About phase transitions in Bose gases at constant density and constant pressure

Velin G. Ivanov, Dimo I. Uzunov

CP Laboratory, G. Nadjakov Institute of Solid State Physics,
Bulgarian Academy of Sciences, BG-1984 Sofia, Bulgaria.

Abstract

The phase transitions in Bose gases at constant volume and constant pressure are considered. New results for the chemical potential, the effective Landau-Ginzburg free energy and the equation of state of the Bose-Einstein condensate in ideal Bose gases with a general form of the energy spectrum are presented. Unresolved problems are discussed.

1. Introduction

The Bose-Einstein condensation (BEC) is a phenomenon due to the quantum statistical correlations (pseudo-interactions) in ideal Bose gases (IBG) of non-interacting bosons. This is a condensation in the momentum space (ℏk) but also it possesses some features of the usual (Van der Waals) condensation [1, 2, 3, 4]. This phenomenon strongly depends on the spatial dimensionality d, and the energy spectrum ε(k) = (ℏ^2k^σ/2m) of the bosons [0 < σ ≤ 2; k = |k|; k̃ = {k_j = (2π/n_j/L_j)}, where j = 1,...,d; n_j = 0, ±1,...] in IBG in volume V = (L_1...L_d) ∼ L^d and periodic boundary conditions [3, 4].

The original Bose-Einstein condensate (BEC) is not superfluid but the latter state is possible in many-body systems of interacting bosons (nonideal Bose gas, or, shortly, NBG) [1, 2, 3, 4, 5]. The phenomena of BEC and superfluidity have a number of similar features and both of them are widely discussed in various problems of astrophysics (see, e.g., Refs. [5, 7, 8, 6]. In particular, BEC and superfluidity are relevant to the treatment of the so-called plasma-solid transition in “astrophysical matter” [7], and for the behaviour of the neutron component of the dense matter in the interior of neutron stars [1, 8, 6, 9]; for applications to cosmological models of dark energy and dark matter, see Ref. [10].

The main properties of BEC are known (see, e.g., Ref. [4, 11, 12, 13, 14, 15]. Recently, BEC at constant density and constant pressure has been reviewed in Ref. [16]. Here we shall discuss the equation of state of IBG and BEC for spinless bosons. The treatment can be generalized for bosons with spin [17, 18].

The superfluidity and the effect of interparticle interactions on BEC can be treated by both the mean-field like Gross-Pitaevskii [19] and the microscopic Beliaev-Popov [20] approaches. We shall discuss the latter within the renormalization group theory [3].
and for this reason we shall consider the following action of NBG [3, 4, 20]:

$$S[\phi] = -\sum_q G_q^{-1}(q)|\psi(q)|^2 - \frac{u}{2\beta N} \sum_{q_1,q_2,q_3} \psi^*(q_1)\psi^*(q_2)\psi(q_3)\psi(q_1 + q_2 - q_3) , \quad (1)$$

where $q = (\omega_l, \vec{k})$ is a $(d+1)$-dimensional frequency-momentum vector, $\omega_l = 2\pi l k_B T / \hbar$ is the (Bose-)Matsubara frequency ($l = 0, \pm 1, ...$), $\psi(q)$ is a C-number Bose field, $u$ is the interaction constant, $N$ is the number of particle and $\beta = 1/k_B T$. The (bare) correlation (Green) function $G_0(q) = \langle |\psi(q)|^2 \rangle_0$ is given by

$$G_0^{-1}(q) = i\omega_l + \varepsilon(k) + r , \quad (2)$$

where $(-r) = \mu \leq 0$ is the chemical potential of IBG ($u = 0$).

Note, that the thermodynamics of NBG is given by the grand canonical thermodynamic potential $\Omega(T, V, \mu) = -\beta^{-1}Z$, where the grand canonical partition function $Z(T, V, \mu)$ is defined by $Z = \int D\phi \exp (S)$ - a functional integral over the possible field configurations. The usual field theoretical investigations of the action (1) are performed in the thermodynamic limit: $N \to \infty$, $V \to \infty$, provided $0 \leq \rho = (N/V) < \infty$.

