The He II Theory Preserving the Symmetry of the Initial Hamiltonian of the System

I.M.Yurin

I.M.Yurin, Fl.61, bld. 7, 22 Festivalnaya St, Moscow, 125581, Russian Federation

(Dated: December 12, 2013)

The article suggests a method for the construction of the He II theory preserving the symmetry of the initial Hamiltonian.

PACS numbers: 67.85.Hj, 67.85.Jk

I. INTRODUCTION

In 1947 Bogoliubov suggested a microscopic description of He II [1]. The main idea of this description is the selection of the two-particle interaction terms in the Hamiltonian

\[ \hat{H} \sim a_0^+ a_0, a_0^+ a_0^+, a_0 a_0, \]

where \( a^+_p \) and \( a_p \) are the creation and annihilation operators for He\(^4\) atoms with momentum \( p \). Accounting for these terms only in order to calculate the physical parameters of the system is not in doubt, because the condensation of a macroscopic number of atoms in a state with zero momentum results in the fact that the transition matrix elements corresponding to the selected terms are far superior in magnitude to the rest of the matrix elements.

However, for the diagonalization procedure Bogolyubov replaced operators \( a^+_0 \) and \( a_0 \) with so-called c-numbers. As a result, the truncated Hamiltonian, in contrast to the initial one, no longer keeps the number of particles in the system, which means the breach of the initial Hamiltonian symmetry (IHS) of the system. This state of affairs will always be a concern in the scientific community [2].

This paper suggests a variant of the construction of the He II theory based on the partial diagonalization of the truncated Hamiltonian suggested recently by Ettouhami [3].

II. DIAGONALIZATION PROCEDURE

So, let us consider the truncated Hamiltonian

\[ \hat{H}_{trunc} = \sum_{q>0} \hat{h}_q, \]  

while

\[ \hat{h}_q = t_q a^+_q a_q + \frac{V}{2t^2} a^+_q a^+_q a_0 a_0 + \frac{V}{2t^2} a^+_q a^+_0 a_q a_0 + \frac{V}{t} a^+_q a^+_q a_q a_0, \]

where \( \Omega \) is the system volume. Hereinafter we will not consider the terms \( \sim V_0 \), because they only add a constant to the energy of the system with a fixed number of particles.

Let us find the ground state of the system \( \Phi_0 \) as

\[ \Phi_0 = \frac{[a^+_0]^N}{\sqrt{N!}} |0\rangle + \frac{1}{2} \sum_{q>0} \sum_{0<m\leq N/2} \alpha^q_m \frac{[a^+_q a^+_q]^m}{m!} \frac{[a^+_0]^N-2m}{\sqrt{(N-2m)!}} |0\rangle, \]

where \( N \) is the number of particles in the system and

\[ \alpha^q_m = \alpha^{-q}_m. \]

Then the diagonalization of \( \hat{H}_{trunc} \) within space of states linked with right hand side of

\[ \Lambda = \left\{ \frac{[a^+_q a^+_q]^m}{m!} \frac{a^+_0^{(N-2m)}}{\sqrt{(N-2m)!}} |0\rangle : 0 \leq m \leq N/2, q > 0 \right\} \]

*Electronic address: yurinoffice@mail.ru
is decoupled into independent diagonalizations of Hamiltonians $\hat{h}_q$ in the subspaces

$$\lambda_q = \left\{ \left[ a_+^q a^-_q \right]_m^m \left[ \alpha_q^+ \right]^{N-2m} \right\},$$

(6)

which gives equations for the eigenvalues $\varepsilon_q$:

$$\begin{align*}
v_q m \sqrt{(N-2m+2)(N-2m+1)} \alpha_{m-1}^q \\
+ 2 mt_q \alpha_m^q + 2 v_q m (N-2m) \alpha_m^q \\
+ \frac{V_q}{\Omega} (m+1) \sqrt{(N-2m-1)(N-2m)} \alpha_{m+1}^q = \varepsilon_q \alpha_m^q.
\end{align*}$$

(7)

An additional definition will be useful in (7):

$$\alpha_{-1}^q = 0, \quad \alpha_0^q = 1$$

(8)

for its convenient connection with (3) at $m = 0$.

Let us now introduce operators $\varphi_+^q$ and $\varphi_q^-$:

$$\begin{align*}
\varphi_+^q &= \frac{u_q^q}{\sqrt{N}} a_+^q a_0^q + \frac{v_q^q}{\sqrt{N}} a^-_q a_q^q, \\
\varphi_q^- &= \frac{u_q^q}{\sqrt{N}} a_0^q a_q^q + \frac{v_q^q}{\sqrt{N}} a_+^q a^-_q a_0^q,
\end{align*}$$

(9)

where

$$\begin{align*}
u_q^q &= \frac{\omega_q^q + t_q}{2 \sqrt{t_q^q}} \\
v_q^q &= \frac{\omega_q^q - t_q}{2 \sqrt{t_q^q}}
\end{align*}$$

(10)

with

$$\omega_q^q = \sqrt{t_q^q (t_q^q + 2V_q N/\Omega)}.$$ 

(11)

Evidently, $u_q^q$ and $v_q^q$ coincide in magnitude with parameters of $u - v$ Bogoliubov’s transformation.

