Abstract—The Hohenberg–Martin dilemma of conserving versus gapless theories for systems with Bose–Einstein condensate is considered. This dilemma states that, generally, a theory characterizing a system with broken global gauge symmetry, which is necessary for Bose–Einstein condensation, is either conserving, but has a gap in its spectrum, or is gapless, but does not obey conservation laws. In other words, such a system either displays a gapless spectrum, which is necessary for condensate existence, but is not conserving, which means that it corresponds to an unstable system, or it respects conservation laws, describing a stable system, but the spectrum acquires a gap, which means that the condensate cannot appear. An approach is described, resolving this dilemma, and it is shown to give good quantitative agreement with experimental data. Calculations are accomplished in the Hartree–Fock–Bogolubov approximation.

1. CONDENSATE EXISTENCE AND STABILITY

The necessary and sufficient condition for Bose–Einstein condensation is the spontaneous breaking of global gauge symmetry $U(1)$ (see [1–3]). This implies that below the Bose condensation temperature $T_c$, the statistical average of a field operator $\langle \hat{\psi} \rangle$ becomes non-zero, since it is proportional to $\sqrt{\rho_0}$, where $\rho_0 \equiv N_0/V$ is the average condensate density. According to the Bogolubov–Ginibre theorem [4–6] the condensate density $\rho_0$ is a minimizer of thermodynamic potential. The same concerns the density of uncondensed particles $\rho_1$ that can be expressed through $\rho_1 = \rho - \rho_0$, with $\rho$ being a fixed average particle density. Keeping this in mind, it is possible to formulate the conditions of condensate existence and stability. Below, we use the system of units, where the Planck and Boltzmann constants are set to one.

The general criterion of Bose–Einstein condensation is the occurrence of a nonzero thermodynamic limit

$$\lim_{V \to \infty} \frac{N_0}{V} = \rho_0 > 0. \quad (1)$$

The number of condensed particles $N_0$ can be defined [7] as the largest eigenvalue of the single-particle density matrix. Denoting the set of these eigenvalues through $n_k$, with $k$ labelling the single-particle states, we have $N_0 = \sup_k n_k$. Then limit (1) implies that

$$\sup_k n_k \propto N \to \infty \quad (N \to \infty). \quad (2)$$

The distribution $n_k = n_k(\epsilon_k)$ is a function of the spectrum of collective excitations $\epsilon_k$. To have the above singularity in the thermodynamic limit, there should exist an index $k_0$, such that $n_k$ would diverge, when $k \to k_0$. Respectively [3], for this index, the spectrum has to tend to zero,

$$\epsilon_k \to 0 \quad (k \to k_0), \quad (3)$$

which means that the spectrum is gapless. For a uniform system, $k$ represents momentum, while $k_0$ becomes zero.

In the case of a uniform system, the gapless spectrum results [5, 8] in the first expression for the chemical potential

$$\mu_1 = \Sigma_{11}(0, 0) - \Sigma_{12}(0, 0), \quad (4)$$

called the Hugenholtz–Pines relation, where $\Sigma_{11}(k, \omega)$ is the normal self-energy and $\Sigma_{12}(k, \omega)$ is the anomalous self-energy.
The system stability requires that the condensate density be the minimizer of thermodynamic potential. This implies for the grand potential the condition

$$\frac{\partial \Omega}{\partial N_0} = 0,$$

which gives [3] the second expression for the chemical potential

$$\mu_0 = \Sigma_{11}(0,0) + \Sigma_{12}(0,0) - 2\rho_0 \Phi_0,$$

where $\Phi_0$ is the Fourier transform of the interaction potential at zero momentum. As is evident, these two expressions $\mu_0$ and $\mu_1$, generally, do not coincide with each other. They may coincide in some approximations (to be considered below) or when $\Sigma_{12}(0,0) = 0$ and $\rho_0 = 0$, if particle interactions are not neglected. But the latter simply means that there is no Bose condensate at all. It is possible to show that equating $\mu_0$ and $\mu_1$, one comes to the conclusion [9] that $\Sigma_{12}(0,0) = 0$.

