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Two-step condensation of interacting bosons in three-dimensional isotropic harmonic traps

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Abstract. The Hartree–Fock–Popov theory of interacting Bose particles in a uniform space is generalized to the interacting boson system in three-dimensional isotropic harmonic traps. At finite temperature T , we find that the Bose condensation of nonideal bosons in three-dimensional isotropic harmonic traps is the two-step condensation. In other words, for a fixed particle number there are two transition temperatures. The first transition temperature is the standard critical temperature T_c . The second transition temperature is the critical temperature T_m , which is smaller than T_c and is determined by the minimum of the curve of condensate fraction versus temperature. The boson system undergoes a first-order phase transition from the normal state to the Bose condensed state.

Keywords: Bose Einstein condensation, cold atoms, rigorous results in statistical mechanics

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1. Introduction

It has currently been recognized that Bose–Einstein condensation (BEC) is a common quantum property of many-particle systems in which the number of particles is conserved. In 1995, the three groups observed the BEC in a vapor of dilute alkali atoms at a temperature of about 170 nK [1–3]. The recent progresses of BEC in dilute atomic gases have been made in many respects. One respect is the trapping geometry. The corresponding trapping geometry can be designed to be harmonic, anharmonic or, recently, even box-like, which mimics a quasi-uniform potential [4, 5]. Another respect is the supersolid state of quantum gases. The supersolid state combines superfluid flow with long-range spatial periodicity of crystals. Pitaevskii and Stringari have calculated the excitation spectrum of a spin–orbit-coupled Bose–Einstein condensate and thereby have found supersolid phenomena in ultracold atomic gases [6]. Han *et al* have predicted a supersolid with nontrivial topological spin textures in spin–orbit-coupled Bose gases [7]. Ketterle and his colleagues have observed supersolid properties in spin–orbit-coupled Bose–Einstein condensates [8]. Léonard *et al* have observed supersolid formation in a quantum gas breaking a continuous translational symmetry [9].

The starting point for our discussion of interacting quantum mechanical assemblies is the Hartree–Fock (HF) approximation. The HF approximation is basically a static mean-field theory, which treats the motion of single particles in an average static field generated by all the other particles. The HF approximation neglects terms like $\langle \hat{a}_{-\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}^\dagger \rangle$ or $\langle \hat{a}_{-\mathbf{k}} \hat{a}_{\mathbf{k}} \rangle$ in the Hamiltonian, which reflect the creation and annihilation of two uncondensed particle pairs due to the interaction and play a crucial role in the BEC theory. The Hartree–Fock–Popov (HFP) approximation includes terms like $\langle \hat{a}_{-\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}^\dagger \rangle$ or $\langle \hat{a}_{-\mathbf{k}} \hat{a}_{\mathbf{k}} \rangle$ in the Hamiltonian. This approach consequently accounts for the low-energy excitations of the system. Originally, the Bogoliubov theory of BEC deals with a weakly interacting boson gas in a uniform space at zero temperature. At small momenta, the elementary excitations of such a boson gas are phonons. However, the original Bogoliubov theory cannot apply to the BEC problem of interacting Bose atoms in an inhomogeneous space at finite temperatures. For this reason, the present paper develops a new theory to investigate the finite-temperature properties of a weakly interacting boson

gas in three-dimensional isotropic harmonic traps. The finite-temperature properties include the transition temperature, elementary excitation spectrum, and depletion of the BEC phase.

The key point in this paper is that the three-dimensional isotropic harmonic potential in coordinate space can be reduced into the zero-point energy in momentum space, so that the energy of an ideal atom in three-dimensional isotropic harmonic traps consists of the kinetic energy and the zero-point energy. In light of the HFP theory of BEC, we investigate the BEC properties of a harmonically trapped, three-dimensional, and weakly interacting gas in the momentum representation. We give a critical analysis of the HFP approximation in the BEC of such an interacting boson. Thereby we derive the transition temperature, elementary excitation spectrum, and depletion of the BEC phase of a harmonically trapped, three-dimensional, and weakly interacting gas. At finite temperature T , we find that the Bose condensation of nonideal bosons in three-dimensional isotropic harmonic traps is the two-step condensation. In other words, for a fixed particle number there are two transition temperatures. The first transition temperature is the standard critical temperature T_c . The second transition temperature is the critical temperature T_m , which is smaller than T_c and is determined by the minimum of the curve of condensate fraction versus temperature. At small momenta k , the elementary excitation is a phonon. At large momenta k , the elementary excitation is a bare atom. Originally, a two-step condensation due to interactions was discovered by Zagrebnov and Bru [10–12]. The present paper gives another model in favor of a two-step condensation due to interactions. Our theory can be verified in the present-day physics laboratories.

