}{m\rho\kappa_T}, \quad (8)$$

where m is the particle mass. The compressibility can also be found from the central value of the structural factor

$$S(0) = \frac{T}{ms^2} = \rho T \kappa_T. \quad (9)$$

And the structural factor

$$S(\mathbf{k}) = 1 + \rho \int [g(\mathbf{r}) - 1] e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r}, \quad (10)$$

in which $g(\mathbf{r})$ is the pair correlation function, can be measured in scattering experiments.

III. THEOREM ON TOTAL FLUCTUATIONS

In some cases, the operators of observables have the form of the sum

$$\hat{A} = \sum_i \hat{A}_i \quad (11)$$

of self-adjoint terms \hat{A}_i . As has been stressed above, we consider here only extensive observables, such that the statistical average $\langle \hat{A} \rangle$ is proportional to the total number of particles N , when the thermodynamic limit $N \rightarrow \infty$ is implied. All parts \hat{A}_i are assumed to have the same dimension as \hat{A} and also to be the operators of extensive observables, so that $\langle \hat{A}_i \rangle \propto N$. For example, $\hat{A}_1 = \hat{K}$ and $\hat{A}_2 = \hat{W}$ could be kinetic and potential energies for a system of N particles. Then, Eq. (11) would give the Hamiltonian $\hat{H} = \hat{K} + \hat{W}$. Or one can consider the operator of the number of particles $\hat{N} = \hat{N}_0 + \hat{N}_1$ as a sum (11) composed of the operators of condensed particles \hat{N}_0 and of noncondensed particles \hat{N}_1 for a system with a Bose-Einstein condensate. For each of the terms, one may consider partial fluctuations quantified by the dispersions $\Delta^2(\hat{A}_i)$. Then, of the principal interest is the problem how the partial dispersions $\Delta^2(\hat{A}_i)$ are correlated with the total dispersion $\Delta^2(\hat{A})$? For instance, could it be that some of the partial dispersions are thermodynamically anomalous, while the total dispersion remains thermodynamically normal, so that the system as a total stays stable? The answer to such questions is given by the following theorem.

Theorem. Let the operator \hat{A} of an extensive observable quantity be represented as a sum of linearly independent self-adjoint operators \hat{A}_i , being of the same dimension and also representing extensive observables, such that $\langle \hat{A}_i \rangle \propto N$ in the thermodynamic limit. Then, the global dispersion $\Delta^2(\hat{A})$ is thermodynamically anomalous, so that $\Delta^2(\hat{A}) \propto N^\alpha$ with $\alpha > 1$, if and only if at least one of the partial dispersions $\Delta^2(\hat{A}_i)$ is thermodynamically anomalous. The power α in the dependence $\Delta^2(\hat{A}) \propto N^\alpha$, as $N \rightarrow \infty$, is defined by the largest power of all partial dispersions $\Delta^2(\hat{A}_i)$. Conversely, the global dispersion $\Delta^2(\hat{A})$ is thermodynamically normal, such that $\Delta^2(\hat{A}) \propto N$ in the thermodynamic limit, if and only if all partial dispersions $\Delta^2(\hat{A}_i)$ are thermodynamically normal.

Proof. First, let us note that it is meaningful to consider only linearly independent terms in the sum (11), since in the opposite case, when some of the terms are linearly dependent, it is straightforward to express one of them through the others, so that to reduce the number of terms in sum (11). For concreteness, in the following proof, the representatives of

observables are called operators, which assumes the case of a quantum system. Of course, the same argumentation is valid for classical systems as well, for which one just has to replace the term ‘‘operator’’ by the term ‘‘classical random variable.’’

The dispersion for the operator sum (11) can be written as

$$\Delta^2(\hat{A}) = \sum_i \Delta^2(\hat{A}_i) + 2 \sum_{i < j} \text{cov}(\hat{A}_i, \hat{A}_j), \quad (12)$$

where the covariance

$$\text{cov}(\hat{A}_i, \hat{A}_j) \equiv \frac{1}{2} \langle \hat{A}_i \hat{A}_j + \hat{A}_j \hat{A}_i \rangle - \langle \hat{A}_i \rangle \langle \hat{A}_j \rangle \quad (13)$$

is employed. The latter enjoys the symmetry property

$$\text{cov}(\hat{A}_i, \hat{A}_j) = \text{cov}(\hat{A}_j, \hat{A}_i).$$

The dispersions are, by definition, semipositive, while the covariances can be positive as well as negative.

It is sufficient to prove the theorem for the sum of two operators, when

$$\Delta^2(\hat{A}_i + \hat{A}_j) = \Delta^2(\hat{A}_i) + \Delta^2(\hat{A}_j) + 2 \text{cov}(\hat{A}_i, \hat{A}_j). \quad (14)$$

This follows from the simple fact that any sum of terms more than two can always be redefined as a sum of two new terms. We assume that in Eq. (14), where $i \neq j$, both terms are operators but not classical functions. If one of the terms were just a classical function, then we would have a trivial equality

$$\Delta^2(\hat{A}_i + \text{const}) = \Delta^2(\hat{A}_i),$$

with the left-hand and right-hand sides being simultaneously either thermodynamically normal or anomalous.

The elements

$$\sigma_{ij} \equiv \text{cov}(\hat{A}_i, \hat{A}_j), \quad (15)$$

having the properties $\sigma_{ii} = \Delta^2(\hat{A}_i) \geq 0$ and $\sigma_{ij} = \sigma_{ji}$, form the covariance matrix $[\sigma_{ij}]$. This matrix is symmetric. For a set of arbitrary real-valued numbers x_i , with $i = 1, 2, \dots, n$, where n is an integer, one has

$$\left\langle \left[\sum_{i=1}^n (\hat{A}_i - \langle \hat{A}_i \rangle) x_i \right]^2 \right\rangle = \sum_{i,j=1}^n \sigma_{ij} x_i x_j \geq 0. \quad (16)$$

The right-hand side of equality (16) is a semipositive quadratic form. The theory of quadratic forms [8] tells us that a quadratic form is semipositive if and only if all principal minors of its coefficient matrix are non-negative. Thus, the sequential principal minors of the covariance matrix $[\sigma_{ij}]$, with $i, j = 1, 2, \dots, n$, are all non-negative. In particular,

$$\sigma_{ii} \sigma_{jj} - \sigma_{ij} \sigma_{ji} \geq 0.$$

This, because of the symmetry $\sigma_{ij} = \sigma_{ji}$, takes the form

$$\sigma_{ij}^2 \leq \sigma_{ii} \sigma_{jj}.$$

Hence, the correlation coefficient

$$\lambda_{ij} \equiv \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}} \quad (17)$$

possesses the property

$$\lambda_{ij}^2 \leq 1.$$

The equality $\lambda_{ij}^2=1$ holds true if and only if \hat{A}_i and \hat{A}_j are linearly dependent. The sufficient condition is evident, since if $\hat{A}_j=a+b\hat{A}_i$, with a and b being any real numbers, then $\sigma_{ij}=b\sigma_{ii}$ and $\sigma_{jj}=b^2\sigma_{ii}$, thence $\lambda_{ij}=b/|b|$, from where $\lambda_{ij}^2=1$. To prove the necessary condition, let us assume that $\lambda_{ij}^2=1$. Therefore, $\lambda_{ij}=\pm 1$. Let us consider the dispersion

$$\Delta^2\left(\frac{\hat{A}_i}{\sqrt{\sigma_{ii}} \pm \frac{\hat{A}_j}{\sqrt{\sigma_{jj}}}\right) = 2(1 \pm \lambda_{ij}) \geq 0.$$

The value $\lambda_{ij}=1$ is possible then and only then, when

$$\Delta^2\left(\frac{\hat{A}_i}{\sqrt{\sigma_{ii}}} - \frac{\hat{A}_j}{\sqrt{\sigma_{jj}}}\right) = 0.$$

The dispersion can be zero if and only if

$$\frac{\hat{A}_i}{\sqrt{\sigma_{ii}}} - \frac{\hat{A}_j}{\sqrt{\sigma_{jj}}} = \text{const},$$

which implies that the operators \hat{A}_i and \hat{A}_j are linearly dependent. In the same way, the value $\lambda_{ij}=-1$ is possible if and only if

$$\Delta^2\left(\frac{\hat{A}_i}{\sqrt{\sigma_{ii}}} + \frac{\hat{A}_j}{\sqrt{\sigma_{jj}}}\right) = 0.$$

And this is admissible then and only then, when

$$\frac{\hat{A}_i}{\sqrt{\sigma_{ii}}} + \frac{\hat{A}_j}{\sqrt{\sigma_{jj}}} = \text{const},$$

which again means the linear dependence of the operators \hat{A}_i and \hat{A}_j . As far as these operators, by assumption, are linearly independent, one has

$$\lambda_{ij}^2 < 1. \quad (18)$$

This inequality is equivalent to

$$\sigma_{ij}^2 < \sigma_{ii}\sigma_{jj},$$

which, employing notation (15), becomes

$$|\text{cov}(\hat{A}_i, \hat{A}_j)|^2 < \Delta^2(\hat{A}_i)\Delta^2(\hat{A}_j). \quad (19)$$

Now, equality (14) can be represented as

$$\Delta^2(\hat{A}_i + \hat{A}_j) = \sigma_{ii} + \sigma_{jj} + 2\lambda_{ij}\sqrt{\sigma_{ii}\sigma_{jj}}, \quad (20)$$

where, as is shown above, $|\lambda_{ij}| < 1$. Altogether, there can occur no more than four following cases. First, both partial dispersions $\sigma_{ii}=\Delta^2(\hat{A}_i)$ and $\sigma_{jj}=\Delta^2(\hat{A}_j)$ are normal, so that $\sigma_{ii}\propto N$ and $\sigma_{jj}\propto N$. Then, from Eq. (20), it is obvious that the total dispersion $\Delta^2(\hat{A}_i + \hat{A}_j)\propto N$ is also normal. Second, one of

the partial dispersions, say $\sigma_{ii}\propto N$, is normal, but another one is anomalous, $\sigma_{jj}\propto N^\alpha$, with $\alpha > 1$. From Eq. (20), using the inequality $(1+\alpha)/2 < \alpha$, one has $\Delta^2(\hat{A}_i + \hat{A}_j)\propto N^\alpha$. That is, the total dispersion is anomalous, with the same power α as σ_{jj} . Third, both partial dispersions are anomalous, such that $\sigma_{ii}\propto N^{\alpha_i}$ and $\sigma_{jj}\propto N^{\alpha_j}$ with different powers, say $1 < \alpha_i < \alpha_j$. Then Eq. (20), with taking account of the inequality $(\alpha_i + \alpha_j)/2 < \alpha_j$, shows that $\Delta^2(\hat{A}_i + \hat{A}_j)\propto N^{\alpha_j}$. Hence, the total dispersion is also anomalous, with the power α_j of the largest partial dispersion σ_{jj} . Fourth, both partial dispersions are anomalous, $\sigma_{ii}\propto c_i^2 N^\alpha$ and $\sigma_{jj}\propto c_j^2 N^\alpha$, where $c_i > 0$ and $c_j > 0$, with the same power α . In that case, Eq. (20) yields $\Delta^2(\hat{A}_i + \hat{A}_j) = c_{ij} N^\alpha$, where

$$c_{ij} \propto (c_i - c_j)^2 + 2c_i c_j (1 + \lambda_{ij}) > 0,$$

which is strictly positive in view of inequality (18). That is, the total dispersion is anomalous, having the same power α of N as both partial dispersions. After listing all admissible cases, we see that the total dispersion is anomalous if and only if at least one of its partial dispersions is anomalous, with the power of N of the total dispersion being equal to the largest power of partial dispersions. Conversely, the total dispersion is normal if and only if all its partial dispersions are normal. This concludes the proof of the theorem.

