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FLUCTUATIONS OF BOSE-CONDENSATE IN THE BOGOLUBOV MODEL

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The Bogolubov theory of nonideal gas Bose-condensation for elucidating ^4He superfluidity was one of the first achievements of quantum statistical physics in studying collective phenomena of the microworld [1]. Not only the repulsion forces between atoms but also the attraction forces [2, 3] were later introduced in the model. Interest in the latter stemed from the problem of quantum crystallization of liquid helium [2]. In the original model, only temperature fluctuations of the Bose-condensate density still remained uninvestigated: the calculation of which, as had been mentioned in [4, 5], gave a nonvanishing value in zero degrees Kelvin.

Interest in the problem of fluctuations of the number of particles under Bose-condensation stems from successful investigations of the dependence of light field fluctuations on the parameters of a system in quantum optics. One of such optical systems, using pairing correlations between photons, has been described in [6, 7] within the zero-dimensional version of Bogolubov's model of condensation of nonideal Bose-gas. We may assume an analogy between this effect and excitation correlations in superfluid liquid ^4He as concerns the existence in the latter of states with different statistics of fluctuations of the number of condensate bosons. This information could be useful for interpreting experiments on measurement of superfluid components in liquid ^4He which, as is known [8], give essentially smaller values than expected from calculations of mean occupation numbers.

In the present paper, in Bogolubov's model of Bose-condensation we have derived formulae for variances of the number of condensate ($k = 0$) and over-condensate ($k \neq 0$) bosons and estimated the intensity of their fluctuations at different temperatures.

1. Partition Function in Bogolubov's Model

The Hamiltonian of Bose-particles in Bogolubov's model has the form

$$\begin{aligned} H &= g_0 \frac{|a|^4}{2V} + \sum_{k \neq 0} \Big[\Omega_k b_k^+ b_k + \frac{g_k}{2V} (b_k^+ b_{-k}^+ a^2 + b_k b_{-k} a^{*2} + \\ &\quad + 2 b_k^+ b_k |a|^2) + \frac{g_0}{V} b_k^+ b_k |a|^2 \Big] , \qquad (1) \\ \Omega_k &= \frac{k^2}{2m}, \qquad \left[b_k, b_{k'}^+ \right] = \delta_{kk'} . \end{aligned}$$

With an accuracy up to processes of higher order in the parameter $g_k(g_0)^{-1}$ assumed small in (1) there holds the integral of motion N of the total number of particles $\hat{N}$

$$\begin{aligned}
\frac{d\hat{N}}{dt} &= \frac{d}{dt}\left(|a|^2 + \sum_{k\neq 0} b_k^+ b_k\right) = \{H, |a|^2\} + i[H, \sum_{k\neq 0} b_k^+ b_k] = 0, \quad (2)\\
\{H, A\} &= i\left(\frac{\partial H}{\partial a}\frac{\partial A}{\partial a^*} - \frac{\partial H}{\partial a^*}\frac{\partial A}{\partial a}\right).
\end{aligned}$$

The partition function Q of the canonical ensemble with allowance for constraints generated by the integral of motion (2) equals

$$Q = Sp\left(e^{-\beta H}\delta_{N,\hat{N}}\right) = \frac{1}{\sqrt{2\pi}}\int d^2a \prod_{k\neq 0}\int Db_k^* Db_k \int_{-\pi}^{\pi} dy \exp(iy\times$$

$$\times (|a|^2 - N)) \exp\left[-\beta\frac{g_0}{2V}|a|^4 + \int_0^\beta dt \begin{pmatrix} b_k^* \\ b_{-k}\end{pmatrix} P \begin{pmatrix} b_k \\ b_{-k}^*\end{pmatrix}\right], \quad (3)$$

$$P_k = \begin{pmatrix} -\frac{d}{dt} - \omega_k & -\gamma_k \\ -\gamma_k^* & \frac{d}{dt} - \omega_k \end{pmatrix},$$

$$\omega_k = \Omega_k + (g_0 + g_k)\frac{|a|^2}{V} - \nu, \qquad \nu = i\frac{y}{\beta}, \qquad \gamma_k = \frac{g_k}{2V}a^2.$$

