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Asymptotic exactness of c-number substitution in Bogolyubov's theory of superfluidity

N.N. Bogolyubov, Jr., D.P. Sankovich

V.A. Steklov Institute of Mathematics, Gubkin Str. 8, Moscow, 119991, Russia

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The Bogolyubov model of liquid helium is considered. The validity of substituting a c-number for the $k = 0$ mode operator $\hat{a}_0$ is established rigorously. The domain of stability of the Bogolyubov's Hamiltonian is found. We derive sufficient conditions which ensure the appearance of the Bose condensate in the model. For some temperatures and some positive values of the chemical potential, there is a gapless Bogolyubov spectrum of elementary excitations, leading to a proper microscopic interpretation of superfluidity.

Key words: *Bose-Einstein condensation, Bogolyubov's Hamiltonian, superfluidity, c-number substitution*

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1. The model

Let us consider a system of N spinless identical nonrelativistic bosons of mass m enclosed in a centered cubic box $\Lambda \subset \mathbb{R}^3$ of volume $V = |\Lambda| = L^3$ with periodic boundary conditions for wave functions. The Hamiltonian of the system can be written in the second quantized form as

$$\hat{H}_\Lambda(\mu) \equiv \hat{H}_\Lambda - \mu\hat{N}_\Lambda = \sum_{k\in\Lambda^*}(\epsilon_k - \mu)\hat{a}_k^\dagger\hat{a}_k + \frac{1}{2V}\sum_{p,q,k\in\Lambda^*}\nu(k)\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_{p+k}\hat{a}_{q-k}\,. \tag{1}$$

Here $\hat{a}_k^\# = \{\hat{a}_k^\dagger \text{ or } \hat{a}_k\}$ are the usual boson (creation or annihilation) operators for the one-particle state $\psi_k(x) = V^{-1/2}\exp(\mathrm{i}kx), k \in \Lambda^*, x \in \Lambda$, acting on the Fock space $F_\Lambda = \oplus_{n=0}^\infty \mathcal{H}_\mathrm{B}^{(n)}$, where $\mathcal{H}_\mathrm{B}^{(n)} \equiv [L^2(\Lambda^n)]_\mathrm{symm}$ is the symmetrized n-particle Hilbert space appropriate for bosons, and $\mathcal{H}_\mathrm{B}^{(0)} = \mathbb{C}$. The sums in (1) run over the dual set

$$\Lambda^* = \left\{k \in \mathbb{R}^3 : k_\alpha = \frac{2\pi}{L}n_\alpha, n_\alpha = 0, \pm1, \pm2, \ldots, \alpha = 1,2,3\right\},$$

$\epsilon_k = |k|^2/(2m)$ is the one-particle energy spectrum of free bosons in the modes $k \in \Lambda^*$ (we propose $\hbar = 1$), $\hat{N}_\Lambda = \sum_{k\in\Lambda^*}\hat{a}_k^\dagger\hat{a}_k$ is the total particle-number operator, μ is the chemical potential, $\nu(k)$ is the Fourier transform of the interaction pair potential $\Phi(x)$. We suppose that $\Phi(x) = \Phi(|x|) \in L^1(\mathbb{R}^3)$ and $\nu(k)$ is a real function with a compact support such that $0 \leqslant \nu(k) = \nu(-k) \leqslant \nu(0)$ for all $k \in \mathbb{R}^3$. Under these conditions the Hamiltonian (1) is superstable [1].

So long as the rigorous analysis of the Hamiltonian (1) is very knotty problem, Bogolyubov introduced the model Hamiltonian of superfluidity theory [2, 3]. He proposed to disregard the terms of the third and fourth order in operators $\hat{a}_k^\#, k \neq 0$ in the Hamiltonian (1),

$$\begin{aligned}\hat{H}_\Lambda^\mathrm{B}(\mu) \;=\; & \sum_{k\in\Lambda^*}(\epsilon_k - \mu)\hat{a}_k^\dagger\hat{a}_k + \frac{1}{2V}\sum_{k\neq0}\nu(k)(\hat{a}_k^\dagger\hat{a}_{-k}^\dagger\hat{a}_0\hat{a}_0 + \hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_{-k}\hat{a}_k) \\ & + \frac{1}{V}\hat{a}_0^\dagger\hat{a}_0\sum_{k\neq0}\nu(k)\hat{a}_k^\dagger\hat{a}_k + \frac{\nu(0)}{V}\hat{a}_0^\dagger\hat{a}_0\sum_{k\neq0}\hat{a}_k^\dagger\hat{a}_k + \frac{\nu(0)}{2V}\hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_0\hat{a}_0\,. \end{aligned}\tag{2}$$

