Original Article

Condensate Density of a Bose Gas Confined between Two Parallel Plates in Canonical Ensemble within Improved Hartree-Fock Approximation

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Abstract: By means of Cornwall-Jackiw-Tomboulis (CJT) effective action approach, the condensate density of a dilute Bose gas is investigated in the canonical ensemble. Our results show that the condensate density is proportional to a *half-integer* power law of the *s*-wave scattering length and distance between two plates. Apart from that, these quantities also depend on the particle number and area of each plate.

Keywords: Condensate density, dilute Bose gas, improved Hatree-Fock approximation, canonical ensemble.

1. Introduction

It is well-known that a number of atoms of a Bose gas will be condensed when the system is cooled to the critical temperature [1] and the Bose-Einstein condensate is formed. The more an atomic number is condensed, the lower the temperature is, therefore all of the atoms are in the same quantum state at the absolute zero temperature. At zero temperature, the wave function of the ground sate of the condensate is the solution of Gross-Pitaevskii (GP) equation [2, 3] and condensate density is defined as the square of the wave function. Within the framework of the GP theory, the condensate density has been studied in many different approximations, such as, linearized order parameter [4], parameterized for the weak and strong separations [5], parameterized order parameter [6], the double parabola approximation [7] and so on.

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In the GP theory, also called mean field theory, the quantum fluctuations are neglected. However, the fluctuations always exist even at absolute zero temperature and are called quantum fluctuations [8, 9]. At zero temperature, they rise from the Heisenberg uncertain principal. To calculate these quantum fluctuations, Bogoliubov transformation was proposed [10], in which the dispersion relation and density of quantum fluctuations were found. Nevertheless, these calculations are very complicate.

Another method to investigate the Bose gas, including the quantum fluctuations is the Cornwall-Jackiw-Tomboulis (CJT) effective action approach [11]. Recently, this method has been widely employed to study the Casimir effect in Bose gas(es) [12, 13] and condensate density [14] in improved Hartree-Fock (IHF) approximation. Furthermore, these works were done in the grand canonical ensemble [15]. In this paper, the CJT effective action approach is invoked in studying of the condensate density in the canonical ensemble.

2. Condensate Density in the Improved Hartree-Fock Approximation

Let us start by considering a Bose gas described by the Lagrangian [9],

$$L = \psi^*(\vec{r},t)\left(i\hbar\frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\nabla^2\right)\psi(\vec{r},t) - \mu|\psi(\vec{r},t)|^2 + \frac{g}{2}|\psi(\vec{r},t)|^4, \tag{1}$$

in which $\hbar$ is the reduced Planck constant, the atomic mass and chemical potential are denoted by m and μ, respectively. In general case, the field operator $\psi(\vec{r},t)$ depends on both the coordinate and time. The strength of interaction between the atoms is featured by the coupling constant g, which relates to the *s*-wave scattering length a_s in form

$$g = \frac{4\pi\hbar^2 a_s}{m}, \tag{2}$$

and $g > 0$ for repulsive interaction.

Let ψ_0 be the expectation value of the field operator, in the tree-approximation the GP potential is read off from Eq. (1)

$$V_{GP} = -\mu\psi_0^2 + \frac{g}{2}\psi_0^4. \tag{3}$$

Without loss of generality, here and hereafter we consider the system without the external field so that ψ_0 is real and it plays the role of the order parameter. Minimizing this potential with respect to the order parameter one arrives at the gap equation

$$\psi_0(-\mu + g\psi_0^2) = 0,$$

and in the broken phase the order parameter has the form

$$\psi_0^2 = \frac{\mu}{g}. \tag{4}$$

In momentum space, the inversion propagator in the tree-approximation has the form

$$D_0^{-1}(k) = \begin{pmatrix} \dfrac{\hbar^2 k^2}{2m} + 2g\psi_0^2 & -\omega_n \\[2mm] \omega_n & \dfrac{\hbar^2 k^2}{2m} \end{pmatrix}, \tag{5}$$

where $\vec{k}$ is the wave vector and ω_n is the Matsubara frequency, for boson, which is defined as $\omega_n = 2\pi n / \beta, \beta = k_B T$ with k_B being Boltzmann constant and T absolute temperature. The Bogoliubov dispersion relation can be attained by requiring the determinant of (5) vanishes [16],

$$\det D_0^{-1}(k) = 0. \tag{6}$$

From Eqs. (5) and (6) we have

$$E_0(k) = \sqrt{\frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + 2g\psi_0^2\right)}. \tag{7}$$

It is obvious that there is the Goldstone boson.