Thus we confront the problem of accepting for the chemical potential either $\mu_0$ or $\mu_1$. However, if we accept $\mu_1$, then the condensate could exist, but it can be not stable. While, if we accept $\mu_0$, the condensate could be stable, but it may not exist. This is, actually, the meaning of the Hohenberg–Martin dilemma [10].

It is important to stress that there is no any thermodynamic requirement that the two expressions for the chemical potential be equal [11, 12]. Thus, from the variation of free energy the equality follows $(\mu_0 - \mu_1) \delta N_0 = 0$. It is only if $N_0$ would be undefined and could be freely varied, the chemical potentials should be equal. However, the number of condensed particles is prescribed by the conditions of the condensate existence and stability, being uniquely defined for fixed temperature and density. Hence $\delta N_0 = 0$, because of which there is no any constraint on the chemical potentials.

As an illustration of the possibility that the condensate could formally exist, being in reality unstable, let us consider a uniform ideal Bose gas in the space of dimensionality $d$. Then, below the condensation temperature

$$T_c = \frac{2\pi}{m} \rho \left[ \frac{\rho}{g_{1/2}(1)} \right]^{-1/d},$$

where $g_{1/2}$ is the modified Bose function [12, 13], formally there occurs Bose–Einstein condensation, when the condensate density becomes nonzero for any dimensionality $d$. However, the stability condition for particle fluctuations

$$0 \leq \frac{\text{var}(\hat{N})}{N} < \infty \quad \left( \text{var}(\hat{N}) = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 \right)$$

is valid not for all dimensionality. It is possible to show [14] that, depending on spatial dimensionality, particle fluctuations scale as

$$\frac{\text{var}(\hat{N})}{N} \propto N^\alpha \quad (\alpha = 1; \alpha = 2; \alpha = 4; \alpha = \text{const})$$

This tells us that the ideal system with a Bose–Einstein condensate can be stable only for $d > 4$.

2. GENERAL SELF-CONSISTENT APPROACH

Here, we describe a general self-consistent approach resolving the Hohenberg–Martin dilemma. The Hamiltonian, in the second-quantized picture, is

$$\hat{H} = \int \hat{\psi}^d(\mathbf{r}) \left[ -\frac{\nabla^2}{2m} + U(r,t) \right] \hat{\psi}(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \hat{\psi}^d(\mathbf{r}) \Phi(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) d\mathbf{r} d\mathbf{r}'$$

where $U = U(r,t)$ is an external field, $\Phi(r)$ is an interaction potential and $\hat{\psi}(\mathbf{r})$ are field operators obeying Bose commutation relations. In the presence of a Bose condensate, the field operator acquires the Bogoliubov shift [4, 5, 15]

$$\hat{\psi}(\mathbf{r}) = \eta(\mathbf{r}) + \psi_1(\mathbf{r})$$

and $\eta$ is the condensate function and $\psi_1$ is the field operator of uncondensed particles. Note that representation (10) is not an approximation but an exact canonical transformation. The variables $\eta$ and $\psi_1$ are mutually orthogonal,

$$\int \eta^d(\mathbf{r}) \psi_1^d(\mathbf{r}) d\mathbf{r} = 0.$$

The condensate function plays the role of an order parameter satisfying equations

$$\eta(\mathbf{r}) = \langle \hat{\psi}(\mathbf{r}) \rangle, \quad \langle \psi_1(\mathbf{r}) \rangle = 0.$$

And the number of uncondensed particles is given by the statistical average

$$N_1 = \langle \hat{N}_1 \rangle \equiv \int \psi_1^d(\mathbf{r}) \psi_1(\mathbf{r}) d\mathbf{r}$$

for the number-of-particle operator of uncondensed particles. Condition $\langle \psi_1^d \rangle = 0$ in a more general form writes as the average

$$\langle \hat{\lambda} \rangle = 0.$$
of the operator

$$\hat{\Lambda} = \int \left[ \lambda(r) \psi_i^*(r) + \lambda^*(r) \psi_i(r) \right] dr.$$  

The grand Hamiltonian, taking into account the normalization conditions (13) and (14) and average (15), becomes

$$H = \hat{H} - \mu_0 N_0 - \mu_1 N_1 - \hat{\Lambda},$$  \hspace{1cm} (16)

in which $\mu_0$, $\mu_1$, and $\lambda(r)$ are the Lagrange multipliers guaranteeing the validity of conditions (13)–(15).