2. Formulism

If $U(\mathbf{r} - \mathbf{r}')$ represents the interaction potential between a boson located at \mathbf{r} and another boson located at \mathbf{r}' , then the finite-size Gaussian potential [13] is

$$U(\mathbf{r} - \mathbf{r}') = g \frac{1}{\pi^{3/2} |s|^3} \exp \left[-\frac{(\mathbf{r} - \mathbf{r}')^2}{s^2} \right], \quad (1)$$

where g and s characterize the strength and range of the interaction, respectively. Both parameters are considered to be tunable. For instance, g can be varied by means of a suitable Feshbach resonance. In the limit of s going to zero, we recover a contact interaction with strength g . We adopt the grand canonical ensemble, in which bosons have a chemical potential μ . Now one can write the Hamiltonian of the nonideal boson system in terms of the boson operators $\hat{a}_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}^\dagger$:

$$\hat{H} = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu^*) \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \frac{1}{2V} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} v(\mathbf{q}) \hat{a}_{\mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\mathbf{k}'-\mathbf{q}}^\dagger \hat{a}_{\mathbf{k}'} \hat{a}_{\mathbf{k}}, \quad (2)$$

where $\varepsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2m$ is the kinetic energy of a boson with wave vector \mathbf{k} and m is the mass of bosons. $\mu^* = \mu - \frac{3}{2} \hbar \omega$ is an effective chemical potential and $\frac{3}{2} \hbar \omega$ is just the zero-point energy of a three-dimensional isotropic harmonic oscillator. ω is the angular

frequency of the trap. $v(\mathbf{q})$ is the Fourier transform of the interaction potential $U(\mathbf{r})$ of bosons and the boson system occupies a volume V .

We need to study the finite-temperature excitations in the system of interacting bosons. The best way to do this study is to use the Beliaev–Green’s function formalism [14, 15]. This technique is the most effective way of calculating the equilibrium thermodynamic properties, as well as single-particle excitations of the system. Our emphasis is on how to include the effects of the non-condensate bosons and is based on the first-order HFP self-energy diagrams. At first, we define the normal and anomalous Green’s function as

$$G_{11}(\mathbf{k}, \tau) = -\langle T_\tau [\hat{a}_{\mathbf{k}}(\tau) \hat{a}_{\mathbf{k}}^\dagger(0)] \rangle, \quad (3)$$

$$G_{12}(\mathbf{k}, \tau) = -\langle T_\tau [\hat{a}_{-\mathbf{k}}(\tau) \hat{a}_{\mathbf{k}}(0)] \rangle, \quad (4)$$

where T_τ is a τ ordering operator. G_{11} and G_{22} represent the propagation of a single boson. G_{12} and G_{21} represent the disappearance and appearance of two non-condensate bosons, respectively. There are two types of proper self-energies for a Bose-condensed system. In the Feynman diagrams, one type of proper self-energies have one particle line going in and one coming out, which are denoted as $\Sigma_{11}(\mathbf{k}, \tau)$ and $\Sigma_{22}(\mathbf{k}, \tau)$. The other ones have two particle lines either coming out, denoted by $\Sigma_{12}(\mathbf{k}, \tau)$, or going in, denoted by $\Sigma_{21}(\mathbf{k}, \tau)$. For simplicity, we use the letter p to represent the four-dimensional vector $(\mathbf{k}, i\omega_n)$.

