Bose–Einstein condensation in self-consistent mean-field theory

V I Yukalov\textsuperscript{1} and E P Yukalova\textsuperscript{2}

\textsuperscript{1} Bogolubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna 141980, Russia
\textsuperscript{2} Laboratory of Information Technologies, Joint Institute for Nuclear Research, Dubna 141980, Russia
E-mail: yukalov@theor.jinr.ru

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Abstract
There is a wide-spread belief in the literature on Bose–Einstein condensation of interacting atoms that all variants of mean-field theory incorrectly describe the condensation phase transition, exhibiting, instead of the necessary second-order transition, a first-order transition, even for weakly interacting Bose gas. In the present paper, it is shown that a self-consistent mean-field approach is the sole mean-field theory that provides the correct second-order condensation transition for Bose systems with atomic interactions of arbitrary strength, whether weak or strong.

Keywords: Bose–Einstein condensation, mean-field theory, critical region

(Some figures may appear in colour only in the online journal)

1. Introduction

A statistical system exhibiting Bose–Einstein condensation is known to pertain to the universality class of the \(XY\)-model \cite{1} or the two-component \(\varphi^4\) theory \cite{2}. Therefore, Bose–Einstein condensation has to be a phase transition of second order, as has been proved for this universality class by renormalization-group techniques \cite{3} and Monte Carlo simulations \cite{4, 5}. Bose–Einstein condensation, accompanied by superfluid transition, has been intensively studied in experiments with liquid \(^4\)He, where it is certainly a phase transition of second order \cite{6}. Numerous experiments with trapped atomic gases also confirm the second order of the condensation phase transition, as summarized in the book \cite{7} and review articles \cite{8–10}.

Contrary to the general requirement for the condensation transition to be of second order, different variants of mean-field theory, applied for describing this transition, lead to a first-order transition, as has been discussed in several articles \cite{11–15}. The fact that such a disruption of the condensation phase transition to that of first order is the general feature of any mean-field theory was emphasized by Baym and Grinstein \cite{16}. This fact was also discussed in recently in \cite{17}, concluding that none of the existing mean-field approaches can correctly describe Bose–Einstein condensation as a second-order phase transition, leading instead to a first-order transition.

Such a fact that no mean-field theory can reasonably describe the condensation transition seems to be quite strange. It is a general situation that for practically all systems there always exists a mean-field approximation that provides a reasonable description of the related phase transition. Yes, it is known that mean-field approximations cannot yield exact critical indices, but in the majority of cases they do correctly characterize phase transitions. Just as one of the many examples, we can mention the magnetization transition in the Heisenberg model, for which there exists a reasonable mean-field theory correctly predicting a second-order phase transition.

It is not difficult to understand why the used mean-field theories fail in correctly predicting the condensation transition \cite{11–17}. Really, the Hartree–Fock approximation, where the global gauge symmetry is not broken, is not able in principle to describe the condensed state with broken gauge symmetry, since the breaking of gauge symmetry is a necessary and sufficient condition for Bose–Einstein condensation \cite{18, 19}. The Bogolubov approximation \cite{20, 21}, by definition, is applicable only at low temperatures, where the Bose-condensed fraction is prevailing. The Shohno trick \cite{22} of omitting anomalous averages is principally not correct,
as far as spontaneous gauge symmetry breaking leads to the simultaneous appearance of the condensate fraction as well as of these anomalous averages. The latter are usually of order or even larger than the normal averages, and in no case can be omitted [23, 24]. Moreover, neglecting the anomalous averages renders the system unstable [9, 10]. One often ascribes the Shohno trick of omitting anomalous averages to Popov, calling this the Popov approximation. It is, however, easy to check from his works [25, 26] that Popov has never suggested such an unjustified trick. In the Girardeau–Arnoult approach [27, 28], an unphysical gap appears in the spectrum of collective excitations. When one employs the number-conserving operator representation [29], one by definition is limited to very low temperatures and weak interactions, when almost all atoms are in the condensed state. The T-matrix approach [30], strictly speaking, is also applicable for low temperatures and weak interactions, but cannot be applied to the transition region, where, as is shown in [17], it leads to the system instability. More detailed discussions of these problems can be found in [16, 17, 31].