This theorem was, first, announced, without proof, in Ref. [9]. The proof, presented above, is rather general, being valid for arbitrary operators and statistical systems. The theorem can be applied to any system. For instance, this can be a multicomponent system, where the index i in Eq. (11) enumerates the components. In recent years, much attention is given to systems with the Bose-Einstein condensate (see review articles [10–12]). The problem of fluctuations in such systems has received a great deal of attention, with a number of papers claiming the existence of anomalous fluctuations everywhere below the condensation point (see discussion in Ref. [13]). In the following sections, the examples of Bose-condensed systems will be considered. In addition to being naturally separated into the condensed and noncondensed parts, Bose systems can also display the coexistence of several coherent topological modes [14–23]. Another possibility is the coexistence of atoms in several internal states, which, e.g., has been studied in collective Raman scattering [24].

IV. IDEAL BOSE GAS

The uniform ideal Bose gas below the condensation temperature is known to exhibit anomalous number-of-particle fluctuations [25,26]. Here, this case will be briefly recalled for the purpose of illustrating the above theorem.

The condensation temperature of the ideal uniform Bose gas is

$$T_c = \frac{2\pi}{m} \left[\frac{\rho}{\zeta(3/2)} \right]^{2/3}, \quad (21)$$

where $\zeta(3/2) \cong 2.612$. Below this temperature, the number-of-particle operator is the sum

$$\hat{N} = \hat{N}_0 + \hat{N}_1 \quad (22)$$

of the terms corresponding to condensed and noncondensed particles, respectively,

$$\hat{N}_0 = a_0^\dagger a_0, \quad \hat{N}_1 = \sum_{k \neq 0} a_k^\dagger a_k,$$

where a_k^\dagger and a_k are the creation and annihilation operators of Bose particles with momentum k .

The dispersion for the total number-of-particle operator \hat{N} can be calculated by means of the derivative over the chemical potential μ , so that

$$\Delta^2(\hat{N}) = T \frac{\partial N}{\partial \mu} \quad (\mu \rightarrow -0). \quad (23)$$

The average number of particles $N = \langle \hat{N} \rangle$ is given by the sum

$$N = N_0 + N_1 \quad (24)$$

of condensed,

$$N_0 \equiv \langle a_0^\dagger a_0 \rangle = (e^{-\beta\mu} - 1)^{-1}, \quad (25)$$

and noncondensed,

$$N_1 \equiv \langle \hat{N}_1 \rangle = \frac{N}{\rho \lambda_T^3} g_{3/2}(e^{\beta\mu}), \quad (26)$$

particles, where $\mu \rightarrow -0$,

$$\lambda_T \equiv \sqrt{\frac{2\pi}{mT}}, \quad \beta \equiv \frac{1}{T},$$

and the Bose-Einstein function is

$$g_n(z) \equiv \frac{1}{\Gamma(n)} \int_0^\infty \frac{z u^{n-1}}{e^u - z} du.$$

Let us stress that the terms \hat{N}_0 and \hat{N}_1 in the sum (23) are linearly independent. Differentiating the sum (24), one has the total dispersion

$$\Delta^2(\hat{N}) = \Delta^2(\hat{N}_0) + \Delta^2(\hat{N}_1), \quad (27)$$

with the partial dispersions

$$\Delta^2(\hat{N}_0) = T \frac{\partial N_0}{\partial \mu}, \quad \Delta^2(\hat{N}_1) = T \frac{\partial N_1}{\partial \mu}.$$

From Eqs. (25) and (26), we find the dispersion for condensed particles,

$$\Delta^2(\hat{N}_0) = N_0(1 + N_0), \quad (28)$$

and for noncondensed particles,

$$\Delta^2(\hat{N}_1) = \frac{N}{\rho \lambda_T^3} g_{1/2}(e^{\beta\mu}), \quad (29)$$

where $\mu \rightarrow -0$. As far as the existence of the Bose-Einstein condensate presupposes that the number of condensed particles N_0 is macroscopic, that is, proportional to N , then from Eq. (28) and the relation $N_0 \propto N \gg 1$, we have $\Delta^2(N_0) \propto N^2$.

Expression (29) in the thermodynamic limit possesses an infrared divergence caused by the integral

$$g_{1/2}(1) \propto \frac{1}{\sqrt{\pi}} \int_{u_{min}}^\infty \frac{du}{u^{3/2}},$$

in which

$$u_{min} = \frac{k_{min}^2}{2mT}, \quad k_{min} \propto \frac{1}{L},$$

with $L \propto V^{1/3}$. Consequently, $g_{1/2}(1) \propto L/\lambda_T$. Thus, dispersion (29) diverges at finite temperatures as

$$\Delta^2(\hat{N}_1) \propto (mT)^2 V^{4/3}. \quad (30)$$

In this way, both dispersions for the number-of-particle operators of condensed as well as noncondensed particles are anomalous

$$\Delta^2(\hat{N}_0) \propto N^2, \quad \Delta^2(\hat{N}_1) \propto N^{4/3}.$$

As a result, the total dispersion (27) is also anomalous, $\Delta^2(\hat{N}) \propto N^2$, with the power of N given by $\Delta^2(\hat{N}_0)$.

The anomalous dispersion $\Delta^2(\hat{N})$ leads, according to Eq. (3), to the divergence of the isothermal compressibility, as $\kappa_T \propto N$, everywhere below T_c , except $T=0$. But the system with a divergent compressibility is not stable. Therefore, the ideal uniform Bose gas below the condensation temperature (21) is a pathological object, being unstable in the whole region $0 < T \leq T_c$. In other words, such a gas does not exist as a stable statistical system [13].

It is worth emphasizing that the anomalous fluctuations of the condensate can be cured by breaking gauge symmetry as will be explained below. However the fluctuations of noncondensed particles remain anomalous, with the dispersion $\Delta^2(N_1) \propto N^{4/3}$ in both ensembles, grand canonical as well as canonical [25,26]. Therefore, the instability of the ideal uniform Bose gas below T_c is not an artifact caused by the choice of an ensemble, but a property peculiar to this system.

V. INTERACTING BOSE GAS

There exists a popular myth that the number-of-particle fluctuations of noncondensed particles in an interacting Bose gas below T_c remain anomalous, corresponding to the dispersion $\Delta^2(\hat{N}_1) \propto N^{4/3}$, of the same type as that for the ideal Bose gas (see discussion in Ref. [13]). If this were true, then according to the theorem of Sec. III, the total dispersion $\Delta^2(\hat{N})$ would also be anomalous, with the power of N not smaller than $\frac{4}{3}$. This would imply that the isothermal compressibility diverges at least as $\kappa_T \propto N^{1/3}$. Hence, the system as a whole would be unstable. In turn, this would mean that there are no stable statistical systems with the Bose-Einstein condensate. Such a conclusion, of course, would be too radical, because of which it is necessary to reconsider the procedure of calculating the number-of-particle dispersions for the Bose-condensed systems.

Let us consider a weakly interacting Bose gas at low temperatures, when the Bogolubov theory [27–29] is applicable.

The main points of this theory are as follows. One starts with the standard Hamiltonian

$$H = \int \psi^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} - \mu \right) \psi(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) d\mathbf{r} d\mathbf{r}' \quad (31)$$

in terms of the Bose field operators $\psi(\mathbf{r})$ and $\psi^\dagger(\mathbf{r})$. The interaction potential is assumed to be symmetric, such that $\Phi(-\mathbf{r}) = \Phi(\mathbf{r})$, and soft, allowing for the Fourier transformation

$$\Phi(\mathbf{r}) = \frac{1}{V} \sum_k \Phi_k e^{i\mathbf{k}\cdot\mathbf{r}}, \quad \Phi_k = \int \Phi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r}.$$

The condensate is separated by means of the Bogolubov shift

$$\psi(\mathbf{r}) = \psi_0 + \psi_1(\mathbf{r}), \quad (32)$$

in which

$$\psi_0 = \frac{a_0}{\sqrt{V}}, \quad \psi_1(\mathbf{r}) = \sum_{k \neq 0} a_k \varphi_k(\mathbf{r}), \quad (33)$$

and, keeping in mind a uniform system, the expansion is over the plane waves $\varphi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$. The gauge symmetry of the Hamiltonian (31) is broken by setting $a_0 = \sqrt{N_0}$. Assuming that $N_0 \approx N$, one omits from the total Hamiltonian the terms of the third and fourth order with respect to the operators a_k of noncondensed particles, where $k \neq 0$. Retaining only the terms up to the second order in a_k , one gets the quadratic Hamiltonian

$$H_2 = \frac{1}{2} N \rho \Phi_0 + \sum_{k \neq 0} \omega_k a_k^\dagger a_k - \mu N + \frac{1}{2} \sum_{k \neq 0} \Delta_k (a_k^\dagger a_{-k}^\dagger + a_{-k} a_k), \quad (34)$$

in which the notation for the quantities

$$\omega_k \equiv \frac{k^2}{2m} + \rho(\Phi_0 + \Phi_k) - \mu \quad (35)$$

and

$$\Delta_k \equiv \rho \Phi_k \quad (36)$$

is employed.