Using the models of IBG ($v \equiv 0$) and NBG defined by Eqs. (1) – (2) we shall consider the equation of state for BEC. For IBG this can be performed exactly, whereas for NBG we must use the loop expansion (see, e.g., Ref. [3]). The main features of BEC can be revealed within the one-loop approximation [3, 21]. We shall discuss the effect of the inter-particle interaction on BEC by using results from preceding works.

We wish to emphasize that the phase transition to BEC cannot be easily put to the usual classification of phase transitions [3]. Above $T_c$ this phase transition resembles certain features of second order phase transitions but is rather different from the standard notion about these transitions [3]. On the other side, the equation of state of IBG below $T_c$ is quite similar to known equations of (almost) first-order phase transitions and tricritical points [3]. There is a close similarity between the phase transition properties of IBG and the spherical model in the ferromagnetism, and this point will be discussed in the remainder of this report. In our consideration we shall essentially use results from preceding works [16, 11, 12, 13, 14, 15] (for a comprehensive reference to original papers, see, e.g., the reviews [3, 4]). We work with general values of $d$ and $\sigma$ but our consideration includes the important case of $d = 3$, $\sigma = 2$.

2. Free energy and thermodynamics

For a convenience we shall introduce a fictitious external field $h$ which is thermodynamically conjugated to the order parameter $\Psi = \langle \psi(0) \rangle$ of uniform BEC. Note, that in case of uniform BEC the $(q = 0)$-mode $\psi(0)$ can be represented by the sum $\psi(0) = \langle \psi(0) \rangle + \delta \psi(0)$, where $\delta \psi(0)$ is the (uniform) fluctuation mode. The consideration of an external uniform field $h$ can be performed by adding a term

$$S_h = \frac{1}{N} [h\psi^*(0) + c.c.] , \quad (3)$$
The thermodynamic potential of IBG can be written in the form

$$
\Omega(T, r, h) = -\beta^{-1} V \lambda_T^{-d} A(d, \sigma) g_{d/\sigma+1}(\beta r) - \frac{1}{N} \frac{hh^*}{r},
$$

(4)

where $g_{\nu}(y)$ is the Bose function \[3, 15, 18\], the thermal wavelength is given by

$$
\lambda_T = \left( \frac{2\pi \hbar^2}{mk_B T} \right)^{1/\sigma},
$$

(5)

and

$$
A(d, \sigma) = \frac{2^{1-d+2d/\sigma} \Gamma(d/\sigma)}{\sigma \pi^{d(1/2-1/\sigma)} \Gamma(d/2)}, \quad A(d, 2) = 1.
$$

(6)

The potential (4) obeys the differential relation $d\Omega = -SdT + Ndr - \Psi dh^* - \Psi^* dh$.

By a suitable Legendre transformation we obtain another thermodynamic potential $\tilde{\Omega}(T, r, \Psi)$, where the natural variable is $\Psi$:

$$
\tilde{\Omega} = -\beta^{-1} V \lambda_T^{-d} A(d, \sigma) g_{d/\sigma+1}(\beta r) + Nr\Psi^2.
$$

(7)

We can restrict ourselves, without a loss of generality, to real $h$ and $\Psi$. The susceptibility is then $\chi_T = \partial \Psi / \partial h = 1/Nr \sim t^{-\gamma}$, where $\gamma$ is the susceptibility critical exponent and $t = (T - T_c)/T_c$ (see, e.g., Ref. \[3\]).

For small $r$ and energies ($\varepsilon \ll k_B T$), which correspond to the critical regime near the phase transition point, the correlation function $\chi(k) = G_0(0, \bar{k})$ takes the form $\chi(k)^{-1} \sim (ck^\sigma + r)$. This gives us the correlation length $\xi = (c/r)^{1/\sigma} \sim t^{-\nu}$ and $\chi(k) \sim k^{-2+\eta}$ at $r = 0$. From $\chi(k) \sim k^\sigma$ we obtain that the Fisher exponent $\eta$, defined by $\chi(k) \sim k^{-2+\eta}$, is equal to $(2 - \sigma)$ for all dimensional ranges and possible constraints (of constant volume $V$ or constant pressure $P$).