Next we discuss the HFP approximation for a gas of N interacting bosons at finite temperatures [16]. We prescribe that at finite temperature T , the number of bosons in the lowest state ($\mathbf{k} = 0$) is given by $N_c(T)$. The N_c bosons form a Bose condensate. In the rest of this paper, we use the superscript ‘(0)’ as a reminder that the quantity is for a noninteracting Bose gas. Now we need to introduce a quantity $\tilde{n}^{(0)}$, which denotes the (temperature-dependent) density of excited bosons in a noninteracting Bose gas and is given by

$$\tilde{n}^{(0)} = \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{1}{\exp[\beta(\varepsilon_{\mathbf{q}} - \mu^{(0)})] - 1}, \quad (5)$$

where $\beta = 1/k_B T$. Consequently, the self-energy Σ_{11} and Σ_{12} can be explicitly written as

$$\Sigma_{11}(\mathbf{k}) = 2n_c v(0) + 2\tilde{n}^{(0)} v(0), \quad (6)$$

$$\Sigma_{12}(\mathbf{k}) = n_c v(0),$$

where $n_c = N_c/V$ is called the condensate density.

In the Bose-condensed phase of $T < T_c$, the chemical potential μ^* of an interacting Bose gas has been shown to satisfy [17–19]

$$\mu^* = n_c v(0) + 2\tilde{n}^{(0)} v(0), \quad T < T_c. \quad (7)$$

By substituting the self-energies in equation (6) and the chemical potential in equation (7) into the Dyson–Beliaev expressions, we obtain G_{11} and G_{12} as

$$G_{11}(p) = \frac{i\omega_n + \varepsilon_{\mathbf{k}} + \Delta}{(i\omega_n)^2 - \varepsilon_{\mathbf{k}}^2 - 2\Delta\varepsilon_{\mathbf{k}}}, \quad (8)$$

$$G_{12}(p) = -\frac{\Delta}{(i\omega_n)^2 - \varepsilon_{\mathbf{k}}^2 - 2\Delta\varepsilon_{\mathbf{k}}}. \quad (9)$$

Here the quantity Δ is defined by $\Delta(T) = n_c(T)v(0)$. Both G_{11} and G_{12} in equations (8) and (9) have identical poles at $\omega = \pm E_{\mathbf{k}}$, where

$$E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + 2\Delta(T)\varepsilon_{\mathbf{k}}}. \quad (10)$$

This gives the energy spectrum of elementary excitations for $T < T_c$. $E_{\mathbf{k}}$ is phonon-like in the long-wavelength limit and the phonon velocity c is given by

$$c \equiv \sqrt{\Delta(T)/2m} = \sqrt{n_c(T)v(0)/2m}. \quad (11)$$

For a given total density n , we have

$$n = n_c + \tilde{n}, \quad (12)$$

where \tilde{n} denotes the density of uncondensed bosons and is given by

$$\tilde{n} = \int \frac{d\mathbf{k}}{(2\pi)^3} \left(\frac{\varepsilon_{\mathbf{k}} + \Delta}{2E_{\mathbf{k}}} \coth \frac{\beta E_{\mathbf{k}}}{2} - \frac{1}{2} \right). \quad (13)$$

For a given n and T , equations (12) and (13) are coupled equations for determining $n_c(T)$.

Then we give a study of BEC of ideal bosons in three-dimensional isotropic harmonic traps. The topic of BEC in a uniform, noninteracting gas of bosons is treated in most textbooks on statistical mechanics [20]. In the grand canonical ensemble, the system under study consists of N ideal bosons in three-dimensional isotropic harmonic traps, which have the energy spectrum $\varepsilon_n = \hbar\omega(n + \frac{3}{2})$ and a chemical potential $\mu^{(0)}$. Based on the first principles of statistical mechanics, one knows that the number N_n of bosons in the n th state of energy ε_n obeys the Bose–Einstein distribution

$$N_n = \frac{1}{e^{\beta(\varepsilon_n - \mu^{(0)})} - 1}. \quad (14)$$

The chemical potential $\mu^{(0)}$ is determined by the constraint that the total number of bosons in the system is N :

$$\sum_{n=0}^{\infty} f_n N_n = N, \quad (15)$$

where $f_n = \frac{1}{2}(n+1)(n+2)$ is the degree of degeneracy for three-dimensional isotropic harmonic traps. The phenomenon of BEC for ideal bosons is fully described by equations (14) and (15).