In order to investigate in Hartree-Fock (HF) approximation, i.e. take into account these fluctuations, the field operator need to expand in terms of two real fields ψ_1, ψ_2 associated with the fluctuations [17],

$$\psi \to \psi_0 + \frac{1}{\sqrt{2}}(\psi_1 + i\psi_2). \tag{8}$$

Plugging (8) into (1) one gets the interaction Lagrangian in HF approximation

$$L_{int} = \frac{g}{2}\psi_0\psi_1(\psi_1^2 + \psi_2^2) + \frac{g}{8}(\psi_1^2 + \psi_2^2)^2. \tag{9}$$

The effective potential can be read-off from (9)

$$V_\beta^{CJT} = -\mu\psi_0^2 + \frac{g}{2}\psi_0^4 + \frac{1}{2}\int_\beta \mathrm{tr}\left[\ln D^{-1}(k) + D_0^{-1}(k)D(k) - \mathbb{1}\right] + \frac{g}{8}(P_{11}^2 + P_{22}^2) + \frac{3g}{8}P_{11}P_{22}, \tag{10}$$

where the notation

$$\int_\beta f(\vec{k}) = \frac{1}{\beta}\sum_{n=-\infty}^{+\infty}\int \frac{d^3\vec{k}}{(2\pi)^3} f(\omega_n, \vec{k}),$$

is used and $D(k)$ is the propagator in this approximation. The momentum integrals P_{aa} will be explained later. In our previous work [12, 14], the CJT effective potential was proved that it violates the Goldstone theorem, i.e. it does not lead to the Goldstone boson. This fact is avoidable if the method proposed by Ivanov *et. al.* [18] is invoked. To do so, an extra term

$$\Delta V = -\frac{g}{4}(P_{11}^2 + P_{22}^2) + \frac{g}{8}P_{11}P_{22}, \tag{11}$$

need be added into the CJT effective (10) and therefore a new CJT effective potential is obtained

$$\tilde{V}_\beta^{CJT} = -\mu\psi_0^2 + \frac{g}{2}\psi_0^4 + \frac{1}{2}\int_\beta \mathrm{tr}\left[\ln D^{-1}(k) + D_0^{-1}(k)D(k) - \mathbb{1}\right] + \frac{g}{8}(P_{11}^2 + P_{22}^2) + \frac{3g}{8}P_{11}P_{22}. \tag{12}$$

Minimizing the CJT effective potential (12) with respect to the order parameter one has the gap equation

$$-\mu + g\psi_0^2 + \Sigma_1 = 0, \tag{13}$$

and, in the same manner, minimizing the CJT effective potential (12) with respect to the elements of the propagator leads to the Schwinger–Dyson (SD) equation

$$M^2 = -\mu + 3g\psi_0^2 + \Sigma_2, \tag{14}$$

In which the self-energies are expressed in terms of the momentum integrals

$$\Sigma_1 = \frac{3g}{2} P_{11} + \frac{g}{2} P_{22},$$
$$\Sigma_2 = \frac{g}{2} P_{11} + \frac{3g}{2} P_{22}, \tag{15}$$

and M is the effective mass. Combining Eqs. (12), (13) and (14), the inversion propagator in this approximation can be derived

$$D^{-1}(k) = \begin{pmatrix} \dfrac{\hbar^2 k^2}{2m} + M^2 & -\omega_n \\[2mm] \omega_n & \dfrac{\hbar^2 k^2}{2m} \end{pmatrix}. \tag{16}$$

Similar to (6), the Bogoluibov dispersion relation associated with (16) is

$$E(k) = \sqrt{\frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + M^2\right)}, \tag{17}$$