The equations of motion can be written as the equation for the condensate function

$$i \frac{\partial}{\partial t} \eta(r, t) = \left( \frac{\delta H}{\delta \eta^*(r, t)} \right)$$  \hspace{1cm} (17)

and for the operator of uncondensed particles

$$i \frac{\partial}{\partial t} \psi_i(r, t) = \frac{\delta H}{\delta \psi_i^*(r, t)}.$$  \hspace{1cm} (18)

The operator Eq. (18) is equivalent to the Heisenberg equation of motion, since it can be proved \[3\] that

$$\frac{\delta H}{\delta \psi_i^*(r, t)} = [\psi_i(r, t), H].$$  \hspace{1cm} (19)

The system chemical potential takes the form

$$\mu = \mu_0 n_0 + \mu_1 n_1 \left( n_0 = \frac{N_0}{N}, n_1 = \frac{N_1}{N} \right).$$  \hspace{1cm} (20)

This general approach includes the particular case, when the chemical potentials $\mu_0$ and $\mu_1$ are equal, which can happen in some simple approximations shown below.

3. QUASICLASSICAL APPROXIMATION

At asymptotically small temperature and weak interactions, when

$$T \to 0, \quad \rho \Phi_0 \to 0; \quad \Phi_0 = \int \Phi(r) dr,$$  \hspace{1cm} (21)

almost all the system is Bose-condensed, hence it is in a coherent state, which is the eigenstate of the field operator,

$$\hat{\psi}(r, t)|\eta\rangle = \eta(r, t)|\eta\rangle.$$  \hspace{1cm} (22)

The condensate function is defined by the coherent field $\eta(r, t)$, for which Eq. (17) yields the nonlinear Schrödinger equation

$$i \frac{\partial}{\partial t} \eta(r, t) = H[\eta] \eta(r, t),$$  \hspace{1cm} (23)

with the nonlinear Hamiltonian

$$H[\eta] = -\frac{\nabla^2}{2m} + U(r, t) - \mu + \int \Phi(r - r')|\eta(r', t)|^2 dr'.$$  \hspace{1cm} (24)

Equation (23) was, first, advanced by Bogolubov in 1949 \[16\] (see also \[4, 5, 15\]).

For a uniform system, considering small deviations of the condensate function

$$\eta(r, t) = \sqrt{\rho_0} + u e^{-i\xi} + v^* e^{i\xi},$$  \hspace{1cm} (25)

one obtains the Bogolubov spectrum

$$\varepsilon_k = \sqrt{c_B^2 k^2 + \left( k^2 / 2m \right)^2} \left( c_B \equiv \sqrt{\rho \Phi_0} \right),$$  \hspace{1cm} (26)

with the Bogolubov sound velocity $c_B$.

In the quasiclassical approximation, the chemical potentials $\mu_0$ and $\mu_1$ coincide, being equal to $\mu = \rho \Phi_0$.

4. BOGOLUBOV APPROXIMATION

This approximation is applicable for temperatures much lower than the condensation temperature, $T \ll T_c$, and weak interactions, such that the characteristic interaction energy be much lower than the characteristic kinetic energy $E_{\text{kin}} \sim 1/2ma^2$, where $a$ is mean interparticle distance. The latter condition gives the inequality

$$m a^{1/3} |\Phi_0| \ll 1.$$  \hspace{1cm} (27)

In the Bogolubov approximation \[4, 5\], one neglects in the Hamiltonian the fourth-order operator terms like $\psi_i^* \psi_i^+ \psi_i \psi_i$. As a result, one gets the spectrum of collective excitations (26) and the same chemical potentials $\mu_0 = \mu_1 = \mu = \rho \Phi_0$. But not all particles are condensed, even at zero temperature, since interactions deplete the condensate, whose density becomes

$$\rho = \rho \left( 1 - \frac{8}{3\sqrt{\pi}} \gamma^{3/2} \right),$$  \hspace{1cm} (28)

where

$$\gamma = \rho^{1/3} a_s = \frac{m}{4\pi} \rho^{1/3} \Phi_0$$

is the dimensionless gas parameter, with $a_s$ being scattering length.