In the majority of cases, the disruption of the phase transition to a discontinuous type is caused by a not self-consistent description resulting in the appearance of an instability caused by what Bogolubov [32, 33] termed the mismatch of approximations. Two important conditions exist that have to be true for a system with a Bose–Einstein condensate. One condition is the condensate existence, formulated in one of the known forms, as is explained in reviews [9, 10], which results in the Hugenholtz–Pines relation [34] leading to a gapless spectrum. The other is the Bogolyubov–Ginibre stability condition [33, 35] requiring that, in an equilibrium system, the condensate fraction would minimize the thermodynamic potential. Both these conditions have to necessarily be treated in the same approximation. But if they are treated in different approximations, this immediately results in the appearance of the system instability.

A novel mean-field approach has recently been advanced [36–38] satisfying the Hohenberg–Martin condition of self-consistency [39], being gapless and conserving. Employing approximate expansions in the vicinity of the critical temperature, it has been shown that the condensation is a second-order phase transition [9, 10, 31, 38]. In the present paper, we accomplish direct numerical calculations explicitly demonstrating the continuous behaviour, at the critical temperature, of the condensate fraction, the fraction of uncondensed atoms, the anomalous average, sound velocity, and superfluid fraction. At the same time, the compressibility diverges at the critical point, as it should be for a continuous transition. These results unambiguously prove that Bose–Einstein condensation, treated in the self-consistent mean-field theory, is a second-order phase transition. To our knowledge, this is the sole mean-field approach correctly characterizing Bose–Einstein condensation as a phase transition of second order.

In section 2, we briefly recall the basic points, which the self-consistent approach is based on. Section 3 presents the resulting formulas for a uniform system. In section 4, numerical calculations for the vicinity of the critical point are demonstrated. Section 5 concludes.

Throughout the paper, the system of units is employed, where the Planck and Boltzmann constants are set to 1.

2. Self-consistent approach

We start with the standard energy Hamiltonian

\[ H = \int \psi^\dagger \left( -\frac{\nabla^2}{2m} \right) \psi \, dr + \frac{1}{2} \Phi_0 \int \psi^\dagger(r) \psi^\dagger(r) \psi(r) \psi(r) \, dr, \]

in which the interaction strength is given by the value

\[ \Phi_0 \equiv 4\pi \frac{\alpha_s}{m}, \]

where \( \alpha_s \) is scattering length and \( m \) atomic mass. The field operators satisfy the Bose commutation relations. Generally, these operators depend on time, which is not shown for brevity.

For describing a system with a Bose–Einstein condensate, we use the Bogolubov shift [33] representing a field operator as the sum

\[ \psi(r) = \eta(r) + \psi_1(r) \]

consisting of a condensate wave function \( \eta(r) \) and the operator of uncondensed atoms \( \psi_1(r) \). Recall that this is not an approximation, but an exact canonical transformation [40], so that no smallness conditions are imposed on the operator \( \psi_1(r) \), except that it satisfies the Bose commutation relations.

Following the Bogolubov method [32, 33], the condensate function and the operators of uncondensed atoms are considered as separate variables that are orthogonal to each other in order to avoid double counting:

\[ \int \eta^\dagger(r) \psi_1(r) \, dr = 0. \]

The statistical average of \( \psi_1(r) \), representing normal atoms, is zero:

\[ \langle \psi_1(r) \rangle = 0. \]

Hence the condensate function is the order parameter

\[ \eta(r) = \langle \psi(r) \rangle. \]

The condensate function is normalized to the number of condensed atoms

\[ N_0 = \int |\eta(r)|^2 \, dr, \]

while the number of uncondensed atoms is

\[ N_1 = \int \langle \psi_1^\dagger(r) \psi_1(r) \rangle \, dr. \]

Thus, the total number of atoms in the system is the sum

\[ N = N_0 + N_1. \]

The evolution equations for the variables are obtained by the extremization of an effective action [9, 10, 31], which yields the equation for the condensate function

\[ i \frac{\partial}{\partial t} \eta(r, t) = \left( \frac{\delta H}{\delta \eta^\dagger(r, t)} \right) \]

and the equation for the operator of uncondensed atoms

\[ i \frac{\partial}{\partial t} \psi_1(r, t) = \frac{\delta H}{\delta \psi_1^\dagger(r, t)}. \]
with the grand Hamiltonian

$$H = \hat{H} - \mu_0 N_0 - \mu_1 \hat{N}_1 - \hat{\Lambda},$$  \hspace{1cm} (12)

in which

$$\hat{N}_1 \equiv \int \psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r})\, d\mathbf{r}$$  \hspace{1cm} (13)

is the number-operator of uncondensed atoms and

$$\hat{\Lambda} \equiv \int \left[ \lambda(\mathbf{r})\psi_1^\dagger(\mathbf{r}) + \lambda^*(\mathbf{r})\psi_1(\mathbf{r}) \right]\, d\mathbf{r}. \hspace{1cm} (14)$$