Here, a trace over quantum variables of over-condensate particles is written as a functional integral along the trajectories $b_k, b_k^*, b_{-k}, b_{-k}^*$ with periodic boundary conditions

$$b_k(0) = b_k(\beta), \qquad b_k^*(0) = b_k^*(\beta)$$

and analogous ones for the trajectories with index $k \longrightarrow (-k)$. Integrals over the Bose-condensate field a and the coupling parameter y are numerical. The Gauss integral over the trajectories b, b^* in the product with respect to k is found from the ratio of functional determinants

$$\frac{Sp\exp(-\beta h_k)}{Sp\exp(-\beta h_k^0)} = \frac{Det P_k}{Det P_k^0} = -\int_0^{g_k} Sp\left(\frac{1}{P_k}\frac{\partial P_k}{\partial x}\right) dx,$$

$$h_k = \frac{\omega_k}{2}\left(b_k^* b_k + b_k^* b_{-k}\right) + \gamma_k b_k^* b_{-k}^* + \gamma_k^* b_k b_{-k},$$

$$h_k^0 = h_k\big|_{g_k=0}$$

$$\begin{pmatrix} b_k \\ b_{-k}^* \end{pmatrix} = P_k^{-1}\begin{pmatrix} \phi \\ \phi^* \end{pmatrix} = e^{-Mt}\int_0^\beta e^{M\tau}\left[\Theta(t-\tau) + \frac{1}{e^{M\beta}-1}\right]\begin{pmatrix} -\phi \\ \phi^* \end{pmatrix} d\tau,$$

$$M = \begin{pmatrix} \omega_k & \gamma_k \\ -\gamma_k^* & -\omega_k \end{pmatrix}, \qquad Spe^{-\beta h_k} = e^{\frac{\omega_k}{2}\beta}\left(4\sinh^2\beta\frac{E_k}{2}\right)^{-1},$$

$$\frac{E_k}{2} = \left(\frac{\omega_k^2}{4} - |\gamma_k|^2\right)^{\frac{1}{2}} = \frac{1}{2}\left[(\omega_k^0)^2 + \frac{2|a|^2}{V}g_k\omega_k^0\right]^{\frac{1}{2}}, \quad (4)$$

$$\omega_k^0 = \omega_k\big|_{g_k=0}.$$

Substituting the result (4) into formula (3) we get the statistical integral in the form

$$Q = V\sqrt{\frac{\pi}{2}}\int d\rho \int_{-\pi}^{\pi} dy \exp\left\{\left[-\beta\frac{g_0}{2}\rho^2 + iy(\rho - R)\right]V\right\} \times \quad (5)$$

$$\times \prod_{k\neq 0}\frac{\exp\omega_k\beta/2}{4\sinh^2(\beta E_k/4)}, \qquad R = \frac{N}{V}, \qquad \rho = \frac{|a|^2}{V}.$$

2. Low-Temperature Approximation

For an approximate calculation of the integral (5) let us divide the half-axis of the integration variable ρ into two parts according to the inequality $\rho \gtrless 4(\beta g_0)^{-1}$. The upper sign of it corresponds to small condensate densities and high temperatures; the lower sign, to large condensate densities and low temperatures. We will restrict ourselves to the last case and will determine more accurately approximation of low temperatures in formula (5) by dividing the plane of variables ω_k^0 and $(E_k^2 - 16/\beta^2)$ into two parts according to the inequality $\beta E_k \gtrless 4$. The roots of the parabola, which divide these parts of the plane

$$(\omega_k^0)_{1,2} = -g_k\rho \pm \left(g_k^2\rho^2 + \frac{16}{\beta^2}\right)^{\frac{1}{2}},$$

determine the regions of applicability of two approximations for the function $\sinh(\beta E_k/4)$

$$\prod_{k\neq 0}\frac{\exp(\omega_k\beta/2)}{4\sinh^2(\beta E_k/4)} \simeq \exp\left[\sum_{k\neq 0}\frac{\omega_k\beta}{2} - \sum_{k\neq 0}\begin{cases} 2\ln\beta\frac{E_k}{2}, & \beta E_k < 4 \\ \beta\frac{E_k}{2}, & \beta E_k > 4\end{cases}\right].$$

Finally, choosing as an expansion parameter of the square root in E_k the ratio $g_k\rho(\omega_k)^{-1}$ or the inverse value, combining all inequalities written down and changing in the spirit of a semiclassical description of over-condensate bosons the sum over k integrals, we derive for (5) the formula

$$Q \simeq V\sqrt{\frac{\pi}{2}}\int_{4/\beta g_0}^{\infty} d\rho \int_{-\pi}^{\pi} dy \exp\Phi, \tag{6}$$

$$\Phi = -\beta V\left(g_0\rho^2/2 - \nu\rho + \nu\rho\right) + cV\int_{\omega_k=-2g_0\rho}^{\omega_k=4/\beta} k^2dk\,[\Omega_k - \nu +$$

$$+\rho(g_0 + g_k)]\,\frac{\beta}{2}, \qquad c^{-1} = 2\pi^2\hbar^3.$$

Note that the integral over k in the limits of $4/\beta < \Omega_k < \infty$ and the term with the function ln in the integral in the interval $-2g_0\rho < \Omega_k < 4/\beta$ give a contribution in the next approximation order in $\rho\beta g_0 > 4$ and are disregarded in (6).