To determine $\mu^{(0)}$, we need to introduce the fugacity z by the definition $z = \exp(\beta\mu^*)$, where we have introduced an effective chemical potential $\mu^* = \mu^{(0)} - \frac{3}{2}\hbar\omega$. One can introduce the parameters $q = \exp(-\beta\hbar\omega)$ and $x = 1 - \mu^*/\hbar\omega$. Because the temperature

T appears in the definition $z = \exp(\beta\mu^*)$, the fugacity z does not parameterize the chemical potential μ^* by much and so z is not a good physical quantity. The quantity x parameterizes the chemical potential μ^* a lot and so x is a good physical quantity. As a result, the quantity x is called the reduced chemical potential. In the same way, the quantity q parameterizes the temperature T a lot and so q is a good physical quantity. In terms of the good physical quantities x and q , equation (15) is cast into an equation of state:

$$\frac{q^{x-1}}{1-q^{x-1}} + P_q(x) = N, \quad (16)$$

$$P_q(x) = F_q(x) + 2G_q(x) + H_q(x), \quad (17)$$

$$F_q(x) = \frac{\ln(1-q) + \psi_q(x)}{\ln q}, \quad (18)$$

$$G_q(x) = \frac{(k_c + 1) \ln(1-q)}{\ln q} + \frac{1}{\ln q} \sum_{k=0}^{k_c} \psi_q(x+k), \quad (19)$$

$$H_q(x) = \frac{k_c(k_c + 1) \ln(1-q)}{2 \ln q} + \frac{1}{\ln q} \sum_{k=1}^{k_c} k \psi_q(x+k), \quad (20)$$

where the upper limit ∞ of summation is replaced by an upper cutoff k_c and in practice we set $k_c = 200$. The numerical calculation demonstrates that the upper cutoff $k_c = 200$ is sufficient for a high precision calculation. $\psi_q(x)$ is the q -digamma function defined by $\psi_q(x) = d[\ln \Gamma_q(x)]/dx$, where $\Gamma_q(x)$ is the q -gamma function defined by

$$\Gamma_q(x) = (1-q)^{1-x} \prod_{n=0}^{\infty} \frac{1-q^{n+1}}{1-q^{n+x}}, \quad (21)$$

when $|q| < 1$ and $x \neq 0, -1, -2, \dots$. The q -gamma function was introduced by Jackson [21] and the q -digamma function was introduced by Krattenthaler and Srivastava [22]. In recent decades the q -gamma function and the q -polygamma function have gained extensive applications in science and technology [23].

$P_q(x)$ represents the number of noncondensed atoms. The reduced chemical potential x can be determined numerically from equation (16). x is a function of temperature T and particle number N . Once x is known, the number of Bose atoms in the ground state can be obtained from the relation $N_0 = q^{x-1}/(1-q^{x-1})$. To satisfy equation (16), it is necessary that $x \geq 1$. When $x = 1$, a three-dimensional atomic gas is in the state of BEC. The critical temperature T_c can now be found by setting $N_0 = 0$ and $x = 1$ in equation (16). This results in the following expression for the critical temperature,

$$P_{q_c}(1) = N, \quad (22)$$

where $q_c = \exp(-\hbar\omega/k_B T_c)$. The function $P_{q_c}(1)$ can be rewritten as $p(q_c) = P_{q_c}(1)$. By virtue of equation (22), from equation (16) we find that the condensate fraction of bosons in the ground state is given by

$$\frac{N_0}{N} = \begin{cases} 1 - \frac{p(q)}{p(q_c)}, & T \leq T_c, \\ 0, & T > T_c. \end{cases} \quad (23)$$

We shall assume that a weakly interacting and a noninteracting Bose gas have the same BEC transition temperature T_c , as given by equation (22).

3. Numerical calculation

In this section we shall make a numerical calculation in the finite-temperature case ($T \leq T_c$). The temperature dependence of the condensate density $n_c(T)$ may be derived from equations (12) and (13). Since their solution requires numerical methods, one can introduce the reduced wave-number $x = \hbar k/2\sqrt{m\Delta}$. We first let $y = n_c(T)/n$ and then derive the following expression,

$$y = 1 - \frac{[2myn^{\frac{1}{3}}v(0)]^{\frac{3}{2}}}{3\pi^2\hbar^3} - \frac{4[myn^{\frac{1}{3}}v(0)]^{\frac{3}{2}}}{\pi^2\hbar^3} \times \int_0^\infty \frac{x(x^2+1)}{\sqrt{x^2+2}} \frac{1}{\exp\left[\frac{y\nu v(0)}{k_B T} \sqrt{x^4+2x^2}\right] - 1} dx. \quad (24)$$

