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RIGOROUS RESULTS IN A NONIDEAL BOSE GAS THEORY

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A method of approach to the problem of the Bose condensation in a nonideal Bose gas based on Bogoliubov's theory of quasi-averages is examined. It is shown that the proof of the existence of a phase transition in this system can be reduced to the proof of some trace-inequality, gaussian domination condition, which is linked with some break of the continuous symmetry group. To prove this condition a special functional integral technique over Bogoliubov's measure defined on some space of continuous functions with a uniform metric is proposed.

1. PHASE TRANSITION IN A NONIDEAL BOSE GAS

In 1961 Bogoliubov proposed a universal method of approach to the phase transitions theory based on the study of a degeneracy of a thermodynamic equilibrium state [1]. This phenomenon arises for a temperature below some critical one $\theta \leq \theta_c$. For $\theta = \theta_c$ a phase transition to a regular nondegenerate state takes place.

In many systems with a continuous symmetry group a phase transition is linked with a break of the law of conservation of total particles number. A typical feature of such system is an emergence of some type of the condensation.

Consider a nonideal Bose gas model. Let in a ν-dimensional cube $V \in R^\nu$ with coordinates $x = (x^1, x^2, \dots, x^\nu), x^j \in (-L/2, L/2), j = 1, 2, \dots, \nu$ and with the volume $|V| = L^\nu$ be N identical spinless particles. The Hamiltonian of the system is

$$\hat{H} = -\frac{1}{2m}\sum_{n=1}^{N} \triangle_{x_n} + \sum_{n<m} \Phi(x_n - x_m), \tag{1}$$

where $\triangle_x$ is a Laplacian operator over x and a potential energy is defined by a real-valued symmetric function $\Phi(x) = \Phi(-x)$.

A superfluidity is a phase transition in a system of bosons accompanied by a long-range order in a coordinate space or by a Bose condensation in a momentum space.

Let $F(x_1, x_2) = \langle \hat{\psi}^+(x_1)\hat{\psi}(x_2)\rangle_V$ be a one-particle density matrix. The average is a Gibbs equilibrium average with the Hamiltonian $\hat{H}$ in the cube V.

An existence of a long-range order in a system means, that

$$\lim_{|x_1-x_2|\to\infty} \lim_{V\uparrow R^\nu} F(x_1,x_2) \equiv n_0 > 0. \tag{2}$$

Passing to the Fourier transformation $w(k) = (2\pi)^{-3}\int F(x)e^{ikx}dx$, one obtains from (2) that $w(k) = n_0\delta(k) + w_1(k)$, where $w_1(k)$ defines a continuous distribution of particles over nonzero momenta and n_0 is a Bose condensate density, i.e.,

$$n_0 = \lim_{V\uparrow R^\nu} \frac{\langle \hat{a}_0^+\hat{a}_0\rangle_V}{|V|} = \lim_{|V|\to\infty} \frac{1}{|V|^2}\iint \langle\hat{\psi}^+(x_1)\hat{\psi}(x_2)\rangle_V\, dx_1dx_2 > 0. \tag{3}$$

So an appearance of a phase transition in a model of a nonideal Bose gas, which is connected with the existence in the system of the long-range order in relation to (2), is determined by an appearance of a nonzero Bose condensate density n_0.

2. GAUSSIAN DOMINATION AND BOSE CONDENSATION

To prove the condition (3) it is necessary to obtain an upper bound for the correlation function $\langle\hat{a}_p^+\hat{a}_p\rangle_V$ for $p \neq 0$. Really we have the sum rule

$$n = \frac{1}{|V|}\sum_p \langle\hat{a}_p^+\hat{a}_p\rangle_V, \tag{4}$$

where n is the average density of the number of particles in the system. Therefore the inequality (3) will take place if from the estimate

$$\langle\hat{a}_p^+\hat{a}_p\rangle_V \leq G_p^{(V)}(\theta), \quad p \neq 0 \tag{5}$$

will result that in the thermodynamic limit $n > |V|^{-1}\sum_{p\neq 0} G_p^{(V)}(\theta)$. In this way the condition $n = \lim_{V\uparrow R^\nu} |V|^{-1}\sum_{p\neq 0} G_p^{(V)}(\theta)$ gives a lower bound for the critical temperature $\theta_c^{(0)}$ of the phase transition.