The quantities $\mu_0$, $\mu_1$ and $\lambda(\mathbf{r})$ are the Lagrange multipliers guaranteeing the validity of conditions (5)–(9). The evolution equations can be shown \[31, 41\] to be equivalent to the Heisenberg equations of motion with Hamiltonian (12). For equilibrium systems, the statistical operator is defined \[9, 10, 31\] by the minimization of the information functional uniquely representing the system, which results in the operator

$$\hat{\rho} = \frac{1}{Z} e^{-\beta H}, \quad Z \equiv \text{Tr} e^{-\beta H}, \hspace{1cm} (15)$$

where $\beta \equiv 1/T$ is inverse temperature.

The average densities of condensed and uncondensed atoms, respectively, are given by the ratios

$$\rho_0 \equiv \frac{N_0}{V}, \quad \rho_1 \equiv \frac{N_1}{V}, \hspace{1cm} (16)$$

with $V$ being the system volume and $\rho$, the total average density

$$\rho \equiv \frac{N}{V} = \rho_0 + \rho_1. \hspace{1cm} (17)$$

The superfluid density is defined \[9, 10\] as

$$\rho_s = \rho - \frac{\text{var}(\hat{P})}{3mTV}, \hspace{1cm} (18)$$

where

$$\hat{P} \equiv \int \hat{\psi}(\mathbf{r})(-iV)\hat{\psi}(\mathbf{r})\, d\mathbf{r}$$  \hspace{1cm} (19)

is the system momentum operator, whose variance is

$$\text{var}(\hat{P}) \equiv \langle \hat{P}^2 \rangle - \langle \hat{P} \rangle^2.$$

For an equilibrium system, the total average momentum is zero, so that the superfluid density reduces to

$$\rho_s = \rho - \frac{\langle \hat{P}^2 \rangle}{3mTV}. \hspace{1cm} (20)$$

3. Uniform system

In the case of a uniform system, the condensate function is the constant

$$\psi_1(\mathbf{r}) = \sqrt{\rho_0}. \hspace{1cm} (21)$$

The operator of uncondensed atoms can be expanded over plane waves,

$$\psi_1(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k a_k e^{i\mathbf{k} \cdot \mathbf{r}}. \hspace{1cm} (22)$$

Note that, because of the orthogonality condition (4), we have

$$\lim_{k \to 0} a_k = 0. \hspace{1cm} (23)$$

The operators $a_k$ in the momentum representation define the momentum distribution

$$n_k \equiv \langle a_k^\dagger a_k \rangle, \hspace{1cm} (24)$$

called the normal average, and the anomalous average

$$\sigma_k \equiv \langle a_k a_{-k} \rangle. \hspace{1cm} (25)$$

Integrating distribution (23) yields the density of uncondensed atoms

$$\rho_1 = \int n_k \frac{dk}{(2\pi \beta)^3}, \hspace{1cm} (26)$$

Respectively, the integral of equation (24) gives

$$\sigma_1 = \int \sigma_k \frac{dk}{(2\pi \beta)^3}, \hspace{1cm} (27)$$

that defines the density $|\sigma_1|$ of pair correlated atoms.

Substituting into Hamiltonian (1) the Bogolubov shift (3) and using expansion (22), we then invoke for the operators $a_k$ the Hartree–Fock–Bogoliubov approximation (see details in \[9, 10, 31, 37\]). Introducing the notation

$$\omega_k \equiv \frac{k^2}{2m} + mc^2, \hspace{1cm} (28)$$

we find the momentum distribution

$$n_k = \frac{\omega_k}{2\pi} \coth \left( \frac{\epsilon_k}{2T} \right) - \frac{1}{2}, \hspace{1cm} (29)$$

and the anomalous average

$$\sigma_k = -\frac{mc^2}{2\pi} \coth \left( \frac{\epsilon_k}{2T} \right), \hspace{1cm} (30)$$

where

$$\epsilon_k = \sqrt{(ck)^2 + \left( \frac{k^2}{2m} \right)^2}. \hspace{1cm} (31)$$

is the spectrum of collective excitations, and the sound velocity is given by the equation

$$mc^2 = (\rho_0 + \sigma_1)\Phi_0. \hspace{1cm} (32)$$

The superfluid density (20) takes the form

$$\rho_s = \rho - \frac{1}{3mTV} \int k^2 (n_k + n_k^* - \sigma_k^2) \, \frac{dk}{(2\pi \beta)^3}. \hspace{1cm} (33)$$