3. Equations of a stationary phase and variances of a condensate density

After the simplifications made let us proceed from the calculation of Q using the stationary phase method as $N \to \infty, V \to \infty$. The low-temperature approximation, that has been formulated in deriving formula (6), is natural for a numerical (nonoperator) description of the

Bose-condensate adopted in the model (1). A description like that is equivalent to the assumption about a large value of the interaction between bosons of the condensate g_0 in comparison with their interaction with over-condensate bosons $g_{k,k\neq 0}$. Perturbation theory in the parameter $g_k(g_0)^{-1}$ connected with this assumption will be used later in the form of iterations with values $g_k \to g_0$ and $\nu \to \nu_0$ in the zero approximation where $\nu_0 = g_0\rho$ is the coupling parameter value providing the Bogolubov phonon spectrum in the formula for E_k. In this case, the integral phase (6) has the form

$$\frac{1}{\beta V}\Phi = -\frac{g_0}{2}\rho^2 + \nu(\rho - R) + \rho_1(2g_0\rho - \nu), \tag{7}$$

and the equations of its stationarity

$$\frac{1}{\beta V}\frac{\partial\Phi}{\partial\rho} = 0 = -g_0\rho + 2g_0\rho_1 + \nu,$$

$$\frac{1}{\beta V}\frac{\partial\Phi}{\partial\nu} = 0 = \rho - R - \rho_1, \qquad \rho_1 = \frac{c}{2}\int_{\Omega_k=0}^{\Omega_k=4/\beta} k^2dk$$

determine extremal values of ρ, ν in first perturbation order according to the equalities

$$\rho_0 + \rho_1 = R, \qquad \rho_0 + \rho = 2R, \qquad \rho_0 = \nu(g_0)^{-1}.$$

In these equalities, the densities of the condensate ρ_0 and over-condensate particles ρ_1 are introduced. Formula (8) coincides with those obtained in first order of the modified perturbation theory [9]. This coincidence is a consequence of the equivalence (in the thermodynamic limit) [1] of a large canonical[9] and canonical (3) Gibbs ensembles.

For the Gauss integral (6) with a simplified phase (7) the solution (8) gives an asymptotically exact at $N \to \infty, V \to \infty$ answer. Formula (6), as has been mentioned, is a low-temperature approximation for the statistical integral (5) of the model (1) that in its turn is an approximation of the Hamiltonian with a pairing four-boson interaction.

[1] If we were interested in dimensional effects of superfluidity at finite V, this equivalence wouldn't hold since the integral of motion in the phase space allows for the binding condition in (3) whereas the chemical potential [9] allows for it as an expectation value

Therefore, proceeding from the calculation of variances of the variable ρ we will be interested only in the main contribution to the phase (7) at $\rho : \rho \sim \rho_0 > \rho_1$

$$D(\rho) = \int d\rho'(\rho'-\rho)^2 \exp\Phi \left(\int d\rho' \exp\Phi\right)^{-1},$$

$$\frac{1}{\beta V} = \Phi_0 - \frac{g_0}{2}(\rho'-\rho)^2, \qquad D(\rho) = \frac{1}{g_0\beta V}.$$

Here, Φ_0 is the value of the phase Φ at the extremal point determined by equations (8); at the fixed density R of the total number of particles these equations result in the equality of variances of all variables

$$D(\rho) = D(\rho_0) = D(\rho_1), \qquad D(R) = 0.$$

4. Temperature Variances of the Condensate

To determine the scale of fluctuations of the condensate and over-condensate bosons one should compare their densities ρ_0, ρ_1 with variances $\mathbf{P}$ of the number of particles normalised to the volume

$$\rho_0 = \frac{n_0}{V}, \qquad \rho_1 = \frac{n_1}{V}, \qquad n_0 + n_1 = N, \qquad \mathbf{P} = \frac{D(n_0)}{V} = \frac{D(n_1)}{V} = \frac{1}{g_0\beta}.$$