Therefore, $n_c(T)/n$ is a universal function of T , N and g , independently of any particular property of the atom system. In order to give a numerical impression of $n_c(T)/n$, we set $\omega/2\pi = 140.0$ Hz, which is accessible to an actual experiment [2]. One can introduce an oscillator length $a = \sqrt{\hbar/m\omega}$, which characterizes the spread of the oscillator wave function in the radial direction. We take into account the gas of ^{23}Na atoms, which are bosons and have a positive scattering length. The mass of ^{23}Na atoms is $m = 23$ a.u. and thereby the oscillator length is calculated as $a = 1.7717 \mu\text{m}$. The trapping volume V of the atom system can be regarded as a cube of side length $L = 15a$. Therefore we have $V = L^3$. Concomitantly, we take the number density of atoms as $n = N/V$. In the following calculation, we take $g = 0.74 \times 10^{-23}$ eV cm³.

According to equation (24), the variation with the temperature T of the condensate fraction $n_c(T)/n$ is shown in figure 1 for $N = 1000\,000$. From equation (22), we find that at $N = 10^6$, the corresponding transition temperature is $T_c = 0.629 \mu\text{K}$. From figure 1, one can see that the Bose condensation of nonideal bosons in three-dimensional isotropic harmonic traps is the two-step condensation [24–26]. In other words, for a fixed N there are two transition temperatures. The first transition temperature is the critical temperature T_c . The second transition temperature is the critical temperature T_m , which is smaller than T_c and is determined by the minimum of the curve. The calculation gives $T_m = 0.536 \mu\text{K}$. The condensate fraction decreases continuously from $n_c(0)/n$ to the minimum as the temperature increases from zero to the transition temperature T_m . In the temperature range $T_m < T \leq T_c$, the condensate fraction increases slowly. The BEC in such a three-dimensional system demonstrates new features: in the temperature range $0 < T \leq T_m$ the equilibrium state is a normal condensate, whereas in the

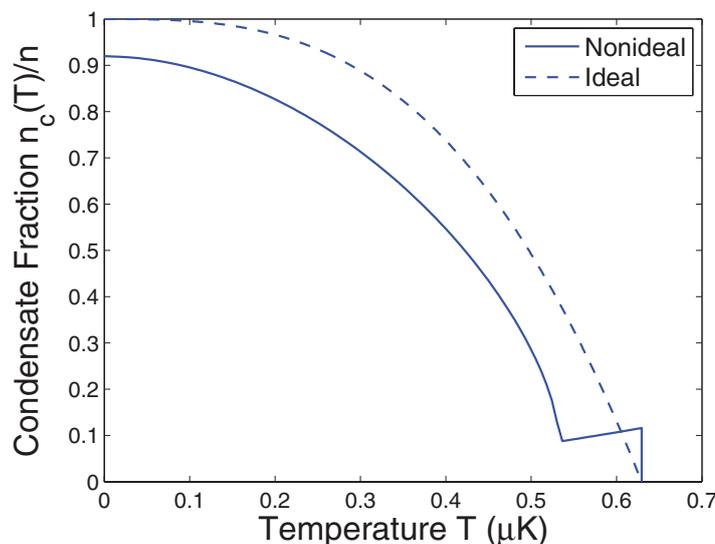


Figure 1. The solid and dashed lines denote the variation of the condensate fraction $n_c(T)/n$ of nonideal and ideal Bose atoms with the temperature T , respectively. The temperature T varies from zero to the transition temperature T_c .

temperature range $T_m < T \leq T_c$ one has a quasi condensate. The quasi condensate is a generalized condensate due to interactions. According to equation (23), figure 1 also shows that the condensate fraction $n_c^{(0)}(T)/n$ of the ideal Bose gas varies with the temperature T . In the temperature range $0 < T \leq T_m$, $n_c^{(0)}(T) > n_c(T)$. This means that the repulsive interaction between bosons kicks off a small fraction of bosons out of the condensate. In the temperature range $T_m < T \leq T_c$, one first has $n_c^{(0)}(T) > n_c(T)$ and then has $n_c^{(0)}(T) < n_c(T)$. This means that the quasi condensation state is metastable. Figure 1 clearly indicates a finite jump in the condensate fraction $n_c(T)/n$ at the transition temperature T_c . This jump is the characteristic of a first-order phase transition.

