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Original Article

The Cloud of Bose-Einstein Condensate in a Harmonic Trap

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Abstract: In this work, we calculate the volume of a Bose-Einstein condensate (BEC) cloud confined within a harmonic trap induced by a magneto-optical trap. Three main factors influencing the volume of the BEC cloud are examined: thermal motion, interatomic interactions, and the uncertainty in momentum and position. These considerations enable the definition of certain thermodynamic variables, leading to the establishment of the thermodynamic equations of state.

Keywords: Bose-Einstein condensate, harmonic trap, thermodynamic volume, thermodynamic pressure, equations of state.

1. Introduction

Nearly 70 years after Einstein's prediction about condensation [1], the first Bose-Einstein condensate was created in an experiment [2]. In this experiment, a Bose-Einstein condensate (BEC) cloud was observed within an apparatus consisting of six laser beams intersecting in a glass cell, forming a magneto-optical trap. The cell measured 2.5 cm in width and 12 cm in length, with the laser beams having a diameter of 1.5 cm. Several technologies now exist to cold the system of Bose gas, such as the low-dimensional traps [3], double wells [4] and optical latices [5].

It is well-known that in the condensed phase, the state of a BEC is governed by the equation of state in the thermodynamic limit [6].

$$p=\frac{\mathrm{Li}_{5/2}(z)}{\lambda_B^3}k_BT, \tag{1}$$

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in which p denotes the pressure of the gas at temperature T, $\lambda_B = \sqrt{2\pi\hbar^2 / mk_B T}$ is the de Broglie wavelength; $\hbar$ and k_B are the reduced Planck constant and Boltzmann constant, respectively. The polylogarithm function is defined as

$$\mathrm{Li}_k(z) = \sum_{l=x,y,z} \frac{z^l}{l^k}. \tag{2}$$

However, this equation is valid only in the thermodynamic limit, meaning it applies exclusively to homogeneous BEC, whereas the BEC in experimental settings have finite sizes. In this paper, based on the phenomenological analogy between theory for BEC and the classical mechanics [7] we propose an alternative equation of state that is applicable to the finite-sized BEC clouds observed in experiments.

2. Volume and Equation of State of the BEC in a Trap

In this Section we establish the equation of state of a BEC confined in a trap with finite size. Analogous to a classical gas, in a uniform or in other words, homogeneous BEC, the volume V, alongside temperature T and particle number N, serves as a mechanical variable that defines the thermodynamic state of the gas. To prevent any potential misunderstandings, we clarify that Eq. (1) pertains to the ideal Bose gas in the thermodynamic limit. This implies that the ratio remains finite as both N and V tend toward infinity.

In experiment, the BEC cloud is usually created in an experimental setup composed of a double magneto-optical trap and a quadrupole– Ioffe-configuration type of trap. A magnetic field caused in the trap by a number of magnetic coils rotating with frequency $\vec{\omega} = (\omega_x, \omega_y, \omega_z)$. In that case, a particle of the system confined in an anisotropic harmonic-oscillator potential [8],

$$U_{\text{ext}}(\vec{r}) = \frac{1}{2} \sum_{i=x,y,x} F_i i^2, \tag{3}$$

in which F_i represents the force acting on the particle in the i-direction, which is assumed to remain constant. In general case, this force is not equal in different directions. Eq. (3) expresses the elastic potential in the classical mechanics. Using the angular frequency of a harmonic oscillator, Eq. (3) can be rewritten in form of the rotating frequency of the magnetic coils

$$U_{\text{ext}}(\vec{r}) = \frac{1}{2}(\vec{\omega}.\vec{r})^2 = \frac{1}{2} m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \tag{4}$$

with m being the mass of the particle. Neglecting the interatomic interaction one can see that each bosonic atom is confined by the harmonic potential (4) thus the average value of its energy

