

Bose-Einstein Condensation of Confined Atomic Gases at Ultra Low Temperatures

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Abstract

In this work I solve the Gross-Pitaevskii equation describing an atomic gas confined in an isotropic harmonic trap by introducing a variational wavefunction of Gaussian type. The chemical potential of the system is calculated and the solutions are discussed in the weakly and strongly interacting regimes. For the attractive system with negative scattering length the maximum number of atoms that can be put in the condensate without collapse begins is calculated

1. Introduction

Bose-Einstein condensation (Pethick & Smith, 2008) is the macroscopic occupation of the lowest momentum state with a finite fraction of particles. This phenomenon had interested both experimental and theoretical physicists from the beginning of the last century since Bose and Einstein conjectured the existing of this phenomenon in the free Bose gas. The first experimental achievement of it came before twenty two years by different experimental groups (Anderson et al., 1995; Davis et al., 1995; Bradley et al., 1995). This achievement had increased the interest in analyzing different aspects related to this phenomenon (Baym & Pethick, 1996; Fetter, 2009; Mateo & Delgado, 2007).

Different theoretical approaches have been used to study these systems that undergoes Bose-Einstein condensation. These methods include mean-field theories (Margetis, 2015), canonical and microcanonical ensemble approaches (Chase, Mekjian, & Zamick, 1999), and numerical calculations including quantum Monte-Carlo techniques (DuBois & Glyde, 2001).

These systems are weakly-interacting ultracold atomic gases confined in an external trap. A good description of these systems is accomplished by the Gross-Pitaevskii equation (Rogel-Salazar, 2013) which is effectively a nonlinear Schrodinger equation. In three dimensions this equation takes the form:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi + N_0g|\psi|^2\psi = \mu\psi \quad (1)$$

where the first term is the kinetic energy, U is the external trap potential and the third term is the nonlinear term arises from the interaction between atoms and μ is the chemical potential and $g = (4\pi\hbar^2a/m)$, a being the scattering length. We take the external trap potential to be isotropic and simple harmonic:

$$U(r) = (1/2)m\omega r^2 \quad (2)$$

where m is the mass of the atom and ω the angular frequency

The approach in this work will be variational. In the next section we make an appropriate ansatz of a trial variational wavefunction of Gaussian type which will be followed by the calculation of the ground state energy which consists of three parts.

2. Variational Wavefunction

In the absence of interactions between the atoms the ground state wave function is Gaussian. Interactions will certainly modify both the wave function and energy. As a trial wavefunction we use a Gaussian function of the form

$$\psi = Ae^{-br^2} \tag{3}$$

Where b is our variational parameter. Normalization of the wavefunction gives $A = (2b/\pi)^{3/4}$

Using the normalized form of the wavefunction to calculate the ground state energy we get first for the kinetic energy:

$$\langle T \rangle = -\frac{\hbar^2}{2m} \int \psi \nabla^2 \psi d^3r = \frac{3\hbar^2}{2m} \tag{4}$$

For the expectation value of the harmonic potential we get:

$$\langle U \rangle = (1/2)m\omega^2 \int r^2 \psi^2 d^3r = \frac{3m\omega^2}{8b}, \tag{5}$$

and finally for the expectation value of the interaction term we get

$$\langle V \rangle = g \int \psi^4 d^3r = g \left(\frac{b}{\pi}\right)^{3/2}. \tag{6}$$

Therefore we get for the chemical potential

$$\mu = \frac{3\hbar^2 b}{2m} + \frac{3m\omega^2}{8b} + N_0 g \left(\frac{b}{\pi}\right)^{3/2}. \tag{7}$$

Now if we define the dimensionless quantities $B = \frac{\hbar b}{m\omega}$ and $\mu^* = \frac{\mu}{\hbar\omega}$ eq.(7) is reduced to

$$\mu^* = \frac{3}{2}B + \frac{3}{8B} + \chi B^{3/2} \tag{8}$$

where $\chi = N_0 (m\omega / \pi\hbar)^{1/2} a$.

Minimization of μ^* gives:

$$\frac{d\mu^*}{dB} = 0 = \frac{3}{2} - \frac{3}{8B^2} + \frac{3}{2}\chi B^{1/2} \tag{9}$$

or equivalently

$$B^2 - 1/4 + \chi B^{5/2} = 0 \tag{10}$$

3. Results and Discussion

In eq.(10) if $\chi = 0$, we obtain $B = 1/2$ or $(b = m\omega/2\hbar)$ which is the ground state of the harmonic trap with chemical

potential $3/2 \hbar \omega$. For $\chi \ll 1$, we get $B = \frac{1}{2} \left(1 - \frac{\chi}{2\sqrt{2}}\right)$, in this case we obtain for the chemical potential

$$\mu = \hbar\omega \left(\frac{3}{2} + \frac{\chi}{2\sqrt{2}}\right)$$

Thus a small repulsive scattering length increases the energy, whereas a small attractive scattering length lowers the energy.

For $\chi \gg 1$, we get $B \approx (1/4\chi)^{2/5} \left(1 - \frac{8}{5} \left[\frac{1}{4\chi}\right]^{4/5}\right)$. Thus the chemical potential equals in this limit

$$\mu \approx \frac{5}{8} (4\chi)^{2/5} \hbar\omega \left(1 - \frac{96}{25} (4\chi)^{-8/5}\right) \tag{11}$$

In this case the kinetic energy is much smaller than the trapping potential energy.

$$\frac{\langle T \rangle}{\langle U \rangle} = 4B^2 = \left(\frac{\sqrt{2}}{\chi}\right)^{4/5} \tag{12}$$

For negative a (attractive interaction), a noncollapsing condensate can exist only for a maximum number of atoms. To find this critical number, we recall that there is no global minimum of the chemical potential at this critical value so the conditions are the vanishing of the first and second derivatives of the chemical potential

$$\mu' = \mu'' = 0 \tag{13}$$

This calculation gives $\chi_c = -0.76$. So we get for the critical number of atoms

$$N_0^c = \frac{\chi_c}{a} \sqrt{\pi \hbar / m \omega} \tag{14}$$

In terms of the oscillator length defined as $d = (\hbar / m \omega)^{1/2}$, $N_0^c = \sqrt{\pi} \chi_c \frac{d}{a}$

And if we substitute the values corresponding to lithium ${}^7\text{Li}$, namely, $a = -1.44 \text{ nm}$, $d = 3.13 \text{ }\mu\text{m}$, we get $N_0^c = 2928$

4. Thomas-Fermi limit

In the Thomas Fermi limit the kinetic energy is ignored for large systems.

In this limit the chemical potential becomes

$$\mu^* = \frac{3}{8B} + \chi B^{3/2} \tag{15}$$

Now we minimize μ^* ,

$$\frac{d\mu^*}{dB} = 0 = -\frac{3}{8B^2} + \frac{3}{2} \chi B^{1/2} \tag{16}$$

And hence $B = (1/4\chi)^{2/5}$.

In this case the chemical potential becomes

$$\mu = \frac{5}{8} (4\chi)^{2/5} \hbar \omega \tag{17}$$

which is the first term of eq. (11)

5. Conclusion

In this work I studied the problem of Bose –Einstein condensation in atomic gases at ultra low temperatures. The system is considered to be confined in an isotropic harmonic potential trap. A Gaussian wavefunction is used to solve the Gross-Pitaevskii equation to calculate the chemical potential of the gas. The solutions were discussed in the strongly as well as the weakly interacting limits.

Without an external trap the system of interacting Bose atoms has a soliton solution (Drake Perez et al., 2005).

In a future work I should take this into account in the variational wavefunction.

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