The quadratic Hamiltonian (34) is diagonalized by means of the Bogolubov canonical transformation

$$a_k = u_k b_k + v_{-k}^* b_{-k}^\dagger,$$

in which

$$u_k^2 - v_k^2 = 1, \quad u_k v_k = -\frac{\Delta_k}{2\varepsilon_k},$$

$$u_k^2 = \frac{\sqrt{\varepsilon_k^2 + \Delta_k^2} + \varepsilon_k}{2\varepsilon_k} = \frac{\omega_k + \varepsilon_k}{2\varepsilon_k}, \quad v_k^2 = \frac{\sqrt{\varepsilon_k^2 + \Delta_k^2} - \varepsilon_k}{2\varepsilon_k} = \frac{\omega_k - \varepsilon_k}{2\varepsilon_k},$$

and ε_k is the Bogolubov spectrum

$$\varepsilon_k = \sqrt{\omega_k^2 - \Delta_k^2}. \quad (37)$$

The condensate separation through the Bogolubov shift (32) is meaningful only when the particle spectrum (37) touches zero at $k=0$, which gives

$$\mu = \rho \Phi_0. \quad (38)$$

Thus, one comes to the Bogolubov Hamiltonian

$$H_B = E_0 + \sum_{k \neq 0} \varepsilon_k b_k^\dagger b_k - \mu N, \quad (39)$$

with the ground-state energy

$$E_0 = \frac{1}{2} N \rho \Phi_0 - \frac{1}{2} \sum_{k \neq 0} (\omega_k - \varepsilon_k). \quad (40)$$

Using the chemical potential (38), for the spectrum (35), one has

$$\omega_k = \frac{k^2}{2m} + \rho \Phi_k. \quad (41)$$

With the diagonal Bogolubov Hamiltonian (39), it is easy to find the normal,

$$n_k \equiv \langle a_k^\dagger a_k \rangle, \quad (42)$$

and anomalous,

$$\sigma_k \equiv \langle a_k a_{-k} \rangle, \quad (43)$$

averages. We have

$$n_k = \frac{\omega_k}{2\varepsilon_k} (1 + 2\pi_k) - \frac{1}{2} \quad (44)$$

and

$$\sigma_k = -\frac{\Delta_k}{2\varepsilon_k} (1 + 2\pi_k), \quad (45)$$

where

$$\pi_k \equiv \langle b_k^\dagger b_k \rangle = (e^{\beta\varepsilon_k} - 1)^{-1}. \quad (46)$$

Now, let us turn to investigating the number-of-particle fluctuations. In the Bogolubov approximation, the number-of-particle operators for condensed \hat{N}_0 and noncondensed \hat{N}_1 particles are uncorrelated, so that

$$\langle \hat{N}_0 \hat{N}_1 \rangle = \langle N_0 \rangle \langle \hat{N}_1 \rangle. \quad (47)$$

Hence, their covariance

$$\text{cov}(\hat{N}_0, \hat{N}_1) = 0.$$

Therefore,

$$\Delta^2(\hat{N}) = \Delta^2(\hat{N}_0) + \Delta^2(\hat{N}_1). \quad (48)$$

Calculating the dispersion $\Delta^2(\hat{N}_1)$ for the number-of-particle operator of noncondensed particles

$$\hat{N}_1 = \sum_{k \neq 0} a_k^\dagger a_k,$$

one has to work out the four-operator expression $\langle a_k^\dagger a_k a_q^\dagger a_q \rangle$ or, after involving the Bogolubov canonical transformation, one needs to treat the four-operator terms $\langle b_k^\dagger b_k b_q^\dagger b_q \rangle$. Such four-operator products are reorganized by means of the Wick decoupling, which yields

$$\Delta^2(\hat{N}_1) = \sum_{k \neq 0} \left\{ \left(1 + \frac{2m^2 c_k^4}{\varepsilon_k^2} \right) \pi_k (1 + \pi_k) + \frac{m^2 c_k^4}{2\varepsilon_k^2} \right\}. \quad (49)$$

Here, the notation

$$c_k \equiv \sqrt{\frac{\rho \Phi_k}{m}}$$

for the effective sound velocity is used, which enters the Bogolubov spectrum (37) as

$$\varepsilon_k = \sqrt{(c_k k)^2 + \left(\frac{k^2}{2m} \right)^2}. \quad (50)$$

Replacing in Eq. (49) the summation by integration, one gets an infrared divergence of the type $N \int dk/k^2$. Limiting here the integration by minimal $k_{min} = 1/L$, with $L \propto N^{1/3}$, one gets $\Delta^2(\hat{N}_1) \propto N^{4/3}$, which is anomalous. Remaining in the frame of the discrete wave vectors \mathbf{k} does not save the situation, and the dispersion $\Delta^2(\hat{N}_1)$ stands anomalous. But, as follows from the theorem of Sec. III, the anomalous partial dispersion yields the anomalous total dispersion $\Delta^2(\hat{N})$, which in the present case is evident from Eq. (48). As a result, the compressibility (3) diverges as $\kappa_T \propto N^{1/3}$, which implies the instability of the system as a whole. Thus, one would come to the strange conclusion that stable Bose-condensed systems do not exist.

However, the conclusion on the appearance of anomalous fluctuations in Bose systems, derived from Eq. (49), is not correct. The mistake here is in the following. A basic point of the Bogolubov theory is the contraction of the total Hamiltonian (31) to the quadratic form (34), omitting all terms of the order higher than two with respect to the operators a_k of noncondensed particles. The Bogolubov theory is a *second-order* theory with respect to a_k . Being in the frame of a second-order theory imposes the restriction of keeping only the terms of up to the second order when calculating any physical quantities, and omitting all higher order terms. In working out the dispersion $\Delta^2(\hat{N}_1)$, one meets the fourth-order terms with respect to a_k . Such fourth-order terms are not defined in the second-order approximation. The calculation of the fourth-order expressions in the second-order approximation is not self-consistent, i.e., it is incorrect.

A correct calculation of $\Delta^2(\hat{N})$ in the frame of the Bogolubov theory can be accomplished in the following way. By invoking the relations (3), (9), and (10), we have

$$\Delta^2(\hat{N}) = N \left\{ 1 + \rho \int [g(\mathbf{r}) - 1] d\mathbf{r} \right\}. \quad (51)$$

The pair correlation function is

$$g(\mathbf{r}_{12}) = \frac{1}{\rho^2} \langle \psi^\dagger(\mathbf{r}_1) \psi^\dagger(\mathbf{r}_2) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \rangle, \quad (52)$$

where $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$.

For the field operators, one assumes the Bogolubov shift (32), which taking into account that in the thermodynamic limit the condensate operator ψ_0 becomes a classical number, can be written as

$$\psi(\mathbf{r}) = \eta + \psi_1(\mathbf{r}), \quad (53)$$

where the first term is the Bogolubov order parameter

$$\eta = \langle \psi(\mathbf{r}) \rangle = \langle \psi_0 \rangle, \quad (54)$$

which can be set as $\eta = \sqrt{\rho_0}$, with $\rho_0 \equiv N_0/V$. Here η does not depend on \mathbf{r} for a uniform system under consideration.

The pair correlation function (52) can be simplified by invoking the Wick decoupling. This, however, must be handled with care. A delicate point is that the Wick decoupling and the Bogolubov shift (53) do not commute with each other. In the present context, the Wick decoupling is equivalent to the Hartree-Fock-Bogolubov approximation. The latter does not commute with the Bogolubov shift. Thus, accomplishing, first, the Bogolubov shift in the pair correlation function (52), and then using the Hartree-Fock-Bogolubov approximation for the operators $\psi_1(\mathbf{r})$, or, what is the same, the Wick decoupling for the operators a_k , with $k \neq 0$, we obtain

$$g(\mathbf{r}_{12}) = 1 + \frac{2\rho_0}{\rho^2} \text{Re}[\rho_1(\mathbf{r}_1, \mathbf{r}_2) + \sigma_1(\mathbf{r}_1, \mathbf{r}_2)] + \frac{1}{\rho^2} [|\rho_1(\mathbf{r}_1, \mathbf{r}_2)|^2 + |\sigma_1(\mathbf{r}_1, \mathbf{r}_2)|^2]. \quad (55)$$

Here the Hartree-Fock-Bogolubov approximation for $\psi_1(\mathbf{r})$ is employed, resulting in

$$\langle \psi_1^\dagger(\mathbf{r}_1) \psi_1(\mathbf{r}_1) \psi_1(\mathbf{r}_2) \rangle = 0,$$

because of the condition $\langle \psi_1(\mathbf{r}) \rangle = 0$, and in

$$\langle \psi_1^\dagger(\mathbf{r}_1) \psi_1^\dagger(\mathbf{r}_2) \psi_1(\mathbf{r}_2) \psi_1(\mathbf{r}_1) \rangle = \rho_1^2 + |\rho_1(\mathbf{r}_1, \mathbf{r}_2)|^2 + |\sigma_1(\mathbf{r}_1, \mathbf{r}_2)|^2.$$

The notation is used for the normal average

$$\rho_1(\mathbf{r}_1, \mathbf{r}_2) \equiv \langle \psi_1^\dagger(\mathbf{r}_2) \psi_1(\mathbf{r}_1) \rangle \quad (56)$$

and for the anomalous average

$$\sigma_1(\mathbf{r}_1, \mathbf{r}_2) \equiv \langle \psi_1(\mathbf{r}_2) \psi_1(\mathbf{r}_1) \rangle \quad (57)$$

in the real space. These averages are related, by means of the Fourier transforms

$$\rho_1(\mathbf{r}_1, \mathbf{r}_2) = \int n_k e^{i\mathbf{k} \cdot \mathbf{r}_{12}} \frac{d\mathbf{k}}{(2\pi)^3}, \quad \sigma_1(\mathbf{r}_1, \mathbf{r}_2) = \int \sigma_k e^{i\mathbf{k} \cdot \mathbf{r}_{12}} \frac{d\mathbf{k}}{(2\pi)^3},$$

with the normal and anomalous averages (42) and (43), respectively, in the momentum space.

Note that function (55) possesses the correct limiting behavior

$$\lim_{\mathbf{r}_{12} \rightarrow \infty} g(\mathbf{r}_{12}) = 1.$$

But, if one, first, would make the Hartree-Fock-Bogolubov approximation for the operators $\psi(\mathbf{r})$ and, after this, would

substitute the Bogolubov shift (53), then one would get another correlation function with a wrong limiting behavior, as is explained in the Appendix A. This is because the usage of the Wick decoupling and Hartree-Fock-Bogolubov approximation for the operators, represented as sums of several terms, is correct if and only if all terms in the sum possess the same commutation relations. However, in the Bogolubov shift (53), the field operators $\psi(\mathbf{r})$ and $\psi_1(\mathbf{r})$ do have the same Bose commutation relations, but the term η does not enjoy such relations. Consequently, the proper way of action is to realize, first, the Bogolubov shift (53) and only after this to invoke the Hartree-Fock-Bogolubov approximation for the operators $\psi_1(\mathbf{r})$. The inverse order, as is explained in the Appendix A, is not correct.