Thus, for the density of uncondensed atoms (25), we have

$$\rho_1 = \int \frac{\omega_k}{2\pi} \coth \left( \frac{\epsilon_k}{2T} \right) - \frac{1}{2} \frac{dk}{(2\pi \beta)^3}, \hspace{1cm} (34)$$

and for the anomalous average (26), we get

$$\sigma_1 = -\int \frac{mc^2}{2\pi} \coth \left( \frac{\epsilon_k}{2T} \right) \, \frac{dk}{(2\pi \beta)^3}. \hspace{1cm} (35)$$

The superfluid density (32) becomes

$$\rho_s = \rho - \frac{1}{12mTV} \int \frac{k^2}{\sinh^2(\epsilon_k/2T)} \frac{dk}{(2\pi \beta)^3}. \hspace{1cm} (36)$$

It is worth stressing that the superfluid density is meaningful only if the anomalous average (29) is taken into account. If in expression (32) this anomalous average were omitted, then the related integral would be divergent leading to the meaningless value $\rho_s \to -\infty$. The principal importance of the anomalous average for the correct definition of the superfluid density is easy to understand: the phenomenon of superfluidity is caused by atomic correlations. And the
anomalous density defines exactly the density of correlated atoms $|\sigma_1|$. Hence, without the anomalous density, there are no correlated atoms, and consequently, there is no superfluidity.

When temperature tends to zero, then equation (34) leads to

$$\sigma_1 \simeq -\int \frac{mc^2}{2\varepsilon} \frac{dk}{(2\pi)^3} \left( T \to 0 \right) .$$

The latter integral is formally divergent but can be regularized, e.g., by means of dimensional regularization that is asymptotically exact for weak interactions [2]. So, at low temperatures and weak interactions, such that

$$\frac{T}{T_c} \ll 1, \quad \frac{\mu \Phi_0}{T_c} \ll 1,$$

where $T_c$ is the critical temperature, one can use the expression

$$\sigma_1 \simeq -\int \frac{mc^2}{2\varepsilon} \frac{dk}{(2\pi)^3} - \int \frac{mc^2}{2\varepsilon} \left[ \coth \left( \frac{\varepsilon_k}{2T} \right) - 1 \right] \frac{dk}{(2\pi)^3} ,$$

with the appropriately regularized first term [9, 10, 31, 37]. The behaviour of the Bose-condensed system at zero temperature, in the frame of the self-consistent approach, has been studied in detail in [10, 37], exhibiting good agreement with Monte Carlo simulations [42–44].

The critical temperature is the temperature, where the condensate density disappears, $\rho_0 \to 0$. Then the gauge symmetry becomes restored, hence, the anomalous average also tends to zero. From the above equations, it follows that this happens at the temperature

$$T_c = \frac{2\pi}{m} \left[ \frac{\rho}{\xi(3/2)} \right]^{2/3} .$$

In the vicinity of the critical temperature (39), equation (31) shows that then $c \to 0$. In this critical region, the anomalous average (34) behaves as

$$\sigma_1 \simeq -\frac{mc^2}{2\pi} T \left( T \to T_c \right) .$$

### 4. Critical region

To study the behaviour of the system in the critical region, where $T \to T_c$, it is convenient to pass to dimensionless quantities, such as the condensate fraction $n_0$ and the fraction of uncondensed atoms $n_1$ given by the ratios

$$n_0 = \frac{\rho_0}{\rho} , \quad n_1 = \frac{\rho_1}{\rho} .$$

Respectively, the superfluid fraction is

$$n_s = \frac{\rho_s}{\rho} ,$$

and we introduce the dimensionless anomalous average

$$\sigma = \frac{\sigma_1}{\rho} .$$

The dimensionless sound velocity is

$$s = \frac{mc}{\rho^{1/3}} .$$

As a dimensionless interaction strength, we use the gas parameter

$$\gamma = \rho^{1/3} \alpha_s .$$

This parameter is very natural, measuring the ratio of potential to kinetic energy. Really, potential energy per atom is proportional to $\rho \alpha_s /m$, while kinetic energy is of order $\rho^{2/3} /m$. Their ratio gives precisely the gas parameter (45).