It is clear that the Goldstone theorem is valid by appearing the Goldstone boson corresponding to the dispersion relation (17). This is the reason why it is called the improved Hartree-Fock approximation. For all above calculations, note that, for the notational simplicity, the same symbols will be used again from (12) to (16) to denote the corresponding quantities, although their expressions are different from those given in Eqs. (10) and (11). The momentum integrals in the IHF approximation are defined as

$$\tag{18}$$
$$P_{11} = \int_\beta D_{11}(k), P_{22} = \int_\beta D_2(k).$$

Based on Eqs. (16) and (18) one has relations

$$P_{11} = \frac{1}{2}\int \frac{d^3\vec{k}}{(2\pi)^3}\sqrt{\frac{\hbar^2 k^2/2m}{\hbar^2 k^2/2m + M^2}},$$
$$P_{22} = \frac{1}{2}\int \frac{d^3\vec{k}}{(2\pi)^3}\sqrt{\frac{\hbar^2 k^2/2m + M^2}{\hbar^2 k^2/2m}}, \tag{19}$$

for the momentum integrals at zero temperature.

We next investigate the condensate density in the IHF approximation. At first, we note that the pressure is defined as the negative of the CJT effective potential at the minimum, i.e. satisfying the gap and SD equations

$$P = -\tilde{V}_\beta \big|_{\text{at minimum}}. \tag{20}$$

The condensate density can be derived from the pressure

$$n_c = -\frac{\partial P}{\partial \mu}. \tag{21}$$

Combining Eqs. (12), (16), (20) and (21), the condensate density is expressed in terms of the order parameter and the momentum integrals [14],

$$n_c = \psi_0^2 + \frac{1}{2}(P_{11} + P_{22}). \tag{22}$$

In order to simplify notations, we use the coherent healing length $\xi = \hbar / \sqrt{2mgn_0}$ with n_0 being density in bulk and henceforth several dimensionless quantities are introduced: the reduced order parameter $\phi_0 = \psi_0 / \sqrt{n_0}$, wave vector $\kappa = k\xi$ and mass effective $\tilde{M} = M / \sqrt{gn_0}$. The momentum integrals (19) reduce

$$P_{11} = \frac{1}{2\xi^3} \int \frac{d^3\vec{\kappa}}{(2\pi)^3} \frac{\kappa}{\sqrt{\kappa^2 + \tilde{M}^2}},$$

$$P_{22} = \frac{1}{2\xi^3} \int \frac{d^3\vec{\kappa}}{(2\pi)^3} \frac{\sqrt{\kappa^2 + \tilde{M}^2}}{\kappa}. \tag{23}$$

3. Density condensate of a dilute Bose gas confined between two parallel plates

In this Section, the effect from the compaction in one-direction, say $0z$, on the density condensate of a dilute Bose gas is studied. The Bose gas is confined between two parallel plates at distance ℓ and perpendicular to $0z$. Owing to this compaction of space, the wave vector can be decomposed

$$k^2 \to k_\perp^2 + k_j^2, \tag{24}$$

in which $\vec{k}_\perp, \vec{k}_j$ are perpendicular and parallel to $0z$, respectively. In dimensionless form, Eq. (24) becomes

$$\kappa^2 \to \kappa_\perp^2 + \kappa_j^2. \tag{25}$$

To proceed further, the periodic boundary condition is applied at the plates, the parallel component of the dimensionless wave vector is quantized as

$$\kappa_j = \frac{2\pi n}{L}, \tag{26}$$

where the dimensionless distance $L = \ell / \xi$. Due to (25) and (26), the momentum integrals in Eq. (23) become

$$P_{11} = \frac{1}{4\pi\xi^3} \int_0^\infty \kappa_\perp d\kappa_\perp \sum_{j=-\infty}^\infty \left(\frac{\kappa_\perp^2 + \kappa_j^2}{\kappa_\perp^2 + \kappa_j^2 + \tilde{M}^2} \right), P_{22} = \frac{1}{4\pi\xi^3} \int_0^\infty \kappa_\perp d\kappa_\perp \sum_{j=-\infty}^\infty \left(\frac{\kappa_\perp^2 + \kappa_j^2 + \tilde{M}^2}{\kappa_\perp^2 + \kappa_j^2} \right). \tag{27}$$