$$\langle E \rangle = 2\langle U_{\text{ext}} \rangle = m\omega^2 r^2. \tag{5}$$

As we know, at ultracold temperature, the kinetic energy is so small that most atoms will be in the ground state. Assuming that in the ground state, our system is in the thermodynamic equilibrium. As yet, BEC is experimentally formed from the condensation of atoms of elements belonging to the alkali metal group. These elements always exist in a monatomic state, so each atom has three degrees of translational freedom corresponding to the three coordinate axes. It is also important to note that the average thermal energy carried by each microscopic degree of freedom is $k_B T / 2$. It turns out that, in the first approximation, the atoms locate in a box with the sizes

$$L_y = \left(\frac{k_B T}{m\omega_y^2}\right)^{1/2}, L_y = \left(\frac{k_B T}{m\omega_y^2}\right)^{1/2}, L_z = \left(\frac{k_B T}{m\omega_z^2}\right)^{1/2}. \tag{6}$$

Eq. (6) is very important to evaluate the effect of finite-size to quantities in experiments [9] by comparing these sizes with the healing length. The volume of the Bose gas cloud caused by thermal motion can be easily computed from (6)

$$V_{\text{ther}} = \left(\frac{k_B T}{m\omega^2}\right)^{3/2}. \tag{7}$$

This result is in excellent agreement with the one in Refs. [9]. According to Equation (6), as the temperature decreases, the thermal volume progressively diminishes. Theoretically, the thermal volume becomes zero at absolute zero temperature. Nevertheless, absolute zero has never been achieved experimentally.

Another factor influencing the volume of the BEC cloud in the trap is the interatomic interaction. Various models describe the interatomic interaction potential, including those where two or three particles interact pairwise through a hard-sphere potential, as well as models involving hard-sphere, soft-sphere, hard-core square-well, or exponential potentials. These models have demonstrated that the contact potential [8]

$$U_{\text{int}}(\vec{r} - \vec{r}\,') = \frac{4\pi\hbar^2 a_s}{m}\delta(\vec{r} - \vec{r}\,'), \tag{8}$$

is sufficiently accurate for characterizing weakly interacting Bose gases. In Eq. (8) a_s represents the *s*-wave scattering length, which is the minimum distance two atoms can approach each other. This allows for the estimation of the volume of a system containing *N* bosonic atoms

$$V_{\text{int}} = \frac{4}{3}\pi a_s^3 N. \tag{9}$$

We now consider the volume of the BEC cloud in a trap due to the Heisenberg uncertain principle. The couple quantities, namely, momentum and coordinate of an atom satisfy an inequality

$$\Delta p.\Delta r \geq \hbar, \tag{10}$$

where Δp and Δr are the uncertainness of the momentum and coordinate, respectively. As already mentioned above, the bosonic atoms of the BEC cloud are confined by the harmonic potential (4). It is well-known that the energy can be written as

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, n = 0,1,2,... \tag{11}$$

Combining Eqs. (10) and (11) yields the uncertainness of the coordinate

$$\Delta r = \sqrt{\frac{2\hbar}{m\omega}}. \tag{12}$$

It is easy to calculate the volume of the BEC owing to the Heisenberg uncertain principle

$$V_{\text{unc}} = \frac{8\sqrt{2}\pi N}{3}\left(\frac{\hbar}{m\omega}\right)^{3/2}. \tag{13}$$

In sum, the total volume of the BEC cloud in the harmonic trap is

$$V = V_{\text{ther}} + V_{\text{int}} + V_{\text{unc}}. \tag{14}$$

We now proceed to examine the equation of state of the BEC cloud within the trap. Most research indicates that thermal motion is the predominant factor contributing to the volume of the BEC cloud in the trap [10]. Equation (7) demonstrates that the volume is inversely proportional to the cubic harmonic frequency. As we know, thermodynamics is a theoretical that addresses a set of global variables so-called the thermodynamic variables. For the BEC cloud one can deduce the role of the inverse of the cube of the geometric average of the frequencies of the harmonic trap as the extensive thermodynamic variable analogous to the volume and called "harmonic volume"

$$\tilde{V} = \frac{1}{\omega^3}. \tag{15}$$

It is important to note that the "thermodynamic volume" should not be identified with the real volume of the system. In fact, it does not even have units of volume. The conjugate quantity of the "harmonic volume" is the "harmonic pressure" and therefore the equation of state has a general form