Then Bogolyubov takes advantage of the most relevant operators in the problem to replace the corresponding creation and annihilation operators $\hat{a}_0^{\#}$ by c-numbers,

$$\frac{\hat{a}_0^{\dagger}}{\sqrt{V}} \to \bar{c}, \qquad \frac{\hat{a}_0}{\sqrt{V}} \to c, \tag{3}$$

where $c \in \mathbb{C}$ and the bar means complex conjugation. This idea has its roots in the work [4]. In §63 of this monograph Dirac analyses a many-body system within the framework of second quantization. Bogolyubov developed the Dirac's idea systematically to study Bose condensation and superfluidity in the model (2).

Let $\hat{H}_{\Lambda}^{\mathrm{B}}(\mu, c)$ be the Hamiltonian (2) after the Bogolyubov approximation (3). This Hamiltonian is a bilinear form in boson operators $\hat{a}_k^{\#} (k \neq 0)$. So, one can diagonalize it by the Bogolyubov canonical transformation. To determine the complex parameter c it is necessary to use some self-consistent procedure.

In [2, 3] Bogolyubov considered the Hamiltonian (2) in the case of zero temperature θ. In the main perturbation order he found that $\mu(\theta = 0) = |c|^2 \nu(0)$, where $|c|^2 = \rho_0$ is the density of Bose condensate. In this case the structure of the collective excitation spectrum of the Hamiltonian $\hat{H}_{\Lambda}^{\mathrm{B}}(\mu, c)$ explains the superfluid properties of the system (2).

It should be noted that the main condition which makes it possible to replace the Hamiltonian (1) by the model Hamiltonian (2) is

$$\frac{N - N_0}{N} \ll 1, \tag{4}$$

where N_0 is the number of condensate particles. Condition (4) means that the interaction is sufficiently weak and the case of very small temperatures must be considered. Thus in 1947 Bogolyubov analysed the model (2) within the framework of (4). The validity of the Bogolyubov approximation (3) has not been rigorously proved.

A rigorous justification for the c-number substitution in the case of the total, correct superstable pair Hamiltonian (1) was done in a classic paper of Ginibre [5]. Recently, this problem was revisited in paper [6]. The authors of [5, 6] did not consider the truncated Bogolyubov's Hamiltonian (2). Nevertheless, Lieb and others [6] mentioned that their device (based on the Berezin-Lieb inequality) can be also used for the Hamiltonian (2). Earlier, in [7–9] the Bogolyubov prescription concerning substitution of the zero-mode annihilation and creation operators by c-numbers and concerning their choice was discussed. The authors of these articles arrived at a conclusion that the Bogolyubov's Hamiltonian (2) is unstable for $\mu > 0$, which is the choice of the Bogolyubov theory. So, from [7–9] it follows that the Bogolyubov's model (2) does not explain the superfluidity. This wrong conclusion is based on the erroneous Proposition 4.3 in [7] and Theorem 3.8 in [9].

Here we revert to the problem of justification of c-number substitution for the Bogolyubov's Hamiltonian (2). We show how to use the Ginibre approach for the non-superstable Hamiltonian (2). To find the stability region of (2), i.e., the domain in a space of independent thermodynamical variables (μ, θ), where the grand-canonical partition function associated for the Hamiltonian (2) is finite, we use the Bogolyubov's inequality [10], which efficiently gives the upper bound for the pressure. Besides, we derive sufficient conditions which ensure the appearance of the Bose condensate in the model.