Such a definition of $\varphi_+^q$ and $\varphi_q^-$ corresponds to the implementation of the equation

$$[\hat{H}, \varphi_+^q] = \omega_q \varphi_+^q$$

(12)

in random phase approximation in the case when all the atoms are condensed at the low energy level, where

$$\hat{H} = \sum_q t_q a_+^q a_q^q + \sum_{p,k,q} \frac{V_q}{2\Omega} a_+^p a_+^q a_+^k a_+^q a_+^p$$

(13)

is the total Hamiltonian of the system.

Obviously, in view of (12) the lowest energy $\varepsilon_q$ is reached when

$$\varphi_q \Phi_0 = 0,$$

(14)

here the action of $\varphi_q$ should be limited to the subspace $\lambda_q$. Thus, in case of $m \geq 0$ we have

$$\alpha_m^q = \left( \frac{t_q^q - \omega_q^q}{t_q^q + \omega_q^q} \right)^m \prod_{i=1}^m \sqrt{\frac{N - 2i + 2}{N - 2i + 1}}$$

(15)

On the other hand, in the same limit, it follows from (7) at $m = 0$ that

$$\Delta_q \alpha_1^q = \varepsilon_q \alpha_0^q,$$

(16)

where

$$\Delta_q = V_q N/\Omega.$$ 

(17)
The combined consideration of (15, 16) gives

$$\varepsilon_q = \omega_q - t_q - \Delta_q.$$  

(18)

and with this choice of $\varepsilon_q$, Eq. (7) is also satisfied at any $m > 0$.

The action of operators $[h^+_{q}]^m [h^-_{q}]^{m-n} / \sqrt{n_q!m_q!}$ on $\Phi_0$ within subspace

$$\tilde{\lambda}_q = \left\{ \frac{[a^+_q]^m [a^-_{-q}]^n}{\sqrt{m!n!}} \frac{[a^+_q]^{N-m-n}}{\sqrt{(N-m-n)!}} |0\rangle : m \geq 0, n \geq 0, m + n \leq N \right\}$$  

gives the excited states of the system. Thus, the system energy $E$ takes the form

$$E = \frac{1}{2} \sum_{q > 0} \varepsilon_q + \sum_{q > 0} n_q \omega_q.$$  

(20)

This is completely consistent with Bogoliubov’s results for the excitation spectrum of the system.

III. VACUUM STATE OF THE PHONON SYSTEM

Refining the obtained approximation of the wave functions of the system stationary states with the use of the standard perturbation theory [3] encountered difficulties due to the appearance of a gap in the phonon spectrum, which is clearly contrary to the Goldstone theorem [4] for such systems. Les us temporarily put aside the Hamiltonian diagonalization procedure and engage the search of the vacuum state of the phonon system. For this purpose let us consider the sequence of states $\Phi_0^{(n)}$ composed by the following rules:

$$\Phi_0^{(-1)} = 0,$$

$$\Phi_0^{(0)} = \frac{[a^+_q]^N}{\sqrt{N!}} |0\rangle,$$

$$\Phi_0^{(n)} = \Phi_0^{(n-1)} + \frac{1}{2} \sum_{q_n > 0} \tilde{G}(q_n) \left( \Phi_0^{(n-1)} - \Phi_0^{(n-2)} \right),$$  

(21)

where

$$\tilde{G}(q) = \sum_{0 < m \leq n_0/2} (-g(q))^m [a^+_q a^-_{-q}]^m \frac{\tilde{n}_q!}{(n_q + m)!} \frac{\tilde{n}^-_{-q}!}{(n^-_{-q} + m)!} [a_0]^m \sqrt{\frac{(n_0 - 2m)!}{n_0!}}.$$  

(22)

$$g(q) = \frac{\omega_q - t_q}{\omega_q + t_q},$$  

(23)

while $q_{i+1} \neq \pm q_i$, if $i > 0$, $n \leq N/2$, and $\tilde{n}_p = a^+_p a^-_p$. Obviously, $\Phi_0^{(1)}$ tends to rhs of (23) as $N \to \infty$. So, the relationship of further discussion with the approach suggested by Etouhami is evident.