For the pair correlation function (55), we find

$$\int [g(\mathbf{r}) - 1] d\mathbf{r} = \frac{2\rho_0}{\rho^2} \lim_{k \rightarrow 0} (n_k + \sigma_k) + \frac{1}{\rho^2} \int (n_k^2 + \sigma_k^2) \frac{d\mathbf{k}}{(2\pi)^3}.$$

In the frame of the Bogolubov theory, we have to set $\rho_0 = \rho$ and to omit the terms of the order higher than two with respect to the operators a_k of noncondensed particles. This means that the terms n_k^2 and σ_k^2 are to be omitted. Therefore, the number-of-particle dispersion (51) in the Bogolubov theory is

$$\Delta^2(\hat{N}) = N[1 + 2 \lim_{k \rightarrow 0} (n_k + \sigma_k)]. \quad (58)$$

Employing Eqs. (44)–(46), we get

$$\lim_{k \rightarrow 0} (n_k + \sigma_k) = \frac{1}{2} \left(\frac{T}{mc^2} - 1 \right),$$

where

$$c \equiv \lim_{k \rightarrow 0} c_k = \sqrt{\frac{\rho\Phi_0}{m}},$$

with

$$\Phi_0 \equiv \lim_{k \rightarrow 0} \Phi_k = \int \Phi(\mathbf{r}) d\mathbf{r}.$$

Then dispersion (58) becomes

$$\Delta^2(\hat{N}) = \frac{T}{mc^2} N, \quad (59)$$

which is, of course, normal, as it should be for a stable system. Respectively, the isothermal compressibility

$$\kappa_T = \frac{\Delta^2(\hat{N})}{\rho TN} = \frac{1}{\rho mc^2} \quad (60)$$

is finite.

According to the theorem of Sec. III, if the total dispersion (59) is normal, then both dispersions of the number-of-particle operators for condensed, $\Delta^2(\hat{N}_0)$, as well as for noncondensed, $\Delta^2(\hat{N}_1)$, particles must be normal. Anomalous fluctuations can arise solely as a result of wrong calculations, when, e.g., one considers the fourth-order terms n_k^2 and σ_k^2 in the second-order Bogolubov theory.

VI. SYSTEMS WITH CONTINUOUS SYMMETRY

It is easy to show that the same fictitious anomalous fluctuations appear, not only for Bose systems, but for arbitrary systems, when one treats the Hamiltonian in the second-order approximation, but intends to calculate fourth-order expressions. This immediately follows from the analysis of susceptibilities for arbitrary systems with continuous symmetry, as has been done by Patashinsky and Pokrovsky [30]. Following Ref. [30], one may consider an operator $\hat{A} = \hat{A}(\varphi)$, which is a functional of a field φ . Let this operator be represented as a sum $\hat{A} = \hat{A}_0 + \hat{A}_1$, where the first term is quadratic in the field φ , so that $\hat{A}_0 \propto \varphi^\dagger \varphi$, while the second term depends on the field fluctuations $\delta\varphi$ as $\hat{A}_1 \propto \delta\varphi^\dagger \delta\varphi$. Let the system Hamiltonian be taken in the hydrodynamic approximation, where only the terms quadratic in the field fluctuations $\delta\varphi$ are retained. The dispersion $\Delta^2(\hat{A}) \propto N\chi$ is proportional to a longitudinal susceptibility χ . The latter is given by the integral $\int C(\mathbf{r}) d\mathbf{r}$ over the correlation function $C(\mathbf{r}) \equiv g(\mathbf{r}) - 1$, with $g(\mathbf{r})$ being the pair correlation function. Calculating $\Delta^2(\hat{A})$, one meets the fourth-order term $\langle \delta\varphi^\dagger \delta\varphi \delta\varphi^\dagger \delta\varphi \rangle$. For the quadratic hydrodynamic Hamiltonian, such fourth-order terms are decoupled by resorting to the Wick theorem. Then one finds

$$C(\mathbf{r}) \propto \frac{1}{r^{2(d-2)}} \quad (61)$$

for any dimensionality $d > 2$. Consequently,

$$\chi \propto \int C(\mathbf{r}) d\mathbf{r} \propto N^{(d-2)/3}$$

for $2 < d < 4$. Hence, the dispersion is

$$\Delta^2(\hat{A}) \propto N\chi \propto N^{(d+1)/3}. \quad (62)$$

For $d=3$, this gives $\Delta^2(\hat{A}) \propto N^{4/3}$, that is, the same anomalous dispersion as $\Delta^2(\hat{N})$ for Bose systems. But this implies that the related susceptibility diverges as $\chi \propto N^{1/3}$, which tells that the considered system is unstable. If this would be correct, it would mean that there are no stable systems with continuous symmetry. For instance, there could not exist magnetic systems, described by the Heisenberg Hamiltonian. Liquid helium also could not exist as a stable system.

The existence or absence of anomalous fluctuations does not depend on the statistical ensemble used. Thus, in the frame of the same calculational procedure, the particle fluctuations are the same, being either anomalous or normal, depending on the chosen procedure, for all ensembles, whether canonical, grand canonical, or microcanonical [31].

It is worth emphasizing that such fictitious anomalous fluctuations arise not just at a phase transition point, which would not be surprising, but everywhere below this point, in the whole region of existence of the considered system. That is, everywhere below the phase transition points such systems would not be stable. As is evident, such a strange conclusion is physically unreasonable. Fortunately, the explanation for the occurrence of anomalous fluctuations is rather

simple: They arise solely due to an incorrect calculational procedure, when the fourth-order terms are treated by a second-order theory, such as the hydrodynamic approximation. No anomalous fluctuations happen, if all calculations are done self-consistently, being defined in the frame of the given approximation.

Another popular way of incorrectly obtaining thermodynamically anomalous particle fluctuations for systems with continuous symmetry is as follows. One uses the representation

$$\psi(\mathbf{r}) = e^{i\hat{\phi}(\mathbf{r})\sqrt{\hat{n}(\mathbf{r})}} \quad (63)$$

for the field operator, in which $\hat{n}(\mathbf{r}) \equiv \psi^\dagger(\mathbf{r})\psi(\mathbf{r})$ is the operator of particle density and $\hat{\phi}(\mathbf{r})$ is the phase operator. The latter is assumed to be Hermitian in order to preserve the correct definition of the density operator,

$$\psi^\dagger(\mathbf{r})\psi(\mathbf{r}) = \sqrt{\hat{n}(\mathbf{r})}e^{-i\hat{\phi}(\mathbf{r})+i\hat{\phi}(\mathbf{r})}\sqrt{\hat{n}(\mathbf{r})} = \hat{n}(\mathbf{r}).$$

It is easy to show that from the representation (63), it follows that the density and phase operators are canonically conjugated, satisfying the commutation relation

$$[\hat{n}(\mathbf{r}), \hat{\phi}(\mathbf{r}')] = i\delta(\mathbf{r} - \mathbf{r}').$$

For the first-order correlation function, one has

$$\langle \psi^\dagger(\mathbf{r})\psi(0) \rangle = \langle \sqrt{\hat{n}(\mathbf{r})}\hat{n}(0)\exp\{-i[\hat{\phi}(\mathbf{r}) - \hat{\phi}(0)]\} \rangle.$$

Then one assumes that the temperature is asymptotically low, $T \rightarrow 0$, such that there are no density fluctuations, and one can replace the operator $\hat{n}(\mathbf{r})$ by its average $\rho(\mathbf{r}) \equiv \langle \hat{n}(\mathbf{r}) \rangle$. This is equivalent to the usage, instead of the representation (63), of the representation

$$\psi(\mathbf{r}) = \sqrt{\rho(\mathbf{r})}e^{i\hat{\phi}(\mathbf{r})}. \quad (64)$$

One also supposes that the phase fluctuations are very small, so that one can employ the following averaging:

$$\langle \exp\{-i[\hat{\phi}(\mathbf{r}) - \hat{\phi}(0)]\} \rangle = \exp\left\{-\frac{1}{2}\langle [\hat{\phi}(\mathbf{r}) - \hat{\phi}(0)]^2 \rangle\right\}. \quad (65)$$

As a result, the first-order correlation function reduces to

$$\langle \psi^\dagger(\mathbf{r})\psi(0) \rangle = \rho(\mathbf{r})\exp\left\{-\frac{1}{2}\langle [\hat{\phi}(\mathbf{r}) - \hat{\phi}(0)]^2 \rangle\right\}.$$

Treating $\hat{\phi}(\mathbf{r})$ as a small quantity, one also expands the exponentials in powers of $\hat{\phi}(\mathbf{r})$. Similarly, one treats the second-order correlation functions. Finally, one comes to the same expressions as in Eqs. (61) and (62), with the thermodynamically anomalous fluctuations, $\Delta^2(\hat{N}_1) \propto N^{4/3}$, for the three-dimensional space.

The main mistake in such calculations is the same as has been made above. All calculations have been based on the assumption that both the density and phase fluctuations are rather weak, so that the hydrodynamic approximation could be invoked. The latter implies that all statistical averages are treated in the hydrodynamic approximation, with a Hamiltonian quadratic in the operators. For instance, it is well

known [32] that Eq. (65) is valid solely for quadratic Hamiltonians. For finding $\Delta^2(\hat{N}_1)$, one needs to consider the fourth-order terms in phase operators. Of course, there is no sense in calculating the fourth-order terms in the frame of a second-order theory, such as the hydrodynamic approximation.

Moreover, the representations (63) and (64), as such, are principally incorrect. This is shown in the Appendix B. A correct definition of the phase operator requires a much more elaborate technique, as can be inferred from the review articles [33–36]. Since the representations (63) and (64), actually, do not exist, all conclusions derived on their basis, even involving no further approximations, are not reliable.

VII. BREAKING OF GAUGE SYMMETRY

In Sec. IV, considering the ideal uniform Bose gas, we found that its particle fluctuations are thermodynamically anomalous, with the corresponding dispersion $\Delta^2(\hat{N}) \propto N^2$. This anomaly is due to the condensate fluctuations, since $\Delta^2(\hat{N}_0) \propto N^2$. Really, for an ideal uniform gas, one has

$$\Delta^2(\hat{N}) = \sum_k n_k(1 + n_k). \quad (66)$$

From here, separating the terms with $\mathbf{k}=0$ and $\mathbf{k} \neq 0$, we get

$$\Delta^2(\hat{N}_0) = N_0(1 + N_0), \quad \Delta^2(\hat{N}_1) = \sum_{k \neq 0} n_k(1 + n_k).$$

Since $N_0 \propto N$, we find $\Delta^2(\hat{N}_0) \propto N^2$.

