# Bose-Einstein condensation of atoms in a trap

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We point out that the local density approximation (LDA) of Oliva is an adaptation of the Thomas-Fermi method, and is a good approximation when $\epsilon = \hbar\omega/kT \ll 1$. For the case of scattering length $a > 0$, the LDA leads to a quantitative result, Eq. (14′), easily checked by experiments. Critical remarks are made about the physics of the many-body problem in terms of the scattering length $a$. [S1050-2947(96)10306-1]

Bose-Einstein condensation (BEC) of free particles was a great contribution to physics and provides one more example of the awesome and daring insight of Einstein. For some 60 years, experimental observation of BEC was considered hopeless. Now, through a series of ingenious developments, BEC has finally been observed [1–3] for trapped bosons. We would like to discuss here BEC of such trapped particles with and without mutual interactions [4]. First some preliminaries.

Four lengths are involved in harmonic traps. They are

$$L_1 = (2\pi m\omega^2\beta)^{-1/2}, \quad L_2 = (\hbar/m\omega)^{1/2},$$

$$\lambda = (2\pi\hbar^2\beta/m)^{1/2}, \quad a, \tag{1}$$

where $\beta = 1/kT$, $L_1$ gives the order of the classical oscillation amplitude of a particle in the oscillator with energy $kT$, $L_2$ is the size of the ground state in the oscillator, $\lambda$ the thermal wave length, and $a$ the $s$-wave scattering length. For recent experiments $\lambda \gg |a|$. We notice also that

$$L_1 : L_2 : \lambda = 1 : \sqrt{2\pi\epsilon} : 2\pi\epsilon, \quad \epsilon = \beta\hbar\omega. \tag{2}$$

## I. THOMAS-FERMI METHOD AND THE LOCAL DENSITY APPROXIMATION, GASEOUS PHASE

For small values of $\epsilon$ and large number of particles, the Thomas-Fermi method for atoms can be adapted to the present problem: We divide space up into cells of volume larger than $(L_2)^3$ but smaller than $(L_1)^3$, and consider the potential energy $V$ of the trap to be a constant in each cell. Each cell contains a collection of particles and mutual interaction described by a scattering length $a$. All particles in a cell have the same external potential $V(r)$ per particle. If $V=0$ this problem for a cell has been studied [5,6] in the 1950s. For the present problem, in each cell we need only replace the fugacity $z$ of the 1950 result by $z\exp(-\beta V)$.

This adaptation of the Thomas-Fermi method to the present problem has been used in a paper by Oliva (see Ref. [4]). We shall follow his terminology and call it the local density approximation (LDA). In this approximation, in the gaseous phase (i.e., without BEC) in each cell, $\rho(r)$ is given by Eq. (20) of [6],

$$\rho(r) = \lambda^{-3}g_{3/2}(\zeta)[1 - (4a/\lambda)g_{1/2}(\zeta)], \tag{3}$$

where

$$\zeta = z\exp(-\beta V), \quad g_\nu(x) = \sum_1^\infty l^{-\nu}x^l \tag{4}$$

and $z$ is the fugacity.

To order $a/\lambda$ we can also write (3) as

$$\rho(r) = \lambda^{-3}g_{3/2}(\xi), \tag{5}$$

$$\xi = z\exp[-\beta V(r) - 4a\lambda^2\rho(r)]. \tag{6}$$

## II. VALIDITY OF LDA FOR CASE $a = 0$

If $a=0$, LDA [i.e., (5) and (6)] gives immediately an explicit expression for $\rho(r)$ provided $z \lesssim 1$. If we pack in more particles, i.e., if we try to increase $z$ beyond 1, since $\xi$ cannot further increase at $r=0$, BEC sets in at $r=0$, in the same way as the original Einstein description of BEC in momentum space at $p=0$. But this case of $a=0$ and $V=\frac{1}{2}m\omega^2r^2$ can be rigorously solved, allowing for an understanding of how LDA approaches the rigorous result. This is what we shall do in the present section.