5. HARTREE–FOCK–BOGOLUBOV APPROXIMATION

In the Hartree–Fock–Bogolubov approximation, the fourth-order operator terms are decoupled into second-order terms, so that for the fourth-order correlators one gets

$$\langle \psi_i^\dagger \psi_j \psi_j^\dagger \psi_i \rangle = \langle \psi_i^\dagger \psi_j \rangle \langle \psi_j^\dagger \psi_i \rangle + \langle \psi_i^\dagger \psi_i \rangle \langle \psi_j^\dagger \psi_j \rangle$$  \hspace{1cm} (29)

$$+ \langle \psi_i^\dagger \psi_i \rangle \langle \psi_j^\dagger \psi_j \rangle.$$
For a uniform system, the self-energies at zero variables become

\[ \Sigma_{11}(0) = (\rho + \rho_0) \Phi_0 + \int \Phi(r) \langle \psi_1^*(0) \psi_1(r) \rangle \, dr, \]

\[ \Sigma_{12}(0) = \rho_0 \Phi_0 + \int \Phi(r) \langle \psi_1^*(0) \psi_1(r) \rangle \, dr. \]

(30)

This yields the chemical potentials

\[ \mu_0 = \rho \Phi_0 + \int \Phi(r) \left( \langle \psi_1^*(0) \psi_1(r) \rangle + \langle \psi_1^*(0) \psi_1(r) \rangle \right) \, dr, \]

\[ \mu_1 = \rho \Phi_0 + \int \Phi(r) \left( \langle \psi_1^*(0) \psi_1(r) \rangle - \langle \psi_1^*(0) \psi_1(r) \rangle \right) \, dr. \]

(31)

that are evidently different [3, 11].

For a dilute gas, it is possible to use the local interaction potential

\[ \Phi(r) = \Phi_0 \delta(r) \left( \Phi_0 = 4\pi \frac{a_s}{m} \right). \]

(32)

This gives the spectrum of collective excitations

\[ \epsilon_k = \sqrt{c^2 k^2 + \left( \frac{k^2}{2m} \right)^2} \]

(33)

that looks similar to the Bogolubov spectrum (26), however with the sound velocity \( c \) defined by the equation

\[ mc^2 = \rho \Phi_0(n_0 + \sigma), \]

(34)

where \( n_0 = \rho_0/\rho \) and \( \sigma \) is the anomalous average

\[ \sigma = \frac{1}{\rho} \langle \psi_1^*(r) \psi_1(r) \rangle. \]

(35)

In dimensionless variables

\[ s \equiv \frac{mc}{\rho^{1/3}}, \quad \gamma \equiv \rho^{1/3} a_s, \]

(36)

the equation for the sound velocity reads as

\[ s^2 = 4\pi \gamma(n_0 + \sigma). \]

(37)

The anomalous average can be represented as the sum of two terms, \( \sigma = \sigma_0 + \sigma_T \), where the first term is the value of \( \sigma \) at zero temperature,

\[ \sigma_0 = \frac{mc^2}{2\rho} \int \frac{1}{\epsilon_k(2\pi)^{3/2}} \, dk. \]

(38)

This term displays an ultraviolet divergence and requires a regularization. We employ the dimensional regularization that is asymptotically exact for small interactions, when \( \Phi_0 \to 0 \). After accomplishing the dimensional regularization, it is necessary to analytically continue the obtained expression to finite interactions. The analytical continuation can be done by means of an iterative procedure [17, 18] starting from the ideal-gas limit, where \( \sigma_0 \to 0 \) for \( \Phi_0 \to 0 \) and respecting the symmetry-restoration limit, when \( \sigma_{05} \to 0 \) for \( n_0 \to 0 \). This procedure results in the expression

\[ \sigma_0 = \frac{s_B^2}{\pi^2} \left( n_0 + \frac{s_B^2}{\pi^2} \sqrt{n_0} \right)^{1/2}, \]

(39)

with the dimensionless Bogolubov sound velocity

\[ s_B \equiv \frac{mc}{\rho^{1/3}} = \sqrt{4\pi \gamma}. \]