Thus the main thing in our approach is to obtain the estimate (5), which is connected with Bogoliubov's quasi-averages theory. Let the Hamiltonian of a system takes the form $\hat{H} = \hat{H}_0 + \hat{H}_1$, where $\hat{H}_0 = \sum \omega_p\hat{a}_p^+\hat{a}_p, \omega_p > 0 (p\neq 0), \omega_0 = 0$ be a free Hamiltonian, $\hat{H}_1$ be an interaction. Consider a one-parameter family of the Hamiltonians $\hat{H}(h) = \hat{H}_0(h) + \hat{H}_1$, where $\hat{H}_0(h) = \sum\omega_p(\hat{a}_p^+ + h_p^*)(\hat{a}_p + h_p)$ and $h_p \in C$ are arbitrary complex numbers. Define the functional (a statistical sum) $Z(h) = \mathrm{Tr}\exp[-\beta\hat{H}(h)]$, where $\beta = \theta^{-1}$ is an inverse temperature. We shall say that the gaussian domination condition [2] takes place if for any $h_p \in C$

$$Z(h) \leq Z(0). \tag{6}$$

If the functional $Z(h)$ has for $h = 0$ a local maximum we shall say that the local gaussian domination condition takes place [3]. The condition of the maximum of $Z(h)$ at zero leads to an inequality [4] for Bogoliubov's inner product (two-point Duhamel function) $(\hat{a}_p^+, \hat{a}_p) \leq (\beta\omega_p)^{-1}$.

It is possible to show, that if the gaussian domination condition (or the more weak local gaussian domination condition) is fulfilled, then in the nonideal Bose gas with the repulsion $\Phi(x) \geq 0$ for $\nu \geq 3$ and $\theta \leq \theta_c^{(0)}$ the Bose condensate is arisen [5], i.e., the phase transition condition (3) is accomplished. In this way we have $\theta_c^{(0)} = \theta_0$, where θ_0 is a temperature of the Bose condensation in an ideal Bose gas. So the London's assumption that the repulsive-type interaction favoured to Bose condensation finds the rigorous substantiation.

To prove the condition (6) in the model (1) use the functional integrals technique [6].

3. GAUSSIAN FUNCTIONAL INTEGRALS OVER BOGOLIUBOV'S MEASURE

Consider a case of the one degree of freedom, the Hamiltonian of a one-dimensional harmonic oscillator

$$\hat{\Gamma} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2,$$

and the chronological average

$$\left\langle T \exp\,[i \sum_{j=1}^{N+1} \nu_j \hat{Q}(s_j)] \right\rangle, \tag{7}$$

with the Hamiltonian $\hat{\Gamma}$. The operator $\hat{Q}(s)$ is given by $\hat{Q}(s) = e^{s\Gamma}\hat{q}e^{-s\Gamma}$, where ν_j are real numbers and $0 = s_1 < s_2 < \cdots < s_N < s_{N+1} = \beta$. It is possible to show, that the average (7) in this case takes the form

$$\left\langle T \exp\,[i \sum_{j=1}^{N+1} \nu_j \hat{Q}(s_j)] \right\rangle = \exp\left(-\frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} A_{jk}\eta_j\eta_k \right), \tag{8}$$

where the covariance matrix A entries are

$$A_{jk} = \frac{1}{2m\omega\,\mathrm{sh}\,\frac{\beta\omega}{2}}\,\mathrm{ch}\left(\frac{\beta\omega}{2} - \frac{\beta\omega}{N}|j-k|\right)$$

and we used the uniform separation of the interval $(0, \beta)$. Taking into account the formula (8), the complex Fourier formula and the fact, that operators commute under the T-product sign, it is possible to show that for an arbitrary T-product average the following formula takes place

$$\left\langle T\left[f\left(\hat{Q}(s_1),\ldots,\hat{Q}(s_{N+1})\right)\right]\right\rangle =$$

$$= \int f(q_1,\ldots,q_{N+1})\rho(q_1,\ldots,q_{N+1})dq_1\ldots dq_{N+1},$$

where

$$\rho(q_1,q_2,\ldots,q_{N+1}) = \frac{1}{(2\pi)^{\frac{N}{2}}}\frac{\delta(q_1-q_{N+1})}{(\det A)^{\frac{1}{2}}}\exp\left[-\frac{1}{2}\sum_{j,k=1}^{N}(A^{-1})_{jk}q_jq_k\right]. \quad (9)$$

It follows from (9) that $\rho \geq 0,\ \int \rho\, dq_1\ldots dq_{N+1} = 1$.

