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DEPLETION DENSITY OF IDEAL GAS BOSE-EINSTEIN CONDENSATE BY TWO PARALLEL PLATES

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Abstract. By means of the second quantization formalism, the condensate density of an infinite Bose gas and finite Bose gas is studied in the broken phase. Our results show that the compactification in one-direction makes the remarkable changes in the condensate density.

Keywords: Bose-Einstein condensate, second quantization, condensate density.

1. Introduction

It is well-known that the system of indistinguishable Bose particles is not affected by the Heisenberg uncertainty principle. Thereby, the particles are allowed to occupy the same state [1]. For a system of Bose gas, a number of the atoms will be condensed when the temperature is decreased to a critical temperature T_C. Theoretically, once the temperature tends to absolute zero temperature, all of the atoms are condensed into the ground state [2, 3]. However, there are always non-condensed atoms even at zero temperature, and the density of non-condensed particles is called the depletion density. The depletion density consists of the quantum depletion associated with the quantum fluctuations [4] and thermal one corresponding to thermal fluctuations [5, 6].

Apart from the temperature, the finite size effect has a remarkable influence on the depletion the density, and thus condensate density of the Bose gas [7]. In the region of low temperature, i.e. $0 < T < T_C$, the depletion is caused by the thermal fluctuations. The main aim of this paper is to investigate the condensate density caused by the thermal fluctuations in the homogeneous Bose gas and the Bose gas confined between two parallel plates.

2. Content

2.1. Chemical potential of weakly interacting Bose gas at finite temperature

To begin with, we consider a weakly interacting Bose gas at finite temperature T. In the grand canonical ensemble, every property of the interacting Bose gas can be subtracted from the partition function [3],

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$$Z = \mathrm{Tr} e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}, \tag{1}$$

in which $\hat{H}$ is the Hamiltonian of trapped many-body boson system in the second quantization formalism, which can be expressed in terms of the field operator $\hat{\Psi}(r,t)$

$$\begin{aligned}\hat{H} = \int d\mathbf{r}\hat{\Psi}^{+}(\mathbf{r},t)\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r})\right]\hat{\Psi}(\mathbf{r},t)\\ +\frac{g}{2}\int d\mathbf{r}\hat{\Psi}^{+}(\mathbf{r},t)\hat{\Psi}^{+}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t).\end{aligned} \tag{2}$$

Here $\hbar$ and m are denoted for the reduced Planck constant and atomic mass, respectively. The strength of repulsive interaction between atoms is determined by the coupling constant $g = 4\pi\hbar^2 a/m > 0$, with a being s-wave scattering length of a particular atomic species (determined from experiments). The effect from an external field is characterized by the external potential $V_{ext}(r)$. The equation of motion for the particle field operator follows directly from the Heisenberg equation and reads

$$i\hbar\frac{\partial\hat{\Psi}(\mathbf{r},t)}{\partial t} = [\hat{\Psi}(\mathbf{r},t),\hat{H}], \tag{3}$$

and Hamiltonian (2) one has

$$i\hbar\frac{\partial\hat{\Psi}(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r})\right]\hat{\Psi}(\mathbf{r},t) + g\hat{\Psi}^{+}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t), \tag{4}$$

which is known as Gross-Pitaevskii time-dependent equation for identical boson systems. We now split the field operator into two parts [9, 10],

$$\hat{\Psi}(\mathbf{r},t) = \psi(\mathbf{r},t) + \delta(\mathbf{r},t).$$

Here, $\psi(\mathbf{r},t) = \left\langle\hat{\Psi}(\mathbf{r},t)\right\rangle$ is the condensate wave-function, $\delta(\mathbf{r},t) = \hat{\Psi}(\mathbf{r},t) - \psi(\mathbf{r},t)$ is non-condensate wave-function, which describes the thermal excitations. These assumptions together with Eq. (4) lead to

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r})\right]\psi(\mathbf{r},t) + g\left\langle\hat{\Psi}^{+}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\right\rangle, \tag{5}$$

and

$$\begin{aligned}i\hbar\frac{\delta(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r})\right]\delta(\mathbf{r},t)\\ +g\left[\hat{\Psi}^{+}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t) - \left\langle\hat{\Psi}^{+}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\right\rangle\right]\end{aligned}. \tag{6}$$

In order to calculate the second terms of the above equations, we use the self-consistent mean-field approximation as follow [11, 12]:

$$\delta^*\delta\delta = 2\left\langle \delta^*\delta \right\rangle \delta + \left\langle \delta\delta \right\rangle \delta.$$