2. Stability of the Hamiltonian

Let us first rewrite the Hamiltonian (2) in the following way:

$$\hat{H}_{\Lambda}^{\mathrm{B}}(\mu) = \hat{H}_{\Lambda 0}^{\mathrm{B}}(\mu, c) + \hat{H}_{\Lambda 1}^{\mathrm{B}}(c), \tag{5}$$

where

$$\hat{H}_{\Lambda 0}^{\mathrm{B}}(\mu, c) \equiv \sum_{k \in \Lambda^*} (\epsilon_k - \mu - \frac{1}{2V}\nu(k)) \hat{a}_k^{\dagger} \hat{a}_k - \frac{\Phi(0)}{2} \hat{a}_0^{\dagger} \hat{a}_0 + \frac{\nu(0)}{2V} \hat{a}_0^{\dagger} \hat{a}_0^{\dagger} \hat{a}_0 \hat{a}_0 + \nu(0)|c|^2 \sum_{k \neq 0} \hat{a}_k^{\dagger} \hat{a}_k \,, \tag{6}$$

$$\hat{H}^{\mathrm{B}}_{\Lambda 1}(c) \quad\equiv\quad \frac{\nu(0)}{V}(\hat{a}^{\dagger}_{0}\hat{a}_{0} - V|c|^{2})\sum_{k\neq 0}\hat{a}^{\dagger}_{k}\hat{a}_{k} + \frac{1}{2V}\sum_{k\neq 0}\nu(k)(\hat{a}^{\dagger}_{0}\hat{a}_{k} + \hat{a}_{0}\hat{a}^{\dagger}_{-k})^{\dagger}(\hat{a}^{\dagger}_{0}\hat{a}_{k} + \hat{a}_{0}\hat{a}^{\dagger}_{-k}). \quad (7)$$

The complex parameter c in formulae (5)–(7) will be defined below. It is easy to see that the Hamiltonian (6) is stable for $\mu \leqslant \nu(0)|c|^{2}$ and any $c \in \mathbb{C}$.

Denoting

$$\delta\hat{a}_{0} \equiv \hat{a}_{0} - c\sqrt{V}, \qquad \delta\hat{a}^{\dagger}_{0} \equiv \hat{a}^{\dagger}_{0} - \bar{c}\sqrt{V}, \qquad \hat{A}_{k} \equiv \hat{a}^{\dagger}_{0}\hat{a}_{k} + \hat{a}_{0}\hat{a}^{\dagger}_{-k}\,, \qquad k \neq 0,$$

we can write (7) in the form

$$\hat{H}^{\mathrm{B}}_{\Lambda 1}(c) = \frac{\nu(0)}{V}\sum_{k\neq 0}\hat{a}^{\dagger}_{k}\hat{a}_{k}\left(\delta\hat{a}^{\dagger}_{0}\delta\hat{a}_{0} + c\sqrt{V}\delta\hat{a}^{\dagger}_{0} + \bar{c}\sqrt{V}\delta\hat{a}_{0}\right) + \frac{1}{2V}\sum_{k\neq 0}\nu(k)\hat{A}^{\dagger}_{k}\hat{A}_{k}\,. \quad (8)$$

Let us prove that

$$\lim_{V\to\infty}\frac{1}{V}\left\langle \hat{H}^{\mathrm{B}}_{\Lambda 1}(c)\right\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu)} \geqslant 0, \quad (9)$$

where c is a solution of the equation

$$|c|^{2} = \frac{1}{V}\langle\hat{a}^{\dagger}_{0}\hat{a}_{0}\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu)}\,.$$

From the Bogolyubov inequality for pressures

$$p\left[\hat{H}^{\mathrm{B}}_{\Lambda}(\mu)\right] \leqslant p\left[\hat{H}^{\mathrm{B}}_{\Lambda 0}(\mu,c)\right] - \frac{1}{V}\langle\hat{H}^{\mathrm{B}}_{\Lambda 1}(c)\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu)}$$

we then obtain that the Hamiltonian (2) is stable for

$$\mu \leqslant \nu(0)|c|^{2}. \quad (10)$$

Let us introduce the Hamiltonian

$$\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu) \equiv \hat{H}^{\mathrm{B}}_{\Lambda}(\mu) - \sqrt{V}(\bar{\nu}\hat{a}_{0} + \nu\hat{a}^{\dagger}_{0})$$