$$\tilde{P} = \tilde{P}(N / \tilde{V}, T), \tag{16}$$

with $\tilde{P}$ denoting the "harmonic pressure". Within defining of the "harmonic volume" (15) one can define the "harmonic density" as

$$\tilde{\rho} = N\omega^3. \tag{17}$$

We emphasize once again that the definitions of "harmonic volume," "harmonic pressure," and "harmonic density" are not identical to their commonly used counterparts. These quantities represent the appropriate thermodynamic parameters for determining the thermodynamic limit, in which both the particle number and the "harmonic volume" tend to infinity, while the "harmonic density" remains finite. To proceed further, we write down the Hamiltonian of the system

$$H = -\frac{\hbar^2}{2m}\nabla^2 + U_{\text{int}} + U_{\text{ext}}. \tag{18}$$

The Helmholtz free energy is read

$$F = k_B T \ln Z, \tag{19}$$

in which the canonical partition function for the ideal Bose gas can be evaluated from the Hamiltonian (18)

$$Z = \frac{1}{N!\lambda_B^{3N}}\left[\int \exp\left(-\beta(U_{\text{int}} + U_{\text{ext}}\right)d^3\vec{r}\right], \tag{20}$$

in which $\beta = 1/k_B T$ and the de Broglie wavelength $\lambda_B = \sqrt{2\pi\hbar^2 / mk_B T}$. Employing Sterling formula to evaluate (20) then plugging into (19) one arrives at the Helmholtz free energy per particle

$$\frac{F}{N} = -k_B T\left\{\ln\left[\frac{1}{N\lambda_B^3}\int \exp\left(-\beta(U_{\text{int}} + U_{\text{ext}}\right)d^3\vec{r}\right] + 1\right\}. \tag{21}$$

By applying the Poisson integral and considering definition (15), Equation (21) is evaluated

$$\frac{F}{N} = -k_B T\left\{\ln\left[\frac{\sqrt{2}\Gamma(3/2)}{\lambda_B^6}\left(\frac{2\pi\hbar^2}{m^2}\right)^{3/2}\frac{\tilde{V}}{N}\right] + 1\right\}, \tag{22}$$

in which $\Gamma(x)$ is the Gamma function. In thermodynamics, the "harmonic pressure" is defined as

$$\tilde{p} = -\left(\frac{\partial F}{\partial \tilde{V}}\right)_{N,T}. \tag{23}$$

Inserting Eq. (22) into (23) yields

$$\tilde{p} = \frac{Nk_BT}{\tilde{V}}. \tag{24}$$

In term of the "harmonic density" (17), this equation becomes

$$\tilde{p} = \tilde{\rho}k_BT. \tag{25}$$

It is evident that Eqs. (24) and (25) share the same form as the equation of state for an ideal gas. It is important to note that these equations represent the "thermodynamic equation of state", which illustrates the relationship among the thermodynamic variables, particularly, "harmonic pressure", "harmonic volume", "harmonic density" and temperature.

3. Conclusion

In the preceding section, we have investigated the thermodynamics of a Bose-Einstein Condensate (BEC) cloud confined within a harmonic trap, typically created using a magneto-optical trap. Our key findings are summarized as follows:

- We estimated the volume of the BEC cloud within the harmonic trap, which is comprised of three components: contributions from thermal motion, interatomic interactions, and the uncertainty principle governing momentum and position. The thermal volume is proportional to the so-called "thermodynamic volume" and $T^{3/2}$. This result enables the evaluation of the homogeneity of a Bose gas in experimental settings, providing a means to verify the validity of homogeneous BEC theory.
- The "thermodynamic equations of state" have been derived. These equations take the same form as those for an ideal gas, known as the Clapeyron-Mendeleev equation.

In conjunction with [7], these results further reinforce the phenomenological analogy between BEC theory and classical physics.

Thirty years have passed since the first experimental realization of BEC [2]. Nevertheless, accurately measuring the size of the BEC cloud in experiments continues to pose significant challenges. We hope that our calculations will offer a reliable method for extracting experimental data on the size of the BEC cloud.

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