Therefore

$$\hat{\Psi}^+(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t) = \left|\psi\right|^2 \psi + 2\left\langle \hat{\Psi}^+\hat{\Psi} \right\rangle \delta + \left\langle \hat{\Psi}\hat{\Psi} \right\rangle \delta^* + 2\psi\delta^*\delta + \psi^*\delta\delta. \tag{7}$$

Note that the average of the thermal fluctuations is equal to zero, i.e $\left\langle \delta \right\rangle = \left\langle \delta^* \right\rangle = 0$, one has

$$\begin{aligned} \left\langle \hat{\Psi}^+(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t) \right\rangle &= \left|\psi\right|^2 \psi + 2\psi\left\langle \delta^*\delta \right\rangle + \psi^*\left\langle \delta\delta \right\rangle \\ &= \left[\left\langle \hat{\Psi}^+\hat{\Psi} \right\rangle + \left\langle \delta^*\delta \right\rangle\right]\psi + \left\langle \delta\delta \right\rangle \psi^*. \end{aligned} \tag{8}$$

Inserting of (8) into (5) leads to

$$\begin{aligned} i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} &= \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r})\right]\psi(\mathbf{r},t) \\ &\quad + g\left[\left\langle \hat{\Psi}^+\hat{\Psi} \right\rangle + \left\langle \delta^*\delta \right\rangle\right]\psi(\mathbf{r},t) + g\left\langle \delta\delta \right\rangle \psi^*(\mathbf{r},t), \end{aligned} \tag{9}$$

neglecting anomalous average $\left\langle \delta\delta \right\rangle$, we obtained

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r})\right]\psi(\mathbf{r},t) + g\left[\left\langle \hat{\Psi}^+\hat{\Psi} \right\rangle + \left\langle \delta^*\delta \right\rangle\right]\psi(\mathbf{r},t). \tag{10}$$

At the zero-temperature limit, thermal excitation vanishes, thus (9) and (10) become the time-dependent Gross-Pitaevskii, which provides solutions to ground state wave-function and quantum fluctuations within Bogoliubov transformation [1].
Subtracting (8) from (7) one gets

$$\hat{\Psi}^+(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t) - \left\langle \hat{\Psi}^+(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t) \right\rangle = 2\left\langle \hat{\Psi}^+\hat{\Psi} \right\rangle \delta + \tilde{\Delta}, \tag{11}$$

here $\tilde{\Delta} = \left\langle \hat{\Psi}\hat{\Psi} \right\rangle \delta^* + 2\psi\left[\delta^*\delta - \left\langle \delta^*\delta \right\rangle\right] + \psi^*\left[\delta\delta - \left\langle \delta\delta \right\rangle\right]$, which included perturbation terms.

Substituting (11) into (6) under Hartree-Fock approximation, in which the perturbation terms are neglected, we find

$$i\hbar\frac{\delta(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r})\right]\delta(\mathbf{r},t) + 2g\left\langle \hat{\Psi}^+\hat{\Psi} \right\rangle \delta(\mathbf{r},t). \tag{12}$$

In the thermodynamic limit, the total density of atoms is fixed, the field operator can be written in the form

$$\hat{\Psi}(\mathbf{r},t)=\sqrt{n_0}e^{-\mathbf{i}\mu t/\hbar}, \tag{13}$$

here $\mathbf{i}^2=-1$, and

$$n_0=\langle\hat{\Psi}^+\hat{\Psi}\rangle=n_c(\mathbf{r})+n_d(\mathbf{r}) \tag{14}$$

is the total atomic density included the condensate density $n_c(\mathbf{r})$ and the thermal excitation density $n_d(\mathbf{r})$, which respectively determined by the condensate wave-function

$$\psi(\mathbf{r},t)=\sqrt{n_c(\mathbf{r})}e^{-\mathbf{i}\mu t/\hbar},\ n_c(\mathbf{r})=|\psi(\mathbf{r},t)|^2, \tag{15}$$

and the non-condensate wave-function

$$\delta(\mathbf{r},t)=\sum_{j\geq 1}\varphi_j(\mathbf{r},t)=\sum_{j\geq 1}\varphi_j(\mathbf{r},t)e^{-\mathbf{i}\varepsilon_j t/\hbar},\ n_d(\mathbf{r})=\langle\delta(\mathbf{r},t)^*\delta(\mathbf{r},t)\rangle \tag{16}$$

with $\mu=\mu(n_0,T)$ is chemical potential, ε_j is energy corresponds to the single-particle wave-function $\varphi_j(\mathbf{r},t)$.

At equilibrium state, $n_c(\mathbf{r})$ and $n_d(\mathbf{r})$ are functions of T, n_0 and μ, thus them respectively replaced by n_c and n_d from now on.