with sources $\nu \in \mathbb{C}$ breaking the symmetry of $\hat{H}^{\mathrm{B}}_{\Lambda}(\mu)$. Using the Cauchy inequality, we get the estimate

$$\langle\delta\hat{a}^{\dagger}_{0}\hat{N}'\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu)}| \leqslant \left[\langle\delta\hat{a}^{\dagger}_{0}\delta\hat{a}_{0}\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu)}\langle\hat{N}'^{2}\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu)}\right]^{1/2} \leqslant \rho V\langle\delta\hat{a}^{\dagger}_{0}\delta\hat{a}_{0}\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu)}\,,$$

where $\hat{N}' \equiv \sum_{k\neq 0}\hat{a}^{\dagger}_{k}\hat{a}_{k}$.

To obtain an upper bound for the average in the last inequality we can apply the usual procedure of the Bogolyubov quasi-average method [11] and Bogolyubov, Jr. technique [12]. Define c by the condition $c = \langle\hat{a}_{0}\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu)}/\sqrt{V}$, $|c| \leqslant M < \infty$. By the Harris inequality [13] one gets

$$\frac{1}{2}\left\langle[\delta\hat{a}^{\dagger}_{0},\delta\hat{a}_{0}]_{+}\right\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu)} \leqslant (\delta\hat{a}^{\dagger}_{0},\delta\hat{a}_{0})_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu)} + \frac{\beta}{12}\left\langle[\delta\hat{a}_{0},[\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu),\delta\hat{a}^{\dagger}_{0}]]\right\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu)}\,,$$

where $[\cdot,\cdot]_{+}$ is the anticommutator and $(\cdot,\cdot)_{\hat{\Gamma}}$ denotes the Bogolyubov inner product (or the Duhamel two-point function) with respect to the Hamiltonian Γ [10]. Literally reiterating the standard for this method of calculations [5], we see that

$$\frac{1}{V}\langle\delta\hat{a}^{\dagger}_{0}\delta\hat{a}_{0}\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu)} \leqslant \frac{\eta}{\sqrt{V}}\,,$$

where η is some positive constant, independent of V. Therefore, it follows from the last inequality that

$$|\langle\delta\hat{a}^{\#}_{0}\hat{N}'\rangle_{\hat{H}^{\mathrm{B}}_{\Lambda}(\mu,\nu)}| \leqslant \rho\sqrt{\eta}V^{5/4}.$$

Thus, using the representation of the Hamiltonian $\hat{H}^{\rm B}_{\Lambda 1}(c)$ in the form (8) one can see that the condition (9) is actually justified. The parameter c should be chosen using the technique stereotyped for the Bogolyubov–Ginibre technique. This parameter is connected with the Bose condensate density as $|c|^2 = \rho_0$.

The above analysis confirms an assertion that if the system is stable after the c-number substitution (3), then so is the original one [6].

3. Self-consistency equation

In the manner similar to the work by Ginibre [5], one can prove that the model Hamiltonian $\hat{H}^{\rm B}_{\Lambda}(\mu)$ is thermodynamically equivalent to the approximating Hamiltonian

$$\begin{aligned}\hat{H}^{\rm B}_{\Lambda}(\mu, c) &= \sum_{k\neq 0}[\epsilon_k - \mu + |c|^2(\nu(0) + \nu(k))]\hat{a}^{\dagger}_k \hat{a}_k \\ &+ \frac{1}{2}\sum_{k\neq 0}\nu(k)(c^2\hat{a}^{\dagger}_k\hat{a}^{\dagger}_{-k} + \bar{c}^2\hat{a}_k\hat{a}_{-k}) + \frac{1}{2}\nu(0)|c|^4 V - \mu|c|^2 V. \qquad (11)\end{aligned}$$

The self-consistency parameter c in the method is determined by the condition that the approximate pressure $p[\hat{H}^{\rm B}_{\Lambda}(\mu, c)]$ should be maximal. At the same time, the stability condition (10) must be fulfilled.