The situation can be made even more dramatic by generalizing it to the case of interacting particles. To this end, let us consider an interacting system that can be treated by perturbation theory starting with a mean-field approximation, such as the Hartree-Fock approximation. In the frame of the latter, the particle dispersion can be shown [37] to have the same form as in Eq. (66). Then, irrespectively of the concrete expression for the momentum distribution of particles n_k , the global dispersion $\Delta^2(\hat{N})$ will be thermodynamically anomalous because of the anomalous term $\Delta^2(\hat{N}_0) \propto N^2$. Hence, one could conclude that all systems with the Bose-Einstein condensate would be unstable.

One often states that the appearance of this anomaly is the defect of the grand canonical ensemble. However, this is not correct. As is mentioned in Sec. IV, the anomalous condensate fluctuations are fictitious and can be removed by breaking the gauge symmetry.

Hohenberg and Martin [38] noticed that the appearance of such fictitious divergences is a common feature of theories possessing gauge symmetry, but breaking the latter would eliminate the divergences resulting from the condensate fluctuations. Ter Haar [25] showed explicitly how the anomalous condensate fluctuations can be removed after breaking the gauge symmetry for an ideal uniform Bose gas. In the present section, we demonstrate that, in general, the gauge-symmetry breaking eliminates the anomalous condensate fluctuations for arbitrary systems, whether interacting or not.

A known method for lifting a system symmetry of any nature is the method of infinitesimal sources, introduced by

Bogolubov [29,39]. There are also several other methods of symmetry breaking, as is reviewed in Ref. [40]. In the case of gauge symmetry, one has to be cautious by choosing the way of its breaking. The standard method of infinitesimal sources may not always lead to the desired symmetry breaking, as is shown by a counterexample in the Appendix C.

To break the gauge symmetry in a Bose system, one has to resort to the Bogolubov shift [29,39]. The latter, keeping in mind the most general statistical system, whether equilibrium or nonequilibrium, uniform or nonuniform, writes as

$$\psi(\mathbf{r}, t) = \eta(\mathbf{r}, t) + \psi_1(\mathbf{r}, t), \quad (67)$$

where t is time. The first term here is the condensate wave function, assumed to be not identically zero in the presence of the Bose-Einstein condensate. The second term in Eq. (67) is the field operator of noncondensed particles, satisfying the same Bose commutation relations as $\psi(\mathbf{r}, t)$. The correct separation of condensed and noncondensed particles presupposes the orthogonality condition

$$\int \eta^*(\mathbf{r}, t) \psi_1(\mathbf{r}, t) d\mathbf{r} = 0, \quad (68)$$

which excludes the double counting of the degrees of freedom. In what follows, just for brevity, we shall write $\psi(\mathbf{r})$ instead of $\psi(\mathbf{r}, t)$, understanding that, generally, the time variable t does enter the dependence of the field operator, $\psi(\mathbf{r}) = \psi(\mathbf{r}, t)$.

For the theory of Bose systems, it is extremely important to specify the spaces of states, which the field operators are defined on. Thus, the field operators $\psi(\mathbf{r})$ and $\psi^\dagger(\mathbf{r})$ are defined on the Fock space $\mathcal{F}(\psi)$ generated by the operator $\psi^\dagger(\mathbf{r})$. This means the following [41]: There exists a vacuum state $|0\rangle$, for which

$$\psi(\mathbf{r})|0\rangle = 0. \quad (69)$$

The Fock space $\mathcal{F}(\psi)$ is the space of all states

$$\varphi = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \int f_n(\mathbf{r}_1, \dots, \mathbf{r}_n) \prod_{i=1}^n \psi^\dagger(\mathbf{r}_i) d\mathbf{r}_i |0\rangle,$$

in which $f_n(\mathbf{r}_1, \dots, \mathbf{r}_n)$ is a square-integrable function symmetric with respect to the permutation of any pair of its variables.

It is easy to notice that the state $|0\rangle$, which is a vacuum state for $\psi(\mathbf{r})$, is not a vacuum for $\psi_1(\mathbf{r})$, since

$$\psi_1(\mathbf{r})|0\rangle = -\eta(\mathbf{r})|0\rangle \neq 0.$$

Consequently, there should exist another state $|0\rangle_1$ satisfying the condition

$$\psi_1(\mathbf{r})|0\rangle_1 = 0, \quad (70)$$

being a vacuum for $\psi_1(\mathbf{r})$. In turn, the state $|0\rangle_1$, which is a vacuum for $\psi_1(\mathbf{r})$, is not a vacuum for $\psi(\mathbf{r})$, as far as

$$\psi(\mathbf{r})|0\rangle_1 = \eta(\mathbf{r})|0\rangle_1 \neq 0.$$

The Bogolubov shift (67) is a particular case of canonical transformations [42]. The operators $\psi(\mathbf{r})$ and $\psi_1(\mathbf{r})$ can be connected with each other by means of the transformation

$$\hat{C} \equiv \exp \left\{ \int [\eta^*(\mathbf{r})\psi(\mathbf{r}) - \eta(\mathbf{r})\psi^\dagger(\mathbf{r})] d\mathbf{r} \right\} \quad (71)$$

and its inverse

$$\hat{C}^{-1} = \exp \left\{ - \int [\eta^*(\mathbf{r})\psi(\mathbf{r}) - \eta(\mathbf{r})\psi^\dagger(\mathbf{r})] d\mathbf{r} \right\}. \quad (72)$$

Using these transformations, one has

$$\psi(\mathbf{r}) = \hat{C} \psi_1(\mathbf{r}) \hat{C}^{-1} \quad (73)$$

and

$$\psi_1(\mathbf{r}) = \hat{C}^{-1} \psi(\mathbf{r}) \hat{C}. \quad (74)$$

Then it becomes clear that the vacuum for $\psi_1(\mathbf{r})$ is

$$|0\rangle_1 = \hat{C}^{-1} |0\rangle. \quad (75)$$

The vacua $|0\rangle$ and $|0\rangle_1$ are mutually orthogonal. This can be shown by employing the Baker-Hausdorff formula, which for two operators \hat{A} and \hat{B} , whose commutator $[\hat{A}, \hat{B}]$ is proportional to the unity operator, reads as

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} \exp \left(- \frac{1}{2} [\hat{A}, \hat{B}] \right).$$

Using this for transformation (72), we have

$$\begin{aligned} \hat{C}^{-1} = & \exp \left\{ \int \eta(\mathbf{r})\psi^\dagger(\mathbf{r}) d\mathbf{r} \right\} \exp \left\{ - \int \eta^*(\mathbf{r})\psi(\mathbf{r}) d\mathbf{r} \right\} \\ & \times \exp \left\{ - \frac{1}{2} \int |\eta(\mathbf{r})|^2 d\mathbf{r} \right\}. \end{aligned} \quad (76)$$

Acting on the vacuum $|0\rangle$, we find

$$\hat{C}^{-1} |0\rangle = \exp \left\{ - \frac{1}{2} \int |\eta(\mathbf{r})|^2 d\mathbf{r} \right\} \exp \left\{ \int \eta(\mathbf{r})\psi^\dagger(\mathbf{r}) d\mathbf{r} \right\} |0\rangle. \quad (77)$$

This is nothing but the coherent state [43], being the eigenstate of the destruction operator,

$$\psi(\mathbf{r})|\eta\rangle = \eta(\mathbf{r})|\eta\rangle, \quad (78)$$

and having in the coordinate representation [44] the form

$$|\eta\rangle = \eta_0 \exp \left\{ \int \eta(\mathbf{r})\psi^\dagger(\mathbf{r}) d\mathbf{r} \right\} |0\rangle, \quad (79)$$

with the normalization factor

$$|\eta_0| = \exp \left\{ - \frac{1}{2} \int |\eta(\mathbf{r})|^2 d\mathbf{r} \right\}.$$

Respectively, the condensate wave function

$$\eta(\mathbf{r}) = \langle \eta | \psi(\mathbf{r}) | \eta \rangle$$

is nothing but the coherent field related to the coherent state $|\eta\rangle$.

In this way, the vacuum (75) is the coherent state (79),

$$|0\rangle_1 = \hat{C}^{-1}|0\rangle = |\eta\rangle. \tag{80}$$

The scalar product of the vacua $|0\rangle$ and $|0\rangle_1$ is

$$\langle 0|0\rangle_1 = \langle 0|\eta\rangle = \exp\left\{-\frac{1}{2}\int |\eta(\mathbf{r})|^2 d\mathbf{r}\right\}. \tag{81}$$

By its definition, the condensate wave function gives the condensate density

$$\rho_0(\mathbf{r}) \equiv |\eta(\mathbf{r})|^2. \tag{82}$$

The number of condensed particles

$$N_0 = \int \rho_0(\mathbf{r}) d\mathbf{r}, \tag{83}$$

in the presence of the condensate, is not zero, but is macroscopic in the sense that $N_0 \propto N \rightarrow \infty$. Therefore, the scalar product

$$\langle 0|0\rangle_1 = \exp\left(-\frac{1}{2}N_0\right) \tag{84}$$

becomes zero in the thermodynamic limit,

$$\langle 0|0\rangle_1 \approx 0 \quad (N \rightarrow \infty). \tag{85}$$

This tells that the vacua $|0\rangle$ and $|0\rangle_1$ are asymptotically orthogonal. The Fock spaces $\mathcal{F}(\psi)$ and $\mathcal{F}(\psi_1)$, generated from the related vacua, are orthogonal to each other, except just the sole state $|0\rangle_1 = |\eta\rangle$, which is the vacuum for $\mathcal{F}(\psi_1)$ and the coherent state, defined by Eq. (78), in $\mathcal{F}(\psi)$. However, having the sole common state for two infinite-dimensional spaces means the intersection of zero measure. Moreover, the influence of this intersection is eliminated by means of the orthogonality condition (68).