It is worth noting that we are considering in the canonical ensemble, in which our system is not connected to any particle reservoir. As a consequence, particle number is fixed and roughly speaking

$$N = n_0 A\ell, \tag{28}$$

with A being the area of the plate. The integration over the wave vector in (27) is ultraviolet divergence and, at the same time, the sum does not converge. This difference can be removed by using a momentum cut-off [12] and Euler-Maclaurin formula [19]. Keeping in mind Eq. (28) one arrives at

$$P_{11} = 0, P_{22} = \frac{mM}{12\hbar^2 \ell}. \tag{29}$$

For a boson system, the chemical potential at zero temperature [17],

$$\mu = gn_0 \left(1 + \frac{32}{3\pi^{1/2}} \sqrt{n_0 a_s^3} \right). \tag{30}$$

In case of a dilute Bose gas, the second term in right hand side of Eq. (30) can be ignored [14]. Combining Eqs. (13)-(30), the gap and SD equations can be rewritten as

$$-1 + \phi_0^2 + \frac{mMA}{24\hbar^2 \ell} = 0,$$

$$-1 + 3\phi_0^2 + \frac{mMA}{8\pi\hbar^2 N} M\ell - \frac{mM^2 A\ell}{4\pi\hbar^2 Na_s} = 0. \tag{31}$$

The solution for Eqs. (31) has the form

$$\phi_0^2 = 1 + \frac{1}{6\hbar} \sqrt{\frac{\pi mA a_s}{N\ell}}, \tag{32}$$

and

$$M = 2\sqrt{2\pi}\hbar \sqrt{\frac{Na_s}{mA\ell}}. \tag{33}$$

Plugging (32) and (33) into (29) and then (22), the condensate density is read

$$n_c = \frac{N}{A\ell} + \frac{1}{3\hbar} \sqrt{\frac{\pi mN}{2A}} \frac{a_s^{1/2}}{\ell^{3/2}}. \tag{34}$$

Let (32) back to the dimensional form one has the condensate density without the quantum fluctuations

$$n_0 = \psi_0^2 = \frac{N}{A\ell} + \frac{1}{6\hbar} \sqrt{\frac{\pi mN}{2A}} \frac{a_s^{1/2}}{\ell^{3/2}}. \tag{35}$$

Eqs. (34) and (35) show many significant differences compared with those in the grand canonical [14]. In grand canonical, the condensate density only depends on gas parameter and the distance between two plates, whereas in canonical ensemble, apart from the gas parameter and the distance, the condensate density is also dependent of the plate geometry, namely, the number of particles N and area A of the each plate.

To illustrate for the above analytical calculations, we do numerical computations for a dilute Bose gas formed by sodium 23 (Na 23) [20] with $m = 22,9897u$ (where $u = 1.66053873 \times 10^{-27}$ kg is atomic mass unit). The total particle number $N = 5 \times 10^5$, plate area $A = 10^{-6}$ m^2 [21]. Figure 1 shows

the evolution of density condensate as a function of the distance between two plates at $a_s = 19.1a_0$ ($a_0 = 0.529 \times 10^{-10} m$ is Borh radius). The blue and red lines correspond to n_c and n_0. It is clear that the condensate density decays fast as the distance between two plates increases and it approaches to zero at large distance. The condensate density is also divergent when the distance tends to zero. This fact is the same in comparison with the one in the grand canonical ensemble.
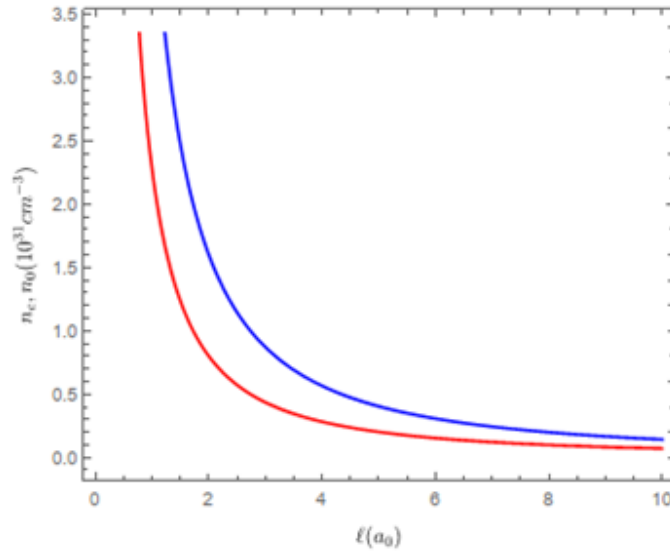