In order to obtain the correlation length exponent $\nu$ and the exponent $\gamma$ of the susceptibility $\chi_T$, we need to calculate the function $r(t)$. The latter is different for the cases $V = \text{const}$ and $P = \text{const}$. In the thermodynamic limit, the constraint of constant volume is equivalent to a constraint of constant density ($\rho = \text{const}$). The results for the critical exponents corresponding to these cases are summarized in Ref. \[16\] for various spatial dimensions $d$. Here we restrict our consideration of the critical exponents and the equation of state to features which demonstrate the difference between the phase transition to BEC and both first and second order phase transitions for the most interesting interval of spatial dimensions $\sigma < d < 2\sigma$ that includes the case $\sigma = 2, d = 3$.

3. Constant density

To consider the effect of the thermodynamic condition of constant density $\rho = (N/V)$ we need the free energy $F = Vf(T, \rho, \Psi)$. To obtain this thermodynamic potential near the phase transition point to BEC we expand the Bose function in (4) in powers of $\beta r$ and express $r$ as a function of $\rho$. This procedure is performed for the potential...
given by Eq. (7). Further we obtain the potential \( F \) with the help of a Legendre transformation of the form:

\[
F = \tilde{\Omega} - N r |_{r=r(\rho)},
\]

\[
\rho = \frac{\partial \tilde{\Omega}}{V \partial r} = \lambda_T^{-d} A(d, \sigma) g_{d/\sigma}(\beta r) + \rho \Psi^2.
\]

The lowest temperature \( T_c \), at which the system does not condensate (\( \Psi = 0 \)) is obtained from Eq. (9). When \( d \leq \sigma \), the Bose function is divergent for \( (\beta r) \to 0 \) which means that BEC may occur only at the absolute zero \( (T_c = 0) \) - a zero temperature BEC \[15\]. When \( d > \sigma \), we obtain that \[4, 14\]

\[
T_c(\rho) = \frac{2\pi \hbar^2}{mk_B} \left[ \frac{\rho}{A(d, \sigma) \zeta(d/\sigma)} \right]^{\sigma/d} > 0,
\]

where \( g_{d/\sigma}(0) = \zeta(d/\sigma) \) is the zeta function. Below the critical temperature \( T_c \), BEC occurs (\( \Psi > 0 \)).

For the most interesting case of dimensions \( \sigma < d < 2\sigma \), the result for the free energy density \( f(T, \rho, \Psi) \) to the lowest order in \( |t| \ll 1 \) is given by:

\[
f = C_f \left( \Psi^2 + \frac{d}{\sigma} t \right)^{d/(d-\sigma)} \),
\]

where

\[
C_f = \left( \frac{d}{\sigma} - 1 \right) \left[ \frac{\zeta(d/\sigma)}{\Gamma(1-d/\sigma)} \right]^{\sigma/(d-\sigma)} (k_B T_c) \rho.
\]

In our derivation of the energy (11) a \( \Psi \)-independent term has been neglected. Such terms can be ignored because they belong to the energy of the disordered phase (\( \Psi = 0 \)). For this reason the net free energy of the BEC can be obtained from (11) by neglecting the \( \Psi \)-independent term of type \( f^{d/(d-\sigma)} \). The free energy (11) is of Landau-Ginzburg type \[3\]; one may easily expand \( f(\Psi) \) in powers of \( \Psi \).

The external field \( h \) is fictitious and can be neglected in studies of the thermodynamics. In this case, the equation of state \( h \sim \partial(f/\partial \Psi) \) becomes \( (\partial f/\partial \Psi) = 0 \). From Eq. (11) we easily obtain the equation of state for \( h = 0 \):

\[
\Psi \left( \Psi^2 + \frac{d}{\sigma} t \right)^{\sigma/(d-\sigma)} = 0.
\]

The solutions of Eq. (13) are: \( \Psi = 0 \) (disordered phase), and \( \Psi^2 = -(d/\sigma)t > 0 \) (corresponding to BEC for \( t < 0 \)). Note, that the chemical potential \( (\mu = -r) \) can be obtained in the form

\[
\mu = -k_B T \left[ \frac{\zeta(d/\sigma)}{\Gamma(1-d/\sigma)} \right]^{\sigma/(d-\sigma)} (\Psi^2 + \frac{d}{\sigma} t)^{\sigma/(d-\sigma)}.
\]
BEC is possible for $t < 0$ under the condition $\mu = 0$. The latter introduces thermodynamically forbidden (unstable) domains in the phase diagram.