A necessary condition for $p[\hat{H}^{\rm B}_{\Lambda}(\mu, c)]$ to be maximum (self-consistency equation) in the case of the Bogolyubov model is

$$\left\langle \frac{\partial \hat{H}^{\rm B}_{\Lambda}(\mu, c)}{\partial c}\right\rangle_{\hat{H}^{\rm B}_{\Lambda}(\mu,c)} = 0. \qquad (12)$$

This equation always has a trivial solution $c = 0$ (no Bose condensation). By explicit calculations, we get the following equation to obtain a nontrivial solution

$$\mu - x\nu(0) = \frac{1}{2V}\sum_{k\neq 0}\left[(\nu(0) + \nu(k))\left(\frac{f_k}{E_k}\coth\frac{\beta E_k}{2} - 1\right) - \nu(k)\frac{h_k}{E_k}\coth\frac{\beta E_k}{2}\right], \qquad (13)$$

where

$$\begin{aligned} u_k &= \sqrt{\frac{1}{2}\left(\frac{f_k}{E_k} + 1\right)}, \qquad v_k = -\sqrt{\frac{1}{2}\left(\frac{f_k}{E_k} - 1\right)}, \\ f_k &= \epsilon_k - \mu + x(\nu(0) + \nu(k)), \qquad h_k = x\nu(k), \qquad E_k = \sqrt{f_k^2 - h_k^2}\end{aligned}$$

and we denote $x \equiv |c|^2$.

Let us first consider the zero temperature case. In this case the right-hand side of (13) is

$$F(x) \equiv \frac{1}{2V}\sum_{k\neq 0}\left[(\nu(0) + \nu(k))\left(\frac{f_k}{E_k} - 1\right) - \nu(k)\frac{h_k}{E_k}\right].$$

One can see that $F'(x) < 0$ and $F''(x) > 0$, i.e., the function $F(x)$ is strictly monotonously decreasing and convex on $[0, \infty)$. Furthermore, it is bounded from below. We are interested in the case where $\mu > 0$ (remind that always $\mu \leqslant x\nu(0)$). For the unique nontrivial solution x^* of the equation (13) to exist, it is necessary that

$$\Delta(\mu) \equiv F\left(x = \frac{\mu}{\nu(0)}\right) \leqslant 0.$$

From now on, we shall use the function

$$\nu(k) = \begin{cases} \nu(0) & \text{for } |k| \leqslant k_0, \\ 0 & \text{for } |k| > k_0 \end{cases} \qquad (14)$$

as the Fourier transform of the pair potential. We suppose that $\nu(0) = 4\pi r_0/m, k_0 r_0 = 1, r_0 = 2.56$ Å$, m = m_{He^4}$. In the case of the potential (14) the nontrivial root μ^* of the equation $\Delta(\mu) = 0$ is

$$\mu^* = \frac{k_0^2}{36m}(4 - \sqrt{1.6})^2.$$

If

$$\nu(0) \geqslant \frac{1}{2V}\sum_{k\neq 0}\frac{\nu^2(k)}{\epsilon_k}\,, \tag{15}$$

for $\theta = 0$ and $0 < \mu \leqslant \mu^*$, where μ^* is the unique nontrivial solution of the equation $\Delta(\mu) = 0$, the Bose condensation can be realized. For $\mu = \mu^*$, the Bose condensate density ρ_0^* has a maximum and is defined by the equation $\mu^* = \rho_0^*\nu(0)$. The stability condition $\mu \leqslant \nu(0)\rho_0$ is fulfilled. Notice that for all $0 < \mu \leqslant \mu^*$, the curve $\rho_0(\mu)$ very little differs from the straight line $\rho_0 = \mu/\nu(0)$ (for the potential (14) the deflection is $\sim 0.1\%$). The condition of the existence of Bose condensate at $0 < \mu \leqslant \mu^*$ is in excellent agreement with the previous estimate of the Bogolyubov theory correctness (see formula (29) in paper [2]) $\nu(0) \ll v/(2mr_0^2)$. Here we must take into account that $v \sim \rho^{-1}$ and suppose (as was conjectured by Bogolyubov) that $\mu = \rho\nu(0)$.