Figure 1. The evolution of the density condensate versus distance between two plates for Na 23 at $a_s = 19.1a_0$.
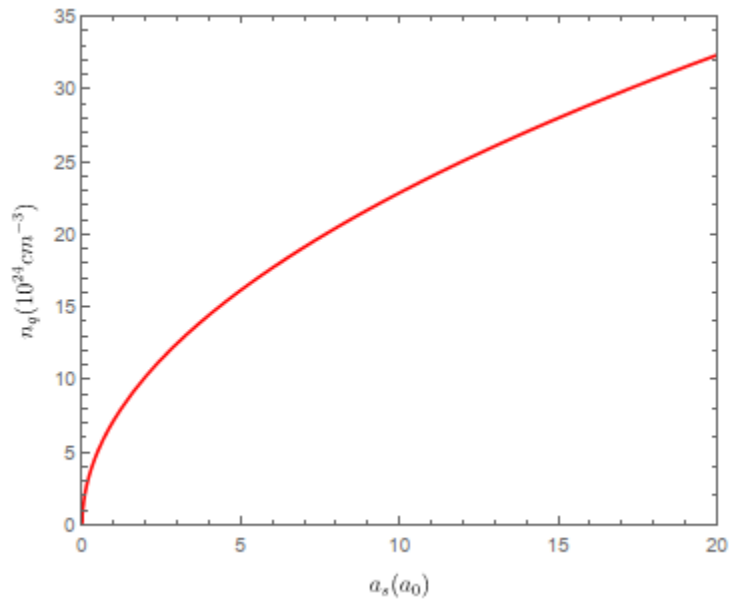

Figure 2. The density of quantum fluctuations as a function of the scattering length a_s at the distance $\ell = 8000a_0$.

Moreover, one important thing is easily seen in Figure 1 is the difference between n_c and n_0. This difference is caused by the quantum fluctuations, which can be read of from Eq. (22),

$$n_q = \frac{1}{2}(P_{11} + P_{22}).$$ (36)

Substituting (33) into (29) and then (36) one has

$$n_q = \frac{1}{6\hbar} \sqrt{\frac{\pi m N}{2A}} \frac{a_s^{1/2}}{\ell^{3/2}}.$$ (37)

Eq. (37) points out that the density of quantum fluctuations is proportional to square root of the scattering length and it decays as a minus half-integer power law of the distance between two plates. This is a very interesting property in compared with the one in the grand canonical ensemble. Figure 2 depicts the quantum fluctuations as a function of the scattering length, which is controlled by the Feshbach resonance [22]. It is shown that the density of quantum fluctuations vanishes as the scattering length tends to zero. It confirms again that the quantum fluctuations in Bose gas are caused by the interaction between atoms.

4. Conclusion

In foregoing sections the condensate density has been investigated by using CJT effective action approach in canonical ensemble. Our main results are in order

- The distance dependence: both condensate density and density of the quantum fluctuations strongly depend on the distance between two plates. However, there are several remarkable differences in compared with those in the grand canonical ensemble. These quantities proportional to the negative half-integer power law of the distance instead of the integer one in the grand canonical ensemble. As the distance is large enough, the condensate density and density of the quantum fluctuations tend to zero whereas they accost the nonzero in the grand canonical ensemble. This fact is understandable by noting that the particle number is kept constant in the canonical ensemble.

- The scattering length dependence: this property is the same for both grand canonical ensemble and the canonical ensemble. In both ensembles, these quantities are proportional to square root of the scattering length. This fact leads to the vanishing of these quantities in an ideal Bose gas.

Besides, a common feature is shown is that the condensate density and density of quantum fluctuations in the canonical ensemble depend on the particle number and area of the plate. It is interesting to extend these results to consider static properties of the Bose gas, such as, the pressure.

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