Using (10), (12) within attention to (14), (15) and (16) one has

$$\mu=g(n_0+n_d)=g(n_c+2n_d), \tag{17}$$

and

$$\varepsilon_j(p)=\frac{p^2}{2m}+V_{\text{eff}}, \tag{18}$$

where effective potential $V_{\text{eff}}=V_{\text{ext}}+2gn_0$, V_{ext} is external potential.

2.2. Depletion density of weakly interacting Bose gas in infinite space

Occupation numbers of j-th state defined by Bose-Einstein statistics [2, 3],

$$n_j(p)=\frac{1}{e^{\beta(\varepsilon_j-\mu)}-1}, \tag{19}$$

in which $\beta=\frac{1}{k_BT}$. Thus, the thermal atomic density is determined in momentum-space as follow [3, 9]:

$$n_d(p) = \frac{1}{(2\pi\hbar)^3} \int_0^\infty d^3\mathbf{p} n_j(p). \tag{20}$$

Inserting (19) into (21) and using transition $\mathbf{p} \to \hbar\mathbf{k}$, one has

$$n_d(k) = \frac{1}{(2\pi)^3} \int_0^\infty \frac{d^3\mathrm{k}}{e^{\beta\left(\frac{\hbar^2k^2}{2m}+2gn_0-\mu\right)}-1}. \tag{21}$$

Note that here we set external potential (V_{ext}) equal to zero.

Substitution (18) into (22), and note that $\int d^d x = \frac{2\pi^{d/2}}{\Gamma(d/2)} \int_0^\infty x^{d-1} dx$ can rewrite Eq. (21) in form

$$n_d(k) = \frac{1}{2\pi^2} \int_0^\infty \frac{k^2 dk}{e^{\beta\left(\frac{\hbar^2k^2}{2m}+gn_c\right)}-1}. \tag{22}$$

Perform above integration one finds

$$n_d(T) = \frac{(mk_BT)^{3/2}}{(2\pi)^{3/2}\hbar^3} Li_{3/2}\left[e^{-\frac{gn_c}{k_BT}}\right]. \tag{23}$$

For ideal Bose gas, $g=0$ and $Li_{3/2}[1]=\zeta[3/2]$ one arrives

$$n_d(T) = \frac{(mk_BT)^{3/2}}{(2\pi)^{3/2}\hbar^3}\zeta\left[3/2\right]. \tag{24}$$

At the critical temperature, $n_d(T)=n_0$, using (24) one finds the critical temperature of the ideal Bose gas is

$$T_c^{(0)} = \frac{2\pi\hbar^2 n_0^{2/3}}{mk_B\zeta\left[3/2\right]^{2/3}}, \tag{25}$$

this coincides with the well-known result in Refs. [2, 3].

2.3. Depletion density of Bose ideal gas confined by two parallel plates

Applying (21) for the ideal Bose gas below the critical temperature we have

$$n_d(k) = \int_0^\infty \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{e^{\beta\frac{\hbar^2k^2}{2m}}-1}. \tag{26}$$

Our system is confined between two parallel plates perpendicular to the *z*-axis and separated at a distance ℓ. Because of the confinement along the *z*-axis, the wave vector is quantized as follows:

$$d^3k \to \frac{1}{\overline{\ell}}\sum_i d^2k, k^2 \to k_\perp^2 + k_j^2, k_j = \frac{i}{\overline{\ell}}, i = 0, \pm1, \pm2, ..., \overline{\ell} = \frac{\ell}{2\pi}, \tag{27}$$

in which, the wave vector component $k_\perp$ is perpendicular to *z*-axis and k_j is parallel with *z*-axis. Note that here the periodic boundary condition is imposed. Using the Taylor series

$$\frac{1}{e^x - 1} = \sum_{j=1}^{\infty} e^{-jx}.$$

Eq. (26) becomes

$$n_d(k) = \frac{1}{2\pi^2\overline{\ell}} \int_0^\infty \sum_{i=0}^\infty \sum_{j=1}^\infty e^{-j\beta\frac{\hbar^2 k^2}{2m}\left(k_\perp^2 + \frac{i^2}{\overline{\ell}^2}\right)} k_\perp dk_\perp. \tag{28}$$

Perform integration in (28) one finds

$$n_d(T) = \frac{mk_BT}{2\pi^2\hbar^2\overline{\ell}} \sum_{i=0}^\infty \sum_{j=1}^\infty \frac{e^{-\frac{\hbar^2 i^2 j}{2mk_BT\overline{\ell}^2}}}{j}. \tag{29}$$

Using Euler-Maclaurin formula to define i-summation we find

$$\sum_{i=0}^\infty e^{-\frac{\hbar^2 i^2 j}{2mk_BT\overline{\ell}^2}} = \frac{\sqrt{\pi}\sqrt{mk_BT}\,\overline{\ell}}{\sqrt{2}\hbar j^{1/2}} + \frac{1}{2}. \tag{30}$$