On the other hand, the structure of wave functions $\Phi_0^{(n)}$ makes it possible to calculate the system parameters as a power series by small parameters $g(q)$. This possibility seems very attractive from the viewpoint of the theory evolution.

Let us redefine operators $\varphi^+_q$ and $\varphi^-_q$ (cf. Eq. (9)):

$$\varphi^+_q = u_q a^+_q a^-_q \frac{1}{\sqrt{n_q}} + \frac{v_q}{\sqrt{n_q}} a^+_q a^-_q,$$  

(25)

$$\varphi^-_q = \frac{u_q}{\sqrt{n_q}} a^+_q a^-_q + \frac{v_q}{\sqrt{n_q}} a^+_q a^-_q \frac{1}{\sqrt{n_q}}.$$  

Evidently, the commutation relations $[\varphi^+_k, \varphi^+_q]$ and $[\varphi^-_k, \varphi^-_q]$ are bosonic. This statement should be understood in the sense that the action of the commutation relations on the state containing at least one atom with zero momentum gives zero for $[\varphi^+_k, \varphi^-_q]$ and does not differ from the action of the corresponding Kronecker delta for $[\varphi^-_k, \varphi^-_q]$. On
the other hand, it is easy to show that the fraction of states not containing atoms with zero momentum for the state with $N_\varphi$ phonons is $\sim \prod_{0<i<N/2-N_\varphi} g(q_i)$. It means that for large systems with $N_\varphi \ll N/2$ the commutation relations under consideration become bosonic with any desired accuracy on the order of small parameters $g(q)$. This allows determining the orthonormal bases of states with any desired accuracy using the formal expansion of the wave functions in the small parameters $g(q)$, if the number of phonons is not too large.

For the construction of the above-mentioned bases of states it is essential that relationships $\varphi_q \Phi_0 = 0$ be fulfilled with high accuracy. On the other hand, for $\Phi^{(n)}_0$ these relationships are true with a precision of $\sim \prod_{i=1}^n g(q_i)$. Therefore, these relationships can be fulfilled with any degree of accuracy: it is enough to choose a sufficiently large $N$.

In the future we shall use $\Phi_0$ to designate the vacuum state of the phonon system.

IV. TRANSITION TO THE FULL HAMILTONIAN OF THE SYSTEM

In systems with very large expectation values of $a_0^+ a_0$ initial operators $a_q^+$ and $a_q$ can be expressed in terms of operators $\varphi_q^+$ and $\varphi_q$ as follows:

$$
a_q^+ = (u_q \varphi_q^+ - v_q \varphi_{-q}) a_0^+ \frac{1}{\sqrt{n_0}},
\quad
a_q = \frac{1}{\sqrt{n_0}} a_0 \left( u_q \varphi_q - v_q \varphi_{-q}^+ \right).$$

This definition should be understood in the sense that the action of the parent operators $a_0^+$ and $a_q$ on the state containing at least one atom with zero momentum does not differ from the action of the operators taken from the lhs of (26). So, (26) can be used to replace the parent operators with the phonon ones in case when it comes to states with a not very large number of phonons. The reasoning here is a little different from the above reasoning on commutation relations $[\varphi_k^+, \varphi_q^+]$ and $[\varphi_k, \varphi_q^+]$.

The operator notation of the Hamiltonian (13) is different from the representation of the Hamiltonian in the creation and annihilation operators of the so-called bogolons, if the creation and annihilation operators of the bogolons are replaced with operators $\varphi_q^+$ and $\varphi_q$, respectively. In this connection let us dwell upon the calculation of the phonon spectrum restricting ourselves to a simplest basis of four states: $\Phi_0$, $\varphi_q^+ \Phi_0$, $\varphi_{-q}^+ \Phi_0$ and $\varphi_q^+ \varphi_{-q}^+ \Phi_0$. The matrix elements of the Hamiltonian for the transitions connecting these states determine the effective Hamiltonian bilinear by the creation and annihilation operators of phonons. Diagonalization of this Hamiltonian leads to the following expression for the spectrum dispersion:

$$\hat{\omega}_q = \sqrt{t_q (t_q + 2V_q \langle \hat{n}_0 \rangle_0 / \Omega)},$$

where $\langle \ldots \rangle_0$ denotes averaging over the vacuum state of the phonon system. It is important to note that for the realistic interatomic potential $V_q$ we have $\langle \hat{n}_0 \rangle_0 \ll N$, which leads to a considerable difference in the dispersion estimates in the suggested theory and the Bogoliubov approach.

At this point it is important to note that in our reasoning we did not have to impose restrictions of the type $N - \langle \hat{n}_0 \rangle_0 \ll N$ on the wave functions (as a rule, these restrictions are used by the authors when considering the He II system [3, 6]). This, apparently, makes possible the in fact first-principle calculation of the spectrum with a realistic interatomic potential.