Thus, there are two different vacua $|0\rangle$ and $|0\rangle_1$ and two mutually orthogonal Fock spaces $\mathcal{F}(\psi)$ and $\mathcal{F}(\psi_1)$, generated by the field operators ψ^\dagger and ψ_1^\dagger , respectively. The operator (71) transforms $\mathcal{F}(\psi_1)$ into $\mathcal{F}(\psi)$, while the operator (72) transforms $\mathcal{F}(\psi)$ into $\mathcal{F}(\psi_1)$. There is no self-adjoint operator \hat{C}^+ that would be defined on the same space as \hat{C} . Therefore, the operator \hat{C} is nonunitary and the transformations (73) and (74) cannot be treated as unitary. The field operators ψ and ψ_1 are defined on different spaces. One says that such operators realize unitary nonequivalent operator representations of canonical commutation relations [45].

Breaking the gauge symmetry by the Bogolubov shift (67), one, actually, passes from the Fock space $\mathcal{F}(\psi)$ to the space $\mathcal{F}(\psi_1)$. Since the left-hand and right-hand sides of Eq. (67) are defined on different spaces, this equation should be understood as a transformation

$$\psi(\mathbf{r}) \rightarrow \eta(\mathbf{r}) + \psi_1(\mathbf{r}).$$

Separating the zero-momentum mode for a uniform Bose gas, with replacing this term by a nonoperator quantity,

$$\psi_0 = \frac{a_0}{\sqrt{V}} \rightarrow \sqrt{\rho_0},$$

as has been done in Sec. V, is mathematically equivalent to the Bogolubov shift [46]. The representation of the operators of observables, expressed through the field operators ψ_1 , and defined on the Fock space $\mathcal{F}(\psi_1)$, can be called the Bogolubov representation.

In the Bogolubov representation, the operator of condensed particles, according to Eqs. (82) and (83), is a non-operator quantity, $\hat{N}_0 = N_0$. Hence, the dispersion of the latter is zero, $\Delta^2(N_0) = 0$. Consequently, the dispersion of the total number-of-particle operator

$$\Delta^2(\hat{N}) = \Delta^2(\hat{N}_1)$$

is completely defined by the dispersion of the operator \hat{N}_1 of noncondensed particles. Thus, the anomalous N^2 dispersion of the condensate particles is removed in the Bogolubov representation.

Considering the ideal uniform Bose gas of Sec. IV in the Bogolubov representation, we do not meet the N^2 -anomalous condensate fluctuations. Nevertheless, particle fluctuations, characterized by the dispersion $\Delta^2(\hat{N}_1) \propto N^{4/3}$, remain thermodynamically anomalous. That is, this gas, anyway, is unstable. This conclusion does not depend on whether the grand canonical or canonical ensemble has been used. Of course, in the latter, where the total number of particles is fixed, the related dispersion is not defined. However, one can calculate the compressibility

$$\kappa_T = -\frac{1}{V} \left(\frac{\partial P}{\partial V} \right)_{TN}^{-1} = \frac{1}{V} \left(\frac{\partial^2 F}{\partial V^2} \right)_{TN}^{-1},$$

where F is free energy. For the ideal uniform Bose gas below T_c , one has [2] $\partial P / \partial V = 0$, hence, $\kappa_T \rightarrow \infty$, which implies instability. The latter is an intrinsic feature of the uniform ideal Bose gas [13]. Including particle interactions stabilizes the gas, as is shown in Sec. V. The ideal Bose gas can also be stabilized by trapping it in an external confining potential, such as the harmonic potential [47,48], though not all power-law potentials are able to stabilize the system [49].

The message of this section is that accurately defining the symmetry properties of the given system helps to avoid the appearance of unphysical instabilities. Although there also exist systems, such as the ideal uniform Bose-condensed gas, which are intrinsically unstable.

VIII. NOTION OF REPRESENTATIVE ENSEMBLES

The consideration of Sec. VII demonstrates the importance of accurately defining the system under investigation. It is not sufficient to chose a statistical ensemble, but often it is also necessary to formulate additional conditions specifying the features of the given system, thus, avoiding the appearance of spurious instabilities. For instance, one can take the grand canonical ensemble without breaking the gauge symmetry or one may employ the grand canonical ensemble with the gauge symmetry breaking. This means that, in gen-

eral, there may exist not just the sole grand canonical ensemble or the sole canonical one, but there can exist several such ensembles. This problem of the ensemble nonuniqueness is just another way of formulating the problem of the nonuniqueness of the Fock space and of the existence of unitary nonequivalent operator representations, which is explained in Sec. VII.

Thus, for the correct description of a physical system, it is necessary to equip the chosen statistical ensemble by additional conditions required for accurately taking account of the system features. Only such an equipped ensemble will correctly represent the considered system, that is, will be a *representative ensemble*.

The idea of the representative ensembles goes back to Gibbs himself [50], who mentioned the necessity of taking into account all additional information known about the considered system, such as the system symmetry, the existence of integrals of motion, and so on. The importance of employing representative ensembles for an adequate description of statistical systems was emphasized by ter Haar [51,52]. A detailed discussion of mathematical techniques, required for the correct definition of representative ensembles, can be found in the review papers [40,53]. In the language of reduced density matrices, the latter have to satisfy specific constraints in order to correctly represent a given statistical system [54].

Systems, exhibiting Bose-Einstein condensation, serve as a very good example demonstrating the importance of taking into account their specific features in order to correctly describe their behavior. Rich properties of these systems are required to be very attentive in formulating the corresponding representative ensemble. Forgetting to impose the appropriate constraints, specifying the system properties, may lead to self-inconsistent calculations and the appearance of spurious instabilities. In Sec. V, the example was given of a weakly interacting equilibrium uniform Bose gas. Now, we shall formulate a general approach to Bose systems with arbitrarily strong interactions, being, in general, nonuniform and not necessarily equilibrium. We shall stress the constraints that are compulsory for defining a self-consistent theory, which, for equilibrium systems, results in a representative ensemble, free of fictitious instabilities.

First of all, as is explained in Sec. VII, we have to break the gauge symmetry by means of the Bogolubov shift, replacing the field operator $\psi(\mathbf{r}, t)$, acting in the Fock space $\mathcal{F}(\psi)$, by the operator

$$\tilde{\psi}(\mathbf{r}, t) \equiv \eta(\mathbf{r}, t) + \psi_1(\mathbf{r}, t), \quad (86)$$

defined on the Fock space $\mathcal{F}(\psi_1)$. In what follows, we shall again omit the time variable in order to simplify the notation. The first term in the right-hand side of Eq. (86) is the condensate wave function and the second term is the field operator of noncondensed particles. The replacement $\psi(\mathbf{r}) \rightarrow \tilde{\psi}(\mathbf{r})$ yields to the passage from the operator representation on the Fock space $\mathcal{F}(\psi)$ to the unitary nonequivalent operator representation, the Bogolubov representation, on the space $\mathcal{F}(\psi_1)$ only if the condensate wave function $\eta(\mathbf{r}, t)$ is not identically zero.

The energy operator has now to be expressed through the field operators (86), which yield the Hamiltonian

$$\hat{H} = \int \tilde{\psi}^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U \right) \tilde{\psi}(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \tilde{\psi}^\dagger(\mathbf{r}) \tilde{\psi}^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \tilde{\psi}(\mathbf{r}') \tilde{\psi}(\mathbf{r}) d\mathbf{r} d\mathbf{r}', \quad (87)$$

in which $U=U(\mathbf{r}, t)$ is an external field. The corresponding Lagrangian is

$$\hat{L} \equiv \int \tilde{\psi}^\dagger(\mathbf{r}) i \frac{\partial}{\partial t} \tilde{\psi}(\mathbf{r}) d\mathbf{r} - \hat{H}. \quad (88)$$

It is important to stress that contrary to a system without condensate, where there is just one field operator variable ψ , in a Bose-condensed system, there appear two variables η and ψ_1 or one can take as two variables η and $\tilde{\psi}$. The condensate wave function defines the condensate density (82). The operator of the total number of particles

$$\hat{N} = \int \tilde{\psi}^\dagger(\mathbf{r}) \tilde{\psi}(\mathbf{r}) d\mathbf{r} \quad (89)$$

is expressed through $\tilde{\psi}$. Respectively, there are two normalization conditions. One condition is for the condensate wave function normalized to the number of condensed particles

$$N_0 = \int |\eta(\mathbf{r})|^2 d\mathbf{r}. \quad (90)$$

And another normalization condition is for $\tilde{\psi}$ normalized to the total number of particles $N = \langle \hat{N} \rangle$, i.e.,

$$N = \int \langle \tilde{\psi}^\dagger(\mathbf{r}) \tilde{\psi}(\mathbf{r}) \rangle d\mathbf{r}. \quad (91)$$

Here and everywhere in this section, the angle brackets imply the averaging over the Fock space $\mathcal{F}(\psi_1)$.

Hamiltonian (87), with the field operator (86), contains the terms linear in ψ_1 , because of which the average $\langle \psi_1 \rangle$ may be nonzero. However, a nonzero $\langle \psi_1 \rangle$ would, in general, lead to the nonconservation of quantum numbers, such as spin and momentum, which would be unphysical. Therefore, it is necessary to impose the constraint for the conservation of quantum numbers,

$$\langle \psi_1(\mathbf{r}) \rangle = 0. \quad (92)$$

In this way, three conditions are to be valid for a Bose-condensed system, two normalization conditions (90) and (91), and the quantum-number conservation constraint (92).