Substituting (30) into (29) yields

$$n_d(T) = \frac{mk_BT}{2\pi^2\hbar^2\overline{\ell}} \sum_{i=0}^\infty \frac{1}{j}\left(\frac{\sqrt{mk_BT}\,\overline{\ell}}{\sqrt{2\pi}\hbar j^{1/2}} + \frac{1}{2}\right) = \frac{(mk_BT)^{3/2}}{\left(\sqrt{2\pi}\hbar\right)^3}\zeta[3/2] + \frac{(mk_BT)^{3/2}\alpha}{4\sqrt{2}\pi^{5/2}\hbar^3}\sum_{j=1}^\infty \frac{1}{j}, \tag{31}$$

in which, $\alpha = \lambda_B / \overline{\ell}, \lambda_B = \sqrt{\frac{2m\hbar^2}{mk_BT}}$ is de Broglie wavelength. When $\ell \to \infty$ then $\alpha \to 0$, the second term in (31) annihilated, and (31) becomes (24), which define depletion condensate density of Bose ideal gas in infinite space.

Finite part of the second term of (31) defined by using a characteristic quantity of system $\alpha << 1$ as follows:

Power series at $\alpha = 0$ one has

$$\sum_{j=1}^\infty \frac{1}{j} = \sum_{j=1}^\infty e^{-j\alpha}\frac{e^{j\alpha}}{j} \approx \sum_{j=1}^\infty \frac{e^{-j\alpha}}{j}\left(1 + j\alpha + \frac{j^2\alpha^2}{2} + \frac{j^3\alpha^3}{6} + ...\right). \tag{32}$$

Perform summation and power series at $\alpha = 0$ once again one finds

$$\sum_{j=1}^{\infty}\frac{1}{j}\approx 2\pi-\ln[\alpha]. \tag{33}$$

Using (33), Eq. (31) can be read

$$n_d\left(T\right)=\frac{\left(mk_BT\right)^{3/2}}{\left(2\pi\right)^{3/2}\hbar^3}\zeta\left[3/2\right]+\frac{\left(mk_BT\right)^{3/2}\alpha}{4\sqrt{2}\pi^{5/2}\hbar^3}\left(2\pi-\ln[\alpha]\right). \tag{34}$$

The condensate density defined by $n_c(T)=n_0-n_d(T)$, together with (34) we have

$$n_c\left(T\right)=n_0-\frac{\left(mk_BT\right)^{3/2}}{\left(2\pi\right)^{3/2}\hbar^3}\zeta\left[3/2\right]-\frac{\left(mk_BT\right)^{3/2}\alpha}{4\sqrt{2}\pi^{5/2}\hbar^3}\left(2\pi-\ln[\alpha]\right). \tag{35}$$

From Eq. (35), we plot the condensate density as functions of the temperature in Figure 1.

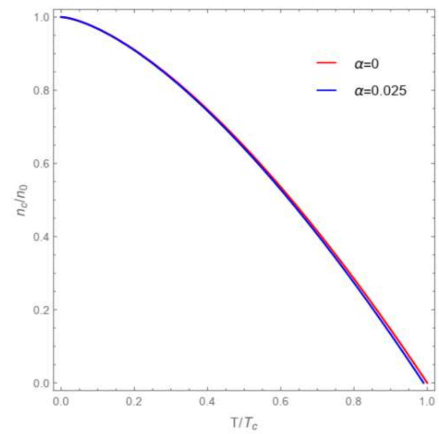

Figure 1. The evolution of condensate density versus temperature for α = 0 and α = 0.025

Figure 1 shows the temperature dependence of the condensate density at $\alpha=0$ and $\alpha=0.025$, which associate with the homogeneous and inhomogeneous systems, respectively. It is easy to see that at zero temperature all of the particles are condensed, whereas at the critical temperature the condensate density vanishes. Below the critical temperature, at a given value of the temperature, the finite size effect makes the condensate density increases.

3. Conclusions

The depletion of the weakly interacting Bose gas has been investigated within the framework of the second quantization formalism. Our main results are the following:

- In the homogeneous Bose gas, the depletion density depends on both the coupling constant and the temperature in the form of a polylogarithm function. Based on this result, the critical temperature for the ideal gas is reproduced in Eq. (25).

- The influence of the compactification of the Oz-direction on the depletion density is investigated. In this case, the depletion density depends on the distance between two parallel plates and temperature, which is included in the parameter α.

These calculations can be extended to consider the temperature dependence of several thermodynamic potentials, in particular, pressure, Helmholtz free energy density, Casimir force in the Bose gas at finite temperature.

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