Thus, analysis indicates a significant difference of the calculated physical quantities that define the limits of applicability of c-numbers in physical theories.

V. DISCUSSION

From the very outset Bogoliubov estimated his method of reviewing the He II system as very rough and approximate [1]. Respectively, the system description was done up to now as follows: on the basis of a rough calculation in the lowest degrees of the perturbation theory in Bogoliubov’s theory conclusions were made about the necessity of introducing of one or other terms in the phenomenological theories.

In contrast, the suggested approach allows both to pose more ambitious problems and to investigate the paradox of the "observability" of the phases of the wave functions of the superconductor and of the superfluid systems.
Immediately, we note that the uncertainty relationship
\[ \Delta N \Delta \varphi < \sim 2\pi \] (28)
in the most cited paper on this subject [7], unfortunately, contains neither references nor substantiation. On the other hand, relationships of this kind are introduced in quantum physics only for the observed quantities, and the phase of the wave function is known to be an unobservable variable.

The paradox of the phase of the wave function of a superconductor is known since 1964. However, it has been described in the available literature for an electronic system comparatively recently [8].

For the case of boson systems this paradox consists in the following. If one replaces in \( u - v \) Bogoliubov transformation parameters \((u_q, v_q)\) with \((u_q \exp(i\varphi), v_q \exp(-i\varphi))\), then the equations used to determine them still remain true. This fact should be related to the unitary transformation of the basis states \( \exp(i\varphi \hat{N}) \), which, as it follows from the fundamentals of the quantum theory, should not change the values of physical quantities.

Let us now consider the following situation. Let us bring into contact two systems of helium with the use of Hamiltonian
\[ \hat{H}_T = \sum_{k,q} T_{k,q} a_k^+ a_q + H.c. \] (29)

We assume that the operators corresponding to the momentum \( k \) are related to the atoms of the first system, and that those corresponding to the momentum \( q \) are related to the atoms of the second system.

Let us apply transformation \( \exp(i\varphi \hat{N}) \) in the space of basis states of one of the systems, that is, let us replace parameters \((u_q, v_q)\) with \((u_q \exp(i\varphi), v_q \exp(-i\varphi))\). It would seem that the observed values of the system should not be changed according to the principles of quantum physics. However, an elementary calculation shows a change, for example, in the total energy of two systems.

The existence of this paradox is unacceptable for a theory which claims to be a scientific theory. It is striking that the followers of the BCS theory use the paradox to interpret the Josephson effect, rather than to resolve it. Previously the Josephson effect could be explained for electronic systems without violating the principles of quantum physics [8]. Unfortunately, this was done beyond the recognized BCS theory [9], which is obviously a descendant of the Bogoliubov approach to the description of He II.

The suggested He II theory, evidently, has no such paradoxes.

**VI. CONCLUSION**

In this paper a He II theory preserving the symmetry of the initial Hamiltonian was created. The absence of paradoxes associated with the "uncertainty" of the phase of the wave function in the suggested approach enables to pose problems attracting calculations of any precision in the model of two-particle interaction for boson systems, in contrast to the Bogoliubov’s approach.

At this point it is appropriate to note that a number of requirements are placed to physical theories. In particular, they should not give results contradicting the foundations of quantum physics. As for various approaches to physical problems in the early stages of their consideration, the requirements for them are not so strict. However, not all approaches necessarily result in the creation of physical theories.

**Acknowledgments**

The author is grateful to Professor A.A. Rukhadze for the moral support of author’s works on theories of superphenomena. In addition, the author thanks D.Sc. S.A. Trigger for criticism of author’s first attempts to solve the problem, which were subsequently refused.

[1] N.N. Bogoliubov. Izv. Akad. Nauk USSR 11 (1947) 77-90.
[2] V.B. Bobrov, S.A. Trigger. J. Low Temp Phys, Vol.170, 31, (2013),
[3] A. M. Ettouhami. Progress of Theoretical Physics, Vol. 127, No. 3, 453 (2012).
[4] J. Goldstone, Nuovo Cim. 19 (1961), 154.
[5] C. Gardiner, Phys. Rev. A 56, 1414-1423 (1997).
[6] Y. Castin and R. Dum, Phys. Rev. A 57, 3008-3021 (1998).
[7] P. W. Anderson, in Lectures on the Many-body Problem, Vol. 2, ed. E. R. Caianiello (Academic Press, New York, 1964), p. 113.
[8] I. M. Yurin. Int. Journal of Mod. Phys. B, Vol. 24, No. 30 (2010) 5847-5860.
[9] J. Bardeen, L. N. Cooper and J. R. Schrieffer. Phys. Rev. 106, 162 (1957).