Consider the space $X \equiv C^\circ[0,\beta]$ of continuous functions $q(s)$, defined on the segment $[0,\beta]$, that satisfy the condition $q(0)=q(\beta)$. This is the metric space with respect to the uniform metric $\rho(q,p)=\sup_{s\in[0,\beta]}|q(s)-p(s)|$. In the space X we can introduce a σ-algebra generated by cylindrical sets. This σ-algebra is the same as the σ-algebra generated by the sets that are open in the metric ρ. Extending the gaussian measure from the cylindrical sets to their Borel closure, we obtain a gaussian measure μ in the space X [7] with the average value equal to zero and with the correlation function

$$B(t,s) = \frac{1}{2m\omega\,\mathrm{sh}\,\frac{\beta\omega}{2}}\,\mathrm{ch}\left(\omega|t-s|-\frac{\beta\omega}{2}\right). \quad (10)$$

An integral corresponding to the measure μ can be defined as an abstract Daniell integral [8]. By means of this integral the Gibbs T-product average for an arbitrary measurable functional can be represented as

$$\left\langle T\left(f(\hat{Q})\right)\right\rangle = \int_X f(x)d\mu(x). \quad (11)$$

4. GAUSSIAN DOMINATION AND FUNCTIONAL INTEGRALS

Consider a system with the Hamiltonian $\hat{H} = \hat{\Gamma} + \hat{V}$, where $\hat{V} = V(\hat{q})$ is an interaction, as well a one-parameter family of the Hamiltonians $\hat{H}(h) = \hat{\Gamma}(h) + \hat{V}, h \in R$ with

$$\hat{\Gamma}(h) = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}(\hat{q}-h)^2.$$

The statistical sum of the system is $Z(h) = \mathrm{Tr}\, e^{-\beta \hat{H}(h)}$. Let the potential of interaction be the nonnegative and symmetric function, i.e., $V(x) \geq 0,\ V(x) = V(-x)$. Using the above-mentioned functional integral (11), we have

$$R(h) = \int_X d\mu(x) \exp\left[-\int_0^\beta ds V\left(x(s) + h\right)\right].$$

Use now the theorem of linear substitution of a variable in an integral over gaussian measure [9], which gives for an integrable functional $F(x)$ and for a function $a \in H$, that

$$\int_X F(x) d\mu(x) = e^{-\frac{1}{2}||a||_H^2} \int_X F(x+a) e^{-(a,x)} d\mu(x).$$

The space H is a linear covering of the eigenfunctions of the kernel (10) that is closed relative to an appropriate norm [7]. Apply this formula for a case of the considered measure and for the constant functions a, which belong to H. We obtain, that

$$R(h) = \exp\left[-\frac{\beta m \omega^2 h^2}{2}\right] \int_X d\mu(x) \exp\left[-\int_0^\beta V(x(t)) dt\right] \cdot \exp\left[m h \omega^2 \int_0^\beta x(t) dt\right].$$

Consider the Fourier–Gauss transformation

$$\tilde{f}(y) \equiv F(f; y) = \int_X d\mu(x) f(x + iy)$$

of the functional $f(x)$ and the Parseval equality

$$\int_X f\left(\frac{x}{\sqrt{2}}\right) g^*\left(\frac{x}{\sqrt{2}}\right) d\mu(x) = \int_X F\left(f; \frac{y}{\sqrt{2}}\right) F^*\left(g; \frac{y}{\sqrt{2}}\right) d\mu(y) \qquad (12)$$

for the case of functionals

$$f(x) = F(x) \equiv \exp\left[-\int_0^\beta dt V(x(t))\right], \quad g(x) = \exp\left[m h \omega^2 \int_0^\beta x(t) dt\right].$$

The equality (12) takes the form

$$\exp\left[-\frac{\beta m h^2 \omega^2}{2}\right] \int_X F\left(\frac{x}{\sqrt{2}}\right) \exp\left[\frac{1}{\sqrt{2}} h m \omega^2 \int_0^\beta x(t) dt\right] d\mu(x)$$
$$= \int_X \tilde{F}\left(\frac{y}{\sqrt{2}}\right) \exp\left[\frac{i}{\sqrt{2}} h m \omega^2 \int_0^\beta y(t) dt\right] d\mu(y)$$

and we see that if for any y

$$\tilde{F}(y) \geq 0, \tag{13}$$

then $R(h) = \tilde{F}(-ih) \leq R(0) = \tilde{F}(0)$. The condition (13) in our case can be proved for symmetric, nonnegative potentials by the Iensen inequality.