The main conclusion which can be drawn from the Ginzburg-Landau free energy (11) of IBG at constant $\rho$ is that the point $t = 0$ resembles a tricritical point [3]. Usually such multicritical points occur on a phase transition line where the phase transition changes from second order to a symmetry conserving first order phase transition (or vice versa). Here this is not the case but the similarity with the usual tricriticality is in the fact that the coefficients of both the $\Psi^2$– and the $\Psi^4$–terms in (11) tend to zero for $t \to 0$. On the other side the phase transition to BEC is a continuous phase transition which exhibits critical exponents identical to the critical exponents known from the Berlin-Kac spherical model in ferromagnetism [22, 23] (see also Refs. [3, 4]). Here the condition of constant density $\rho$ plays the role of the spherical condition for the spins in the spherical model.

**Interaction effect.** Most of these exceptional properties of the phase transition to BEC in IBG are not present in systems of interacting bosons described by NBG. In this case an additional term of type $u\Psi^4$ will appear in the effective free energy $f(T, \rho, \Psi)$ and the respective coefficient of the $\Psi^4$–term will remain finite at $T_\lambda$ – the critical temperature to superfluid state in interacting Bose fluids (gases and liquids). The generalization of our treatment to the case of interacting bosons described by the action (1) may lead to new thermodynamic properties. A similar generalization for the spherical model was made in Ref. [23]. Another way of treatment of NBG may be performed within the loop expansion [21]. It is believed that the $\lambda$–transition described by NBG belongs to the so-called XY universality class of standard second order phase transitions [3].

Recent studies of interacting bosons indicated discrepancies in the theoretically predicted values of the critical temperature $T_\lambda$ [24, 25, 26, 27]. The problem for the calculation of the phase transition temperature of interacting many-body systems is a hard and still unresolved problem of the theory [3]. The fluctuation shifts of the critical temperature that are usually calculated from field models (see, e.g., Ref. [3] are very small and do not include essential contributions due to the large-momentum (high-energy) fluctuations of the order parameter field $\psi$. Therefore, the correct treatment of the phase transition temperature in many-body systems with interparticle interactions requires new theoretical methods.

**4. Constant pressure**

The only papers where the effect of the constraint of constant pressure on the phase transition properties of IBG has been investigated so far are Refs. [13, 14, 4, 16]. This case should be taken in mind in interpretations of real experiments, in particular, in low-temperature experiments on BEC in trapped atomic gases (see, e.g., Ref. [19]), where the density $\rho$ varies but the pressure $P$ is (almost) fixed. In this case BEC occurs at finite temperatures ($T_c > T > 0$) for all spatial dimensions $d > 0$. The
critical temperature will be \[ T_c(P) = \left( \frac{\lambda_0^d P}{\zeta(1 + d/\sigma)A(d, \sigma)k_B} \right)^{(d+\sigma)/(d+\sigma)}, \tag{15} \]

where \( \lambda_0 \) is given by \( \lambda_0 = \lambda T^{1/\sigma} \) and Eq. (5). For \( d = \sigma = 2 \) one obtains the result for \( T_c \) known from Ref. [13].

Although a number of results are known from preceding works, in particular, for the two-dimensional case \((d = 2)\) [13], the entire picture of the phase transition to BEC at constant pressure is not still clear for all spatial dimensions \( d \). In particular, this is the case of interacting bosons. We have no information about research papers devoted to this problem.

5. Concluding remarks

We have presented a brief discussion of several properties of the phase transition to BEC. New results have been obtained for the effective Landau-Ginzburg free energy (11), the equation of state (13) and the chemical potential (14) of BEC in ING for general values of \( d \) and \( \sigma \).

The effects of the constraints of constant density and constant pressure on BEC in ING and the condensation to a superfluid phase in systems of interacting bosons (NBG) are not yet clarified in a comprehensive way. The renormalization group methods [3, 4] reveal a dimensional (quantum to classical crossover) in interacting Bose systems and other basic universality features of the so-called quantum phase transitions at zero and very low temperatures but the equation of state below the phase transition point is not investigated in details. This is the situation for the whole variety of Bose systems known in condensed matter physics [3, 4] and, in particular, for Bose fluids of real atoms.