Using the definition of the gas parameter \( \gamma \), we find

\[ \sigma_0 = \frac{8}{\sqrt{\pi}} \gamma^{3/2} \left( n_0 + \frac{8}{\sqrt{\pi}} \gamma^{3/2} \sqrt{n_0} \right)^{1/2}. \]

(40)

6. NUMERICAL CALCULATIONS

The theory presented in the previous section has been applied for calculating the condensate density \( n_0 \) and superfluid fraction \( n_s \) in uniform and harmonically trapped systems \([17, 19, 20]\). The results are shown in Figs. 1–5. In Fig. 1, the condensate fraction \( n_0 \), for a uniform system, as a function of temperature, in the vicinity of the condensation temperature, demonstrates that the Bose–Einstein condensation transition is of second order for any interaction strength, as it should be. Temperature here is measured in units of \( m/\rho^{2/3} \), and the interaction strength is characterized by the gas parameter \( \gamma \). The superfluid fraction \( n_s \),
appears at the same critical point, as is seen in Fig. 2. In Fig. 3, we study the calculated condensate density \( n_0 \), for a uniform system at zero temperature as a function of the gas parameter and compare it with the Monte Carlo simulations [21] and the Bogolubov approximation \( n_B \). In Fig. 4, we show the effect of local condensate depletion at trap center occurring for the gas parameter \( \gamma > 0.3 \). And Fig. 5 shows the average condensate density in a harmonic trap as a function of the gas parameter, compared with the Bogolubov approximation [22] and the Monte Carlo simulations [23]. The calculated results, based on the Hartree–Fock–Bogolubov approximation, are in good agreement with experiments and Monte Carlo simulations, contrary to the Bogolubov approximation valid only for weak interactions, where \( \gamma < 0.1 \).
REFERENCES

1. E. H. Lieb, R. Seiringer, J. P. Solovej, and J. Yngvason, *The Mathematics of the Bose Gas and Its Condensation* (Birkhäuser, Basel, 2005).

2. V. I. Yukalov, Laser Phys. Lett. *4*, 632–647 (2007).

3. V. I. Yukalov, Phys. Part. Nucl. *42*, 460–513 (2011).

4. N. N. Bogolubov, *Lectures on Quantum Statistics* (Gordon and Breach, New York, 1967) Vol. 1.

5. N. N. Bogolubov, *Lectures on Quantum Statistics* (Gordon and Breach, New York, 1970) Vol. 2.

6. J. Ginibre, Commun. Math. Phys. *8*, 26–51 (1968).

7. O. Penrose and L. Onsager, Phys. Rev. *104*, 576–584 (1956).

8. N. M. Hugenholtz and D. Pines, Phys. Rev. *116*, 489–506 (1959).

9. A. A. Nepomnyashchii and Y. A. Nepomnyashchii, JETP Lett. *21*, 3–6 (1975).

10. P. C. Hohenberg and P. C. Martin, Ann. Phys. (N.Y.) *34*, 291–359 (1956).

11. V. I. Yukalov, Ann. Phys. (N.Y.) *323*, 461–499 (2008).

12. V. I. Yukalov, Laser Phys. *26*, 062001 (2016).

13. V. I. Yukalov, Phys. Rev. A *72*, 033608 (2005).

14. V. I. Yukalov, Symmetry *11*, 603 (2019).

15. N. N. Bogolubov, *Quantum Statistical Mechanics* (World Scientific, Singapore, 2015).

16. N. N. Bogolubov, *Lectures on Quantum Statistics* (Ryadyanska Shkola, Kiev, 1949) [in Ukrainian].

17. V. I. Yukalov and E. P. Yukalova, Phys. Rev. A *90*, 013627 (2014).

18. V. I. Yukalov and E. P. Yukalova, Laser Phys. Lett. *16*, 065501 (2019).

19. V. I. Yukalov and E. P. Yukalova, J. Phys. B *47*, 095302 (2014).

20. V. I. Yukalov and E. P. Yukalova, J. Phys. B *51*, 085301 (2018).

21. M. Rossi and L. Salasnich, Phys. Rev. A *88*, 053617 (2013).

22. J. Javanainen, Phys. Rev. A *54*, 3722 (1996).

23. J. L. DuBois and H. R. Glyde, Phys. Rev. A *68*, 033602 (2003).