The density of atoms is $\rho(r) = \langle r|D|r \rangle$, where $D$ is the density matrix equal to $ze^{-\beta H}(1 - ze^{-\beta H})^{-1} = \sum_1^\infty z^l e^{-\beta Hl}$. The matrix elements of $e^{-\beta Hl}$ are known explicitly from [7]. (Using it we avoid the tedious process of summing over squares of Hermite polynomials.) We thus obtain

$$\rho(r) = \epsilon^{3/2}\lambda^{-3}\sum_1^\infty (\sinh l\epsilon)^{-3/2}z^l\exp[-\sigma^2\tanh(l\epsilon/2)], \tag{7}$$

where $\sigma = r/L_2$. The summand in (7) behaves at large $l$ like a geometrical series with the ratio of successive terms equal to

$$z_1 = ze^{-3\epsilon/2}. \tag{8}$$

Thus the summation converges at all $r$ for $z_1 < 1$ and becomes divergent at $z_1 = 1$ for all $r$. To study how it diverges we write the summation as $\sum_1^\infty a_l$ where

$$\ln a_l = l(\ln z) - \tfrac{3}{2}\ln(\sinh l\epsilon) - \sigma^2 \tanh(l\epsilon/2)$$

$$= l[\ln z - 3\epsilon/2] + (\tfrac{3}{2}\ln 2 - \sigma^2) + C_l,$$

where $C_l \to 0$ as $l \to \infty$.

Thus $a_l = 2^{3/2}e^{-\sigma^2}z_1^l + 2^{3/2}e^{-\sigma^2}z_1^l(e^{C_l}-1)$. Therefore the summation is equal to

$$\sum a_l = 2^{3/2}e^{-\sigma^2}\frac{z_1}{1-z_1} + 2^{3/2}e^{-\sigma^2}\sum z_1^l(e^{C_l}-1). \quad (9)$$

The first term on the right is the divergent part as $z_1 \to 1$. We notice happily that it is exactly proportional to $|\psi_0(r)|^2$, where $\psi_0$ is the normalized ground-state wave function of the harmonic oscillator. Thus (7) becomes

$$\rho(r) = \frac{z_1}{1-z_1}|\psi_0(r)|^2 + \rho_n(r), \quad (10)$$

showing that the BEC is in the ground state. $\rho_n$ is the normal fluid part of the density function $\rho(r)$. It is the last term of (9) multiplied by $\lambda^{-3}\epsilon^{3/2}$:

$$\rho_n(r) = \lambda^{-3}(2\epsilon)^{3/2}\sum_1^\infty z_1^l \left\{ \frac{1}{(1-e^{-2l\epsilon})^{3/2}} \right.$$

$$\left. \times \exp[-\sigma^2\tanh(\epsilon l/2)] - \exp[-\sigma^2] \right\}. \quad (11)$$

So far (10) and (11) are exact. Notice that for large $l$, the sum in (11) is convergent for $z_1 = 1$, unlike the first term of (10). Now we go to the case of $\epsilon \ll 1$. The contribution to the sum in (11) for $\epsilon l > 1$ is negligible. For $\epsilon l < 1$, we can drop the last term in the curly brackets and replace $1-e^{-2l\epsilon}$ by $2l\epsilon$ and $\tanh(\epsilon l/2)$ by $\epsilon l/2$, obtaining

$$\rho(r) \cong \frac{z_1}{1-z_1}|\psi_0(r)|^2 + \lambda^{-3}g_{3/2}(z_1 e^{-(1/2)\beta m\omega^2 r^2}). \quad (12)$$

The second term here is the result of LDA with the replacement of $z$ by $z_1$. See (8). For $\epsilon \ll 1$, this replacement creates negligible errors.

In the gaseous phase, i.e., $1-z_1 \approx O(1)$, the second term in (12) dominates and the LDA is good.

In the BEC phase, the first term is the condensate, with $1-z_1 \approx O(N^{-1})$. Thus we can put $z_1 = 1$ in the second term, obtaining exactly the result of LDA, except for the fact that in the rigorous result the condensate has the spatial dependence of $|\psi_0(r)|^2 = \text{const} \times \exp[-\sigma^2]$ while in the LDA the condensate has a $\delta$-function dependence on $\mathbf{r}$. But this is hardly surprising since in LDA each cell has a linear dimension large compared with $L_2$, so that any structure of the order of $L_2$ is shrunk to a point. This fact also means that in LDA the cells should not be chosen to be $\leq O(L_2)$.

To further check the error in (12) we evaluated numerically its error divided by the second term on the right for certain cases and found that the ratio is generally of the order of $\sqrt{\epsilon}$. For example, if $\epsilon = 0.05$, the ratio is $<0.28$, and for $\epsilon = 0.01$, the ratio is $<0.12$.