For Bose fluids the concept of universality of the quantum critical phenomena seems to be invalid and mainly for this reason the quantum phase transitions of second order can be classified in two groups: as universal and non-universal (see Ref. [4]). However, a number of examples indicate that the quantum phase transitions are often of first order or are described by multicritical points which are different from the critical points of standard second order phase transitions.

In astrophysics, a quantum phase transition \((T_c \sim 0)\) may occur in cases of very low density or very low pressure of the respective Bose fluid; see Eqs. (10) and (14). For the matter in the interior of neutron stars one should investigate the so-called classical limit [4] in which the quantum fluctuations are irrelevant. This is the case of \( T_c > 0 \) discussed in the prevailing part of our report.

BEC of spin bosons [17] can be treated within the framework of a generalization of our treatment. For this aim one may consider a complex vector field \( \vec{\psi}(q) = \{\psi_{\alpha}; \alpha = 1, \ldots, n/2\} \). For \( n = 2 \) one obtains the complex scalar field in Eq. (1). When such a system is placed in an external magnetic field, essentially new results can be ob-
tained [17]. The unresolved problem about the superfluidity of interacting spin bosons in external magnetic field is of special interest in astrophysics.

References

[1] Huang,K.: 1963, Statistical Physics, Wiley, New York.

[2] Landau,L.D. and Lifshits,E.M.: 1980, Statistical physics, Part I, Pergamon, London.

[3] Uzunov,D.I.: 1993, Theory of critical phenomena, World Scientific, Singapore.

[4] Shopova,D.V. and Uzunov,D.I.: 2003, Phys.Rep.C, 379, 1-67.

[5] Tilley,D.R., Tilley,J.: 1974, Superfluidity and Superconductivity, Van Nostrand Reinhold Company, New York.

[6] Link,B.: 2003, Phys.Rev.Lett., 91, 101101.

[7] Celebonovic,V. and Daæppen, in: 2000, 20th SPIG Conference, Ed. by Petrovic,Z. et al, Faculty of Physics and INN,Vinca, Beograd, Yugoslavia; see also astro-ph/0007337 and astro-ph/0102284.

[8] Tsuruta,S.: 1998, Phys.Rep.C, 292, 1.

[9] Pérez Rojas,H., Pérez Martínez,A. and Mosquera Cuuesta,H.J.: 2004 cond-mat/0407047.

[10] Nishiyama,M., Morita,M-a. and Morikawa,M.: 2004 astro-ph/0403571.

[11] Gunton,J.D. and Buckingham,M.J.: 1968, Phys.Rev., 166, 152.

[12] Cooper,M.J. and Green,M.S.: 1968, Phys.Rev., 176, 302.

[13] Gunther,L., Imry,Y. and Bergman,D.J.: 1974, J.Stat.Phys., 10, 425.

[14] Lacour-Gayet,P. and Toulouse,G.: 1974, J.Physique(Paris), 35, 425.

[15] Busiello,G., De Cesare,L. and Uzunov,D.I.: 1985, Physica A, 132, 199.

[16] Ivanov,V.G., in: 2004, Meetings in Physics at Sofia University, Ed. by A. Proykova, Heron Press, Sofia; cond-mat/0405537.

[17] Yamada,K.: 1982, Progr.Theor.Phys., 67, 443.

[18] da Frota,H.O., Silva,M.S., Goulart Rosa Jr,S.: 1984, J. Phys.C:Solid St. Phys., 17, 1669.
[19] Dalfovo, F., Giorgini, S., Pitaevskii, L. P. and Stringari, S.: 1999, Rev. Mod. Phys., 71, 463.

[20] Popov, V. N.: 1983, Functional integrals in quantum field theory and statistical physics, Riedel, Dordrecht.

[21] Toyoda, T.: 1982, Ann. Phys. (N.Y.), 141, 154.

[22] Berlin, T. H. and Kac, M.: 1952, Phys. Rev., 86, 821.

[23] Langer, J. S.: 1963, Phys. Rev., 137, No. 5A, A1532.

[24] Baym, G., Blaizot, J.-P., Holzmann, M. et al: 1999, Phys. Rev. Lett., 83, 1703.

[25] Huang, K.: 1999, Phys. Rev. Lett., 83, 3770.

[26] Schakel, A. M. J.: 2000, cond-mat/0004142

[27] Schakel, A. M. J.: 2003, J. Phys. Studies, 7, 140; cond-mat/0301050