The condensate density ρ_0 takes the largest value at zero temperature. This value, equal to R, can be estimated from the equality

$$R = \frac{c}{2}\int_0^{\Omega_k = 4/\beta_0} k^2 dk = \frac{c}{2}(8mk_0T_0)^{\frac{3}{2}}, \qquad \beta_0 = \frac{1}{k_0T_0},$$

where k_0 is the Boltzmann constant, and T_0 is critical temperature. Taking this temperature equal to 2 K, the density of liquid helium equal to 0,13$gr \cdot cm^{-3}$ and the Avogadro number equal to $6 \cdot 10^{23}$, we have

$$R \simeq 10^{20} cm^{-3} = 3 \cdot 10^{21} (mol)^{-1} = 0{,}5 \cdot 10^{-2} (atom)^{-1}.$$

The interaction constant g_0 between atoms of the condensate has the dimension (energy · volume). For one atom the energy $\mathcal{E}$ of the van der Waals interaction [10] for light atoms can be taken equal to 0,01eV

so that variance $\mathbf{P}$ of the number of condensate and over-condensate particles equals

$$\mathbf{P} = \frac{k_0T}{g_0} = T\frac{10^{-4} eV}{\mathcal{E} eV \cdot atom \cdot \ K} = 0{,}8 \cdot 10^{-2}\frac{T}{atom \cdot \ K}.$$

The comparison of numerical estimates for R and ρ shows that at temperature larger than 1 K, the variance $\mathbf{P}$ of the number of particles of any component exceeds the density of its number of particles. At temperature smaller than 1 K, the density of the number of particles of the condensate exceeds the variance, and in this case, one may speak about small fluctuations of the number of bosons with zero momentum. As for the over-condensate component, at the lowest temperatures both its density and its variance are small. Thus, the question of a possible suppression of variances of phonon excitations in an equilibrium system remains open.

One expects that at temperature close to critical the above estimates are incorrect. This is due to the statement of the problem with the Hamiltonian (1) and low-temperature approximation being limited. It seems inexpedient to raise the accuracy within the model (1) as it, as has been noted in [4, 5] and as it follows from the form of E_k in formula (4), leads to the appearance of a gap in the phonon spectrum which is not observed experimentally and is absent in perturbation theory with a four-boson interaction. In the last case, besides a possible more accurate calculation, one can consider quantum fluctuations of the condensate which are disregarded in the above statement of the problem.

Using the analogy with quantum optics, one can note that the situation with small variances of the density of the number of particles of the Bose-condensate corresponds to the so-called sub-Poisson statistics of the light field. At temperatures close to the phase transition temperature, density fluctuations of the number of particles of the condensate are large. In this case, to study their statistics , it may be effective to use the theory of the Bose-field phase operator [11].

Thus for the Bogolubov model, we have given the estimates of the density of the number of particles of the Bose-condensate and their variances. The comparison of these quantities with each other shows that temperature fluctuations of the number of particles of the condensate are rather small in the vicinity of zero degree Kelvin and large in the vicinity of transition temperature. This means that the way of interpreting experimental data should depend on temperature. Indeed, in experiments with liquid ^4He one observes the scattering cross section of neutrons as a function of transferred energy. The results are presented as two Gaussian contours [8] associated with the condensate and over-condensate components. The density of the number of particles is determined by areas restricted by these curves. Therefore, the accuracy of their construction is of great importance. In the case with strong fluctuations of the condensate, reconstruction of the envelope by the experimental results needs apparently a special technique of data processing.

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Ярунин В.С E17-92-348

Флуктуации бозе-конденсата
в модели Боголюбова

Методом стационарной фазы в каноническом ансамбле со связью вычислена статистическая сумма модели Боголюбова по надконденсатным (квантовым) и конденсатным (классическим) переменным. Получены формулы для стационарных значений и дисперсий числа частиц обеих компонент. Численные оценки показывают превышение уровнем тепловых флуктуаций конденсата его числа заполнения при температурах 1 K < T < T_0 и обратную ситуацию при 0 < T < 1 K, где T_0 - температура фазового перехода. Обсуждается значение обнаруженного обстоятельства для интерпретации экспериментов по нахождению плотности сверхтекучей компоненты в жидком ^{4}He.

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Yarunin V.S. E17-92-348

Fluctuations of Bose-Condensate
in the Bogolubov Model

The stationary phase method in the canonical ensemble with constraints is used to calculate the statistical sum of Bogolubov's model with respect to over-condensate (quantum) and condensate (classical) variables. Formulae are derived for expectation values and variances of the particle number of both components. Numerical estimations show that the level of thermal fluctuations exceeds its occupation number at temperatures 1 K < T < T_0 and that the opposite situation is at 0 < T <1 K, where T_0 is the phase transition temperature. The importance of the observed fact for interpretation of experiments in searching for the density of a superfluid component in liquid ^{4}He is discussed.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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