Consider now the case $\theta > 0$. Denote by $F_\beta(x)$ the right-hand side of the equation (13). As a function of x, this function is strictly monotonously decreasing, convex and bounded from below on $[0, \infty)$ for any β. As shown above, we reach a conclusion that if

$$\Delta_\beta(\mu) \equiv F_\beta\left(x = \frac{\mu}{\nu(0)}\right) \leqslant 0$$

then the equation (13) will have a nontrivial unique solution for $\mu > 0$. The function $\Delta_\beta(\mu)$ increases if β decreases. The "critical curve" $\theta = \theta_0(\mu)$ is determined by the equation $\Delta_\beta(\mu) = 0$. One can verify that $\partial^2\theta_0/\partial\mu^2 < 0$. On this curve, the Bose condensate density has a maximum $\rho_0 = \mu/\nu(0)$. The curve $\theta = \theta_0(\mu)$ is illustrated in figure 1.

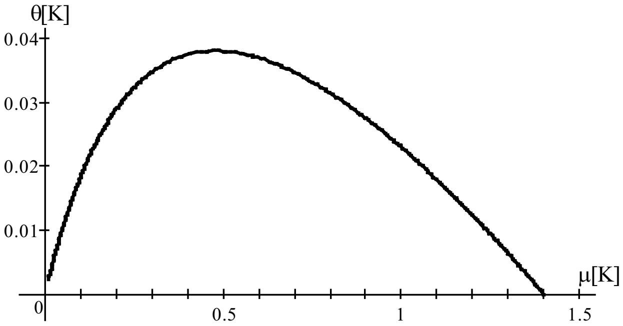

Figure 1. Phase diagram.

Let $\mu \leqslant 0$ and the potential $\nu(k)$ satisfies (15). Then, the self-consistency equation for the Bogolyubov model for any θ has a trivial solution only. In this case, the Bogolyubov model is thermodynamically equivalent to the ideal Bose gas.

4. Conclusion

We have shown that if the potential $\nu(k)$ in the Bogolyubov model of superfluidity (2) satisfies the condition (15), then there exists a domain of stability on the phase diagram $\{0 < \mu \leqslant \mu^*, 0 \leqslant \theta \leqslant \theta_0(\mu)\}$, where the nontrivial solution of self-consistency equation takes place. In this domain, there is a non-zero Bose condensate. At the boundary $\theta = \theta_0(\mu)$ of this domain, the Bose condensate density equals $\rho_0 = \mu/\nu(0)$. In this case, the quasi-particles spectrum of the Bogolyubov

Hamiltonian (2)

$$E_k = \sqrt{\epsilon_k(\epsilon_k + 2\rho_0\nu(k))}$$

is of a gapless type, and the famous criterion of superfluidity $\min_k(E_k/|k|) > 0$ holds.

As we have noted earlier, the Bogolyubov's theory is a theory of a dilute weakly interacting Bose gas at temperatures far below the λ-point. This is particularly evident from the phase diagram. By contrast to the pair Hamiltonian (1), the Bogolyubov's Hamiltonian (2) does not correspond to some pair interaction and it is not superstable. Nevertheless, Bogolyubov's approach forms the basis for a systematic application of quantum theory to an interacting system of bosons (for a review, see [14]).

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Асимптотична точність підстановки c-чисел в теорії надплинності Боголюбова

Н.Н. Боголюбов (мол.), Д.П. Санковіч

Математичний інститут ім. В.А.Стєклова Російської академії наук, Москва, Російська Федерація

Розглядається модель Боголюбова для рідкого гелію. Обґрунтованість підстановки c-числа для $\boldsymbol{k} = \mathbf{0}$ модового оператора $\hat{\boldsymbol{a}}_{\mathbf{0}}$ строго встановлюється. Знайдено область стабільності гамільтоніану Боголюбова. Ми виводимо достатні умови, що забезпечують появу бозе-конденсату в цій моделі. Для деяких температур та значень хімічного потенціалу існує безщілинний боголюбівський спектр елементарних збуджень, що приводить до належної мікроскопічної інтерпретації надплинності.

Ключові слова: *бозе-ейнштейнівська конденсація, гамільтоніан Боголюбова, надплинність, підстановка c-числа*