Under the validity of inequalities (37), when the second of them reads as $\gamma \ll 0.3$, one can use the low-temperature form (38) of the anomalous average. But in the critical region, one has to employ the anomalous average (40).

Let us measure temperature in units of $\rho^{2/3} /m$, so that in what follows $T$ implies the dimensionless quantity, such that the transformation to the dimensional temperature corresponds to the change

$$T \to \frac{mT}{\rho^{2/3}} .$$

Thus, for the critical temperature we have

$$T_c \to \frac{T_c \rho^{2/3}}{\rho^{2/3}} = \frac{2\pi}{[\xi(3/2)]^{2/3}} = 3.312 498 .$$

Our aim is to investigate the behaviour of the characteristic quantities in the critical region close to the critical temperature $T_c$. We shall study the behaviour of the condensate fraction

$$n_0 = 1 - n_1 ,$$

expressed through the normal fraction

$$n_1 = \frac{s^3}{3\pi^2} \left[ 1 + \frac{3}{2\sqrt{2}} \int_0^\infty \left( \sqrt{1 + x^2} - 1 \right) \frac{dx}{x} \right] ,$$

the dimensionless anomalous average

$$\sigma = -\frac{sT}{2\pi} ,$$

and sound velocity $s$ given by the equation

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

![Figure 1. Condensate fraction $n_0$ as a function of dimensionless temperature (in units of $\rho^{2/3}/m$) in the critical region.](image_url)
and the superfluid fraction

$$n_s = 1 - \frac{s^5}{6\sqrt{2}\pi^2 T} \int_0^\infty \frac{(\sqrt{1 + x^2} - 1)^{3/2} x \, dx}{\sqrt{1 + x^2}\sinh^2(s^2x/2T)}.$$  (50)

Solving the system of equations (46)–(50), we find that all these characteristics of interest are continuously varying in the vicinity of the critical temperature. The results of numerical calculations are presented for the condensate fraction in figure 1, the fraction of uncondensed atoms, in figure 2, for the anomalous average, in figure 3, for the sound velocity, in figure 4, and for the superfluid fraction, in figure 5. The continuous variation is a typical feature of the phase transition of second order. Let us stress that, as is seen from our calculations, the order of the phase transition does not depend on the atomic interaction strength, being of second order for any value of the gas parameter $\gamma$.

At the point of a second-order phase transition, the compressibility should be divergent. The isothermal compressibility can be calculated by invoking different representations [45], for instance

$$\kappa_T = \frac{\var(\hat{N})}{\rho T N} \quad (\hat{N} = N_0 + \hat{N}_1).$$

In the used approximation, we obtain

$$\kappa_T = \frac{1}{mpc^2}.$$
Since the sound velocity $c$ tends to zero at $T_c$, the compressibility diverges, as it should be for a second-order phase transition.

5. Conclusion

We have shown that in the self-consistent mean-field theory [9, 10, 31, 36–38] Bose–Einstein condensation is a second-order phase transition. This is proved by the direct numerical investigation for the critical behaviour of the most important quantities characterizing the condensation phase transition: the condensate fraction, the fraction of uncondensed atoms, the anomalous average, the sound velocity, and the superfluid fraction. The condensate fraction, anomalous average, sound velocity, and the superfluid fraction continuously tend to zero at the same critical temperature $T_c$. Respectively, the isothermal compressibility, inversely proportional to the sound velocity squared, diverges at the critical point. All this behaviour unambiguously demonstrates the second order of the Bose–Einstein condensation transition.

It is worth emphasizing that all other known mean-field approximations, as is discussed in [11–17, 31], incorrectly describe the Bose condensation as a first-order phase transition. In [17] it is claimed that in the self-consistent mean-field theory [9, 10, 31, 36–38] the condensation transition is also of first order. However, this claim is caused by an error: in their calculations, the authors of [17] have taken the low-temperature approximation for the anomalous average, instead of the correct form (48) valid for the critical region. As we have shown in the present paper by straightforward numerical calculations, in the self-consistent mean-field theory [9, 10, 31, 36–38] the Bose–Einstein condensation is undoubtedly a second-order phase transition, independent of the strength of atomic interactions. To our knowledge, this is the sole variant of the available mean-field approaches qualifying this transition as a second-order one.

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