According to equation (24), the variation with the boson number N of the condensate fraction $n_c(T)/n$ is shown in figure 2 for $T = 0.17 \mu\text{K}$. From equation (22), we find that at $T = 0.17 \mu\text{K}$, the critical boson number is $N_c = 18949$. From figure 2, one can see that for a fixed T there are two critical boson numbers. The first critical boson number is N_c . The second critical boson number is N_m , which is larger than N_c and is determined by the minimum of the curve. The calculation gives $N_m = 2 \times 10^5$. In the boson number range $N_c \leq N \leq N_m$, the condensate fraction decreases to the minimum very fast. The condensate fraction first increases from the minimum to the maximum and then decreases as the boson number increases from N_m . The BEC in such a three-dimensional system demonstrates new features: in the boson number range $N > N_m$ the equilibrium state is a normal condensate, whereas in the boson number range $N_c \leq N \leq N_m$ one has a quasi condensate. The quasi condensate is a generalized condensate due to interactions. According to equation (16), figure 2 also shows that the condensate fraction $n_c^{(0)}(T)/n$ of the ideal Bose gas varies with the boson number N . In the boson number range $N > N_m$, $n_c^{(0)}(T) > n_c(T)$. This means that the repulsive interaction between bosons kicks off a small fraction of bosons out of the condensate.

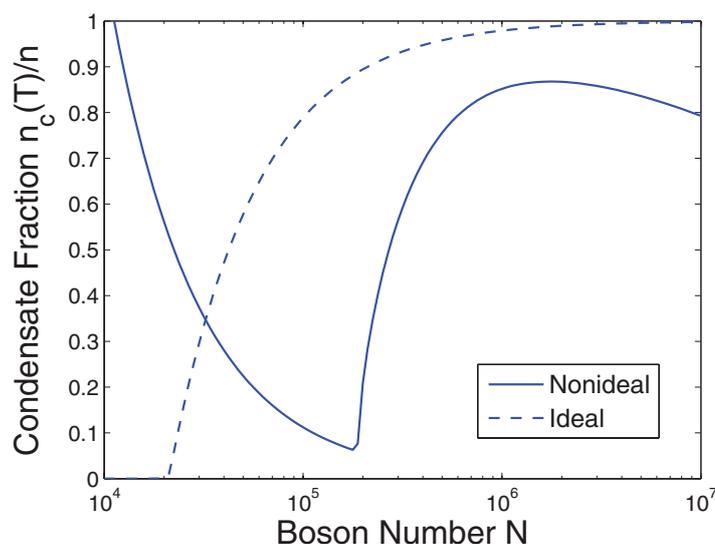


Figure 2. The solid and dashed lines denote the variation of the condensate fraction $n_c(T)/n$ of nonideal and ideal Bose atoms with the boson number N , respectively.

In the boson number range $N_c \leq N \leq N_m$, one first has $n_c^{(0)}(T) < n_c(T)$ and then has $n_c^{(0)}(T) > n_c(T)$. This means that the quasi condensation state is metastable.

4. Conclusions

Just over 24 years after the discovery of BEC in ultracold dilute atomic gases, it is clear that much important progress still remains to be made. A lot of experiments clearly show that the interaction between bosons can indeed play an important role in the BEC of bosons. The existing BEC theory is highly relevant to all basic features revealed in the BEC of dilute atomic gases. An ongoing viewpoint about the BEC mechanism in three-dimensional anisotropic harmonic traps is that the Bose condensation is the two-step condensation. Our study has pointed out that the Bose condensation of interacting bosons in three-dimensional isotropic harmonic traps is also the two-step condensation. In the temperature range $0 < T \leq T_m$ the equilibrium state is a normal condensate, whereas in the temperature range $T_m < T \leq T_c$ one has a quasi condensate. The quasi condensate is a generalized condensate due to interactions. In fact, the condensation phase of dilute atomic gases shows some features of normal Bose–Einstein condensation along with others of generalized Bose–Einstein condensation.

In summary, we have proposed a BEC theory of nonideal bosons in three-dimensional isotropic harmonic traps within the HFP approximation. The BEC of trapped nonideal bosons within the HFP approximation possesses some peculiar properties. The Bose condensation in three-dimensional isotropic harmonic traps is the two-step condensation. The boson system undergoes a first-order phase transition from the normal state to the BEC state. These features reveals some secrets of the condensation phase of trapped nonideal bosons.

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