The most general procedure of deriving the equations of motion is by looking at the extrema of the action, under the given additional conditions. In our case, the effective action is

$$A[\eta, \psi_1] = \int (\hat{L} + \mu_0 N_0 + \mu \hat{N} + \hat{\Lambda}) dt. \quad (93)$$

Here, \hat{L} is the Lagrangian (88). The second and third terms in the integral (93) preserve the normalization conditions (90) and (91). And the role of the term

$$\hat{\Lambda} \equiv \int [\lambda(\mathbf{r}) \psi_1^\dagger(\mathbf{r}) + \lambda^*(\mathbf{r}) \psi_1(\mathbf{r})] d\mathbf{r} \quad (94)$$

is to satisfy the quantum-number conservation constraint (92). The Lagrange multipliers $\lambda(\mathbf{r})$ have to be chosen so that to cancel, in Eq. (87), the terms linear in ψ_1 . The absence of such linear terms in the Hamiltonian, as is known [42], is necessary and sufficient for the validity of condition (92). By introducing the effective grand Hamiltonian

$$H[\eta, \psi_1] \equiv \hat{H} - \mu_0 N_0 - \mu \hat{N} - \hat{\Lambda} \quad (95)$$

and the resulting Lagrangian

$$L[\eta, \psi_1] = \int \left[\eta^*(\mathbf{r}) i \frac{\partial}{\partial t} \eta(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}) i \frac{\partial}{\partial t} \psi_1(\mathbf{r}) \right] d\mathbf{r} - H[\eta, \psi_1], \quad (96)$$

the effective action (93) can be rewritten as

$$A[\eta, \psi_1] = \int L[\eta, \psi_1] dt. \quad (97)$$

According to the standard prescription, the equations of motion are obtained from the variational principle determining the extremum of the action functional (97). These variational equations are

$$\frac{\delta A[\eta, \psi_1]}{\delta \eta^*(\mathbf{r}, t)} = 0, \quad (98)$$

where, for generality, the time variable is written explicitly, and

$$\frac{\delta A[\eta, \psi_1]}{\delta \psi_1^\dagger(\mathbf{r}, t)} = 0. \quad (99)$$

From Eqs. (95)–(97), it follows that Eqs. (98) and (99) are identical to the variational equations

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \frac{\delta H[\eta, \psi_1]}{\delta \eta^*(\mathbf{r}, t)}, \quad (100)$$

with the effective grand Hamiltonian (95), and

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \frac{\delta H[\eta, \psi_1]}{\delta \psi_1^\dagger(\mathbf{r}, t)}. \quad (101)$$

Explicitly, Eq. (100) is

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left(-\frac{\nabla^2}{2m} + U - \varepsilon \right) \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') [|\eta(\mathbf{r}')|^2 \eta(\mathbf{r}) + \hat{X}(\mathbf{r}, \mathbf{r}')] d\mathbf{r}', \quad (102)$$

where $\varepsilon \equiv \mu_0 + \mu$ and again, for short, the time dependence is omitted. Equation (101) yields

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \left(-\frac{\nabla^2}{2m} + U - \mu \right) \psi_1(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \times [|\eta(\mathbf{r}')|^2 \psi_1(\mathbf{r}) + \eta^*(\mathbf{r}') \eta(\mathbf{r}) \psi_1(\mathbf{r}') + \eta(\mathbf{r}') \eta(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') + \hat{X}(\mathbf{r}, \mathbf{r}')] d\mathbf{r}'. \quad (103)$$

Here the notation

$$\hat{X}(\mathbf{r}, \mathbf{r}') \equiv \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \eta(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}') \eta(\mathbf{r}') \psi_1(\mathbf{r}) + \eta^*(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \quad (104)$$

is used. Averaging Eq. (102), we obtain the equation for the condensate wave function

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left(-\frac{\nabla^2}{2m} + U - \varepsilon \right) \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') [\rho(\mathbf{r}') \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') + \langle \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle] d\mathbf{r}', \quad (105)$$

in which the total density of particles

$$\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \rho_1(\mathbf{r})$$

is the sum of the condensate density (82) and of the density of noncondensed particles

$$\rho_1(\mathbf{r}) \equiv \langle \psi_1^\dagger(\mathbf{r}) \psi_1(\mathbf{r}) \rangle;$$

also, the notation is used for the normal density matrix

$$\rho_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}) \rangle,$$

and the so-called anomalous density matrix

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

which is nonzero because of the broken gauge symmetry.

It is not our goal to study here particular consequences of the approach sketched above. The sole aim of the example of this section is to illustrate the way of constructing a representative ensemble for a rather nontrivial system. This is done by accurately specifying the basic system properties, such as the broken gauge symmetry, normalization conditions, and the quantum-number conservation condition. Following the most general procedure of action variation, under the specified conditions, one automatically obtains an effective Hamiltonian and the related exact equations of motion. It is possible to show [37] that the latter guarantee the correct behavior for the spectrum of collective excitations, the validity of all conservation laws, and the absence of unphysical instabilities.

It may happen in some lower-order approximations that there is no need to invoke all of the conditions discussed above. This, for instance, occurs in the Bogolubov approximation of Sec. IV. In this approximation, one assumes that $N_0 \rightarrow N$, hence $\mu_0 \rightarrow 0$. Also, for a uniform gas, the Hamiltonian term of the first order in ψ_1 vanishes itself, while the terms of the third and fourth order in ψ_1 are neglected in the Bogolubov second-order approximation. Because of this, there is no necessity of introducing the term (94). However, all these conditions are to be taken into account when going to higher-order approximations. In the other case, the defined ensemble may occur to be nonrepresentative, which can result in physical inconsistencies and fictitious instabilities.

Correctly defining a representative ensemble is also crucially important for the problem of equivalence of statistical ensembles, which is discussed in Sec. IX.

IX. PROBLEM OF ENSEMBLE EQUIVALENCE

The examples of the previous sections show that the stability properties of a system can be different in different ensembles. More generally, the same physical quantity may be different, being calculated in two different ensembles. Does this mean the failure of the basic principle of statistical mechanics, stating the equivalence of ensembles for large systems? This question is analyzed in the present section.

First of all, let us stress that, as is clear from the previous sections, a physical system and a describing ensemble do not exist separately, but they are intimately connected. A correct formulation of an ensemble does presuppose that it includes the information on the main system features. An ensemble, which is adequate for the given physical system, is only that, which properly represents the system, that is, a *representative ensemble*. But if there are two representative ensembles for the same system, then, by their definition, they must yield identical results for the same physical quantities. In the other case, at least one of these ensembles does not correctly describe the system, hence, is not representative. Also, in the case of equilibrium, it is meaningful to talk only about stable systems, as far as an unstable system cannot be in absolute equilibrium. Thus, in terms of representative ensembles, the following statement is straightforward: *Two ensembles are equivalent if and only if both of them are representative for the given stable system*. Conversely, when two ensembles are not equivalent, then at least one of them is not representative. An ensemble that is not representative for the given system may be representative for some other system. However, there is not any reason to require that two ensembles applied to two different physical systems be equivalent. Ensemble non-equivalence, vaguely formulated, is a rather artificial non-physical problem caused by an improper usage of ensembles not representing the considered system.

To be more correct, let us recall that, generally, one distinguishes two types of ensemble equivalence—thermodynamic and statistical. In thermodynamics, a physical system is characterized by thermodynamic potentials, each of which is a function of its natural thermodynamic variables [1–7]. The system is stable, when thermodynamic potentials enjoy the property of convexity or concavity with

respect to the appropriate variables. The thermodynamic potentials, expressed through different thermodynamic variables, are connected with each other by Legendre transforms [1–7]. All thermodynamic characteristics are defined as derivatives of thermodynamic potentials. When the latter are connected by Legendre transforms and correspond to a stable (in the sense of the convexity or concavity property of the potentials) system, then the thermodynamic characteristics, calculated in different ensembles, coincide with each other. Summarizing, the concept of thermodynamic equivalence can be formulated as follows:

Thermodynamic equivalence. Two ensembles, representing a stable physical system, are thermodynamically equivalent if and only if their thermodynamic potentials are mutually connected by Legendre transforms.

A rigorous proof of this statement for the case of the macrocanonical and canonical ensembles can be found in Refs. [55,56]. Several examples of systems with long-range interactions have been considered, whose microcanonical entropy is not a concave function of energy [55–58]. The internal energy of such systems, though being nonadditive, can be made extensive by means of the Kac-Uhlenbeck-Hemmer normalization [59] yielding a well-defined thermodynamic limit. The canonical free energy is a concave function of inverse temperature, but the microcanonical entropy is not a concave function of energy. This does not allow us to use the Legendre transform in both directions [55,56]. The nonconcavity of the microcanonical entropy results in the appearance, for some range of energies, of negative specific heat, while in the canonical ensemble, specific heat is always positive. Because of this, one tells that, for such models with long-range interactions, the microcanonical and canonical ensembles are not equivalent. However, a microcanonical ensemble with a nonconcave entropy does not represent a stable physical system, i.e., this ensemble is not representative. As is explained above, there is no sense to compare nonrepresentative ensembles, which are not obliged to be equivalent. To make the microcanonical ensemble representative, it must be complimented by the concavity construction rendering stability again. After this, it becomes representative and completely equivalent to the canonical ensemble.

Nonconcave microcanonical entropy and negative specific heat are also known for gravitating systems, as is reviewed in Refs. [60,61]. To avoid the negative specific heat, one can again invoke a concavity construction or to use the canonical ensemble. However, contrary to other models with long-range interactions, the energy of gravitating systems, being proportional to $N^{5/3}$, cannot be made extensive, which does not allow the existence of the thermodynamic limit. For gravitating systems, the condition of global equilibrium [62]

$$\frac{E}{N} \geq \text{const} < 0 \quad (106)$$

is not valid. Therefore, they may be in principle unstable, which makes questionable the application for their description of equilibrium statistical mechanics.

The notion of statistical equivalence of ensembles is based on the comparison of the averages of observable quantities calculated in different ensembles. To concretize this, let

us consider the operators of observables \hat{A} defined on a Fock space \mathcal{F} . The set of all these operators forms the algebra of observables $\mathcal{A} \equiv \{\hat{A}\}$. The statistical state is defined [44,63] as the set $\langle \mathcal{A} \rangle \equiv \{\langle \hat{A} \rangle\}$ composed of all statistical averages for the algebra of observables. The calculation of the averages is defined in the standard way as the trace of \hat{A} , with a statistical operator corresponding to the chosen ensemble. Let us define as $\langle \mathcal{A} \rangle_\mu$, the statistical state related to the grand canonical ensemble, with a chemical potential μ . For short, the dependence of the state on temperature T and volume V is not shown explicitly. For instance, the average density is

$$\rho = \frac{N}{V}, \quad N = \langle \hat{N} \rangle_\mu. \quad (107)$$

Suppose, we wish to compare the grand canonical and canonical ensembles. Recall that the general structure of the Fock space is a direct sum

$$\mathcal{F} = \sum_{n=0}^{\infty} \mathcal{H}_n \quad (108)$$

of the n -particle Hilbert spaces \mathcal{H}_n . The pertinent mathematical details can be found in Refs. [41,42,44,63]. Define a restriction of the operator \hat{A} on \mathcal{H}_n as \hat{A}_n . Then the statistical state in the canonical ensemble can be denoted as $\langle \mathcal{A}_N \rangle_\rho$, with a fixed density ρ and the number of particles N . In view of the structure (108), the states $\langle \mathcal{A} \rangle_\mu$ and $\langle \mathcal{A}_N \rangle_\rho$ are related through the integral

$$\langle \mathcal{A} \rangle_{\mu(\rho)} = \int_0^\infty K(\rho, x) \langle \mathcal{A}_{N(x)} \rangle_\rho dx, \quad (109)$$

in which $\mu = \mu(\rho)$ is a solution of Eq. (107) and $N(x) \equiv xV$. The kernel $K(\rho, x)$ is called the Kac density. The corresponding states coincide, when in the thermodynamic limit

$$K(\rho, x) \rightarrow \delta(\rho - x).$$

Then, one has

$$\langle \mathcal{A} \rangle_{\mu(\rho)} = \langle \mathcal{A}_N \rangle_\rho, \quad (110)$$

which signifies the *statistical equivalence* of grand canonical and canonical ensembles.