Up to here we considered a case of one degree of freedom. For situation which is interesting in the nonideal Bose gas theory there is a system of N spinless particles of the mass m everyone of which interact with each other by means of the pairwise symmetric potential $\hat{H} = \hat{\Gamma} + \hat{V}$, where

$$\hat{\Gamma} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2, \quad \hat{V} = V(\hat{q}) = \sum_{i<j=1}^{N} \Phi(\hat{q}_i - \hat{q}_j) = V(-\hat{q})$$

and by now $\hat{p} = (\hat{p}_1, \hat{p}_2, \ldots, \hat{p}_N), \hat{q} = (\hat{q}_1, \hat{q}_2, \ldots, \hat{q}_N)$. Let us assume also, that $\hat{V} \geq 0$.

In this case all our arguments and proofs are true. In this situation the multiple integral over a gaussian measure is defined on the direct product of N copies of the space $X^N \equiv X \times X \times \cdots \times X$. An appropriate measure $\mu^N = \bigotimes_{k=1}^{N} \mu$ is a Cartesian product of the gaussian measures μ and as well as the measure μ is σ-additive [10]. The functional integral in this case is

$$\int_{X^N} F(x) d\mu^N(x),$$

where $x = (x_1, x_2, \ldots, x_N)$ is a function on $\bigotimes_1^N C^\circ[0, \beta]$. The gaussian domination condition takes the form $R(h) \leq R(0)$, where $h = (h_1, h_2, \ldots, h_N)$ is an arbitrary vector in R^N.

Consider construction of a functional integral over Bogoliubov's measure when an integrand function depends not only on coordinates but on momenta also. In this case instead of the expression (7) let us consider the average

$$\left\langle T \exp\left[i \sum_{j=1}^{N+1} \left(\sqrt{2m\omega}\, x_j \hat{Q}(s_j) + \sqrt{\frac{2}{m\omega}}\, y_j \hat{P}(s_j) \right) \right] \right\rangle,$$

with the Hamiltonian $\hat{\Gamma}$ again. This average is $\exp\left[-\Omega\left(\{x_j, y_j\}\right)\right]$, where the quadratic form on the variables x_j, y_j is

$$\Omega\left(\{x_j, y_j\}\right) = \sum_{j,k=1}^{N+1} S_{jk}(x_j x_k + y_j y_k) + \sum_{j,k=1}^{N+1} R_{jk} x_j y_k$$

and matrices are

$$S_{jk} = \frac{\omega}{\beta} \sum_{n=-\infty}^{\infty} \frac{e^{2\pi i n \beta^{-1}(s_j - s_k)}}{\omega^2 + \left(2\pi n \beta^{-1}\right)^2} = S_{kj},$$

$$R_{jk} = \frac{4\pi}{\beta^2} \sum_{n=-\infty}^{\infty} \frac{n e^{2\pi i n \beta^{-1}(s_j - s_k)}}{\omega^2 + (2\pi n \beta^{-1})^2} = -R_{kj}.$$

The Gibbs T-product average for an arbitrary measurable functional can be written down as $\langle T(f(\hat{Q},\hat{P}))\rangle = \int_X f(\xi)d\mu(\xi)$ with the gaussian measure defined on the space X of continuous functions of two variables that satisfy the conditions $x(0) = x(\beta), y(0) = y(\beta)$. The correlation function takes the form

$$M(t,s) = \left[\mathrm{ch}\left(\frac{\beta\omega}{2} - \omega|t-s|\right) + i\epsilon(t-s)\,\mathrm{sh}\left(\frac{\beta\omega}{2} - \omega|t-s|\right)\right] / \,\mathrm{sh}\,\frac{\beta\omega}{2},$$

where

$$\epsilon(x) = \begin{array}{rl} 1, & x > 0; \\ 0, & x = 0; \\ -1, & x < 0. \end{array}$$

The formula of linear substitution of a variable in integral over gaussian measure in this case takes the form

$$\int_X F(\xi)d\mu(\xi) = e^{-\frac{1}{2}(a,a)} \int_X F(\xi + a)e^{-(a,\xi)}d\mu(\xi),$$

where the linear measurable functional is defined as $(a,\xi) = \tilde{a}M\xi$.

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