Comparing the statistical states, one has to be very cautious, remembering that it may happen that there is not just the sole canonical or grand canonical ensemble, but there could be several such ensembles depending on additional constraints specifying the properties of the considered system. This is related to the nonuniqueness of the Fock space (108) and the existence of nonequivalent operator representations, as is discussed in Secs. VII and VIII. Therefore, one has, first of all, to define the appropriate representative ensembles and only after this one can compare the related averages. If at least one of the ensembles is not representative, then there is no sense to compare the averages and equality (110) does not need to be valid.

As an example, let us take a Bose-condensed system, which, according to the previous sections, can be considered either using an operator representation on the gauge-symmetric space $\mathcal{F}(\psi)$ or employing the Bogolubov repre-

sentation on the space $\mathcal{F}(\psi_1)$, with broken gauge symmetry. In the former case, some fictitious instabilities may arise and Eq. (110) may become invalid. However, this would not imply nonequivalence of the ensembles, but would simply mean that nonrepresentative ensembles are involved.

Recall as well that a representative ensemble is assumed to represent a stable system. For unstable models, Eq. (110) does not have to be always valid. For instance, if we consider the ideal Bose gas in a box, which, as has been explained above, is not stable, then there is no reason to require that Eq. (110) be true. This is really so below the condensation point [64,65], where the Bose-condensed gas becomes unstable. This instability is manifested by thermodynamically anomalous density fluctuations. The ideal Bose gas is also shown [65] to be unstable with respect to boundary conditions, whose slight variation leads to a dramatic change of the spatial particle distribution, even in the thermodynamic limit. This is contrary to the behavior of realistic stable systems, for which the influence of boundary conditions disappears in the thermodynamic limit. Changing, for the ideal Bose gas, the boundary conditions from repulsive to attractive [65] transforms the Bose-Einstein condensation from the bulk phenomenon to a strange surface effect, when the condensate is localized in a narrow domain in the vicinity of the system surface, being mainly concentrated at the corners of an infinite box. It is clear that a system, in which the condensate is localized somewhere at the corners of an infinite volume, is a rather unphysical object.

Thus, formally comparing two ensembles, one sometimes can arrive at their seeming nonequivalence. This, however, in no way invalidates the basic principle of statistical mechanics stating the ensemble equivalence. This just means that at least one of the compared ensembles is not representative, which also includes that the system may be intrinsically unstable. *The principle of equivalence holds only for representative ensembles, which represent stable systems.*

X. CONCLUSION

The analysis is given of the relation between the stability properties of statistical systems and the fluctuations of observable quantities. The emphasis is made on the composite observables that are represented by the sums of several terms. The main result of the paper is the theorem connecting the global fluctuations of an observable with the partial fluctuations of its components. The theorem is general, being formulated for an arbitrary operator represented as a sum of linearly independent self-adjoint operators. These operators can be associated with the total and partial observable quantities of a statistical system. The theorem tells us that: The total dispersion of an operator, being a sum of linearly independent self-adjoint operators, is thermodynamically anomalous if and only if at least one of the partial dispersions is anomalous, with the power of N in the total dispersion defined by the largest partial dispersion. Conversely, the total dispersion is thermodynamically normal if and only if all partial dispersions are normal.

The theorem allows us to understand the relation between the fluctuations of partial observables and the fluctuations of

the total observable. Respectively, the character of partial fluctuations turns out to be directly related to the stability of statistical systems. Several examples illustrate the practicality of the theorem, helping to avoid wrong conclusions that could happen when studying the behavior of partial observables. In particular, the fluctuations of condensed, as well as noncondensed particles, in a Bose-condensed system must be normal, if the system is assumed to be stable. In the same way, fluctuations in systems with continuous symmetry are also thermodynamically normal.

Breaking of gauge symmetry helps to eliminate fictitious instabilities arising in Bose-condensed systems. Generally, it is crucially important that a system be characterized by its representative ensemble. This makes it possible to avoid artificial contradictions in the theory and the related unphysical instabilities. One of the basic principles of statistical mechanics, the principle of ensembles equivalence, holds only for representative ensembles correctly representing stable statistical systems.

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APPENDIX A: NONCOMMUTATIVITY OF BOGOLUBOV SHIFT

This appendix illustrates the noncommutativity of the Bogolubov shift and the Hartree-Fock-Bogolubov (HFB) approximation. When one accomplishes in function (52), first, the Bogolubov shift (53) and then the HFB approximation for $\psi_1(\mathbf{r})$, one gets expression (55), with the correct limiting behavior. But in the other way round, employing, first, the HFB approximation for $\psi(\mathbf{r})$ and, after this, substituting the Bogolubov shift (53), one gets

$$g(\mathbf{r}_{12}) = 1 + \frac{2\rho_0^2}{\rho} + \frac{2\rho_0}{\rho^2} \text{Re}[\rho_1(\mathbf{r}_1, \mathbf{r}_2) + \sigma_1(\mathbf{r}_1, \mathbf{r}_2)] \\ + \frac{1}{\rho^2} \{ |\rho_1(\mathbf{r}_1, \mathbf{r}_2)|^2 + |\sigma_1(\mathbf{r}_1, \mathbf{r}_2)|^2 \}.$$

The limiting behavior of this pair correlation function is not correct, since here

$$\lim_{\mathbf{r}_{12} \rightarrow \infty} g(\mathbf{r}_{12}) = 1 + \frac{2\rho_0^2}{\rho^2},$$

which would be true only when $\rho_0 \equiv 0$. But when $\rho_0 \neq 0$, we confront the problem of the condensate overcounting. Thence, these procedures are not commutable. And one has, first, to introduce the Bogolubov shift (53) and only after this to resort to the HFB approximation.

APPENDIX B: NONEXISTENCE OF PHASE OPERATOR

To show that the representation (63) does not exist, we may use the method of reduction to absurdity. Suppose that

this representation is correct. Then, from the commutation relation

$$[\hat{n}(\mathbf{r}), \hat{\phi}(\mathbf{r}')] = i\delta(\mathbf{r} - \mathbf{r}'),$$

we obtain for the number-of-particle operator,

$$\hat{N} \equiv \int \hat{n}(\mathbf{r}) d\mathbf{r},$$

the commutation relation

$$[\hat{N}, \hat{\phi}(\mathbf{r})] = i.$$

From here, taking the matrix element with respect to the number basis $\{|n\rangle\}$, for which $\hat{N}|n\rangle = n|n\rangle$, we find

$$(n - n') \langle n | \phi(\mathbf{r}) | n' \rangle = i \delta_{nn'}.$$

Setting here $n = n'$, we get the senseless equality $i = 0$. Thus, the representation (63) does not exist.

Now, suppose that the representation (64) is correct. Then for the density operator, we have

$$\hat{n}(\mathbf{r}) \equiv \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) = \rho(\mathbf{r}).$$

Hence, the number-of-particle operator becomes identical to the total number of particles,

$$\hat{N} = \int \rho(\mathbf{r}) d\mathbf{r} = N.$$

At the same time, there is an exact relation

$$[\psi(\mathbf{r}), \hat{N}] = \psi(\mathbf{r}).$$

Using this for $\hat{N} = N$, we get the senseless equality $\psi(\mathbf{r}) = 0$. Hence, the representation (64) is wrong.

In this way, neither representation (63) nor representation (64) are correct. The phase operator, defined through these representations, does not exist. To introduce correctly a kind of a quasiphas operator, one should employ the Pegg-Barnett technique [36].

APPENDIX C: GAUGE-SYMMETRY BREAKING

The simple method of infinitesimal sources may not always break gauge symmetry. To illustrate this, it is sufficient to give at least one counterexample. For this purpose, let us consider the Hamiltonian

$$H = \int \psi^\dagger(\mathbf{r}) \omega(\mathbf{r}) \psi(\mathbf{r}) d\mathbf{r},$$

with a positive function $\omega(\mathbf{r}) > 0$. This Hamiltonian is invariant under the gauge transformation

$$\psi(\mathbf{r}) \rightarrow e^{i\alpha} \psi(\mathbf{r}),$$

where α is any real-valued number. Hence $\langle \psi(\mathbf{r}) \rangle = 0$. To break the gauge symmetry, following the standard method of infinitesimal sources, one adds to the Hamiltonian H a term lifting the symmetry. For instance, the Hamiltonian

$$H_\varepsilon \equiv H - \varepsilon \int [\lambda^*(\mathbf{r})\psi(\mathbf{r}) + \lambda(\mathbf{r})\psi^\dagger(\mathbf{r})]d\mathbf{r},$$

where $\lambda(\mathbf{r})$ is a complex-valued function, is not gauge invariant. The latter Hamiltonian can be diagonalized by means of the canonical transformation

$$\psi(\mathbf{r}) = \varepsilon \frac{\lambda(\mathbf{r})}{\omega(\mathbf{r})} + \bar{\psi}(\mathbf{r}),$$

in which the new field operator $\bar{\psi}(\mathbf{r})$ enjoys the same commutation relations as $\psi(\mathbf{r})$. Then, we have

$$H_\varepsilon = E_\varepsilon + \int \bar{\psi}^\dagger(\mathbf{r})\omega(\mathbf{r})\bar{\psi}(\mathbf{r})d\mathbf{r},$$

with the notation

$$E_\varepsilon \equiv -\varepsilon^2 \int \frac{|\lambda(\mathbf{r})|^2}{\omega(\mathbf{r})}d\mathbf{r}.$$

For the diagonal in $\bar{\psi}(\mathbf{r})$ Hamiltonian H_ε , one has $\langle \bar{\psi}(\mathbf{r}) \rangle = 0$. Therefore,

$$\langle \psi(\mathbf{r}) \rangle = \varepsilon \frac{\lambda(\mathbf{r})}{\omega(\mathbf{r})}.$$

According to the method of infinitesimal sources, after calculating the averages, one should set $\varepsilon \rightarrow 0$. But then

$$\langle \psi(\mathbf{r}) \rangle \rightarrow 0 \quad (\varepsilon \rightarrow 0),$$

because of which the gauge symmetry has not been broken. Contrary to this, the Bogolubov shift (67) is a sufficient condition for gauge-symmetry breaking.

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