In summary, as $\epsilon \to 0$, the LDA expression for $\rho(r)$ approaches the rigorous result at every fixed $\sigma_1 = r/L_1$.
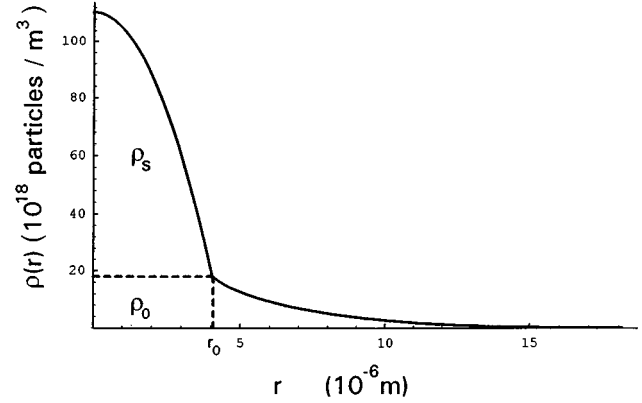


FIG. 1. Example of $\rho(r)$ as a function of $r$ for $a>0$ according to Eq. (14′). The curve is for a harmonic trap. Notice that the first and second derivatives are both finite but discontinuous at $r_0$. $\rho_0 = \lambda^{-3}g_{3/2}(1)$ is the normal part of $\rho$, and $\rho_s$ the condensate part. For smaller total number of particles ($=N$), $r_0$ becomes smaller. It eventually shrinks to zero and the condensate disappears.

We mention here that with $a=0$, there is the well-known basic symmetry in the Hamiltonian between the coordinate and the momentum. To be precise, if we keep $\hbar$, $\omega$, and $\beta$ unchanged, but replace $m$ with $(m\omega^2)^{-1}$ and switch $x$ and $p$, the problem is unchanged (for $a=0$). Thus we easily obtain the exact momentum space density distribution $n(p)$. The condensate is of course in the state $|\psi_0(p)|^2$.

## III. CONDENSATE FOR THE CASE $a>0$ IN LDA

For $a>0$, the thermal equilibrium in each cell can be studied as in [6]. For large enough density, condensation takes place in the cell. The cell then consists of a saturated gaseous part with density $\rho_0 = \lambda^{-3}g_{3/2}(1)$ plus a super part with density $\rho-\rho_0 = \rho_s$. The free-energy density then becomes, according to Eq. (33) of Ref. [6],

$$f(r) = -kT\lambda^{-3}g_{3/2}(1) + 2a\lambda^2 kT\rho^2 - a\lambda^2 kT\rho_s^2. \quad (13)$$

From this free energy we obtain the chemical potential, which should be equated with $kT\ln[z\exp(-\beta V)]$ giving

$$kT\ln z - V = 4\pi a[\rho+\rho_0]\hbar^2/m \quad (r<r_0). \quad (14)$$

At $r=r_0-$, $\rho_s = 0$ and $\rho = \rho_0$. Thus

$$V(r) + 4\pi a\rho(r)\hbar^2/m = V(r_0) + 4\pi a\rho_0\hbar^2/m. \quad (14')$$

This simple equation is valid in the LDA for any trap potential $V(\mathbf{r})$ and should be *testable experimentally* (see Fig. 1).

Outside of $r_0$, (5) and (6) give the dependence of $\rho$ on $r$. At $r_0$, $\xi = 1$ and $\rho = \rho_0$ on both sides; i.e., $\rho$ is continuous. The value of $d\rho/dr$ is finite also but discontinuous at $r_0$, a fact already emphasized by Oliva [4]. $d^2\rho/dr^2$ is also finite and discontinuous.

## IV. REMARKS

The pseudopotential interaction [5] is, in $q$-number language,

$$V_{pp} = \frac{4\pi a \hbar^2}{m} \frac{1}{2} \int d\mathbf{r}_1 \, d\mathbf{r}_2 \, \psi^\dagger(\mathbf{r}_1) \psi^\dagger(\mathbf{r}_2)$$

$$\times \delta(\mathbf{r}_1 - \mathbf{r}_2) \frac{\partial}{\partial r_{12}} [r_{12} \psi(\mathbf{r}_1) \psi(\mathbf{r}_2)]. \qquad (15)$$

The commonly used $\delta$-function interaction [5] is, also in $q$-number language,

$$V_\delta = \frac{4\pi a \hbar^2}{m} \frac{1}{2} \int d\mathbf{r} \, \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) \psi(\mathbf{r}). \qquad (16)$$

(a) We point out that there has been great confusion in the theoretical literature of factors of two about $V_{pp}$ and $V_\delta$. Furthermore, the approximate one-particle $c$-number equation written down from (16) also has confusions of factors of two in the literature.

(b) Strictly speaking (16) does not make sense: The two-body interaction $A\Delta(\mathbf{r}_1 - \mathbf{r}_2)$ for $A < 0$ is not defined and for $A > 0$ it is equivalent to zero. To prove the first statement, we calculate the $s$-wave phase shift for such a case. The interaction is considered as the limit $R \to 0$ of a potential well of magnitude $U$ and radius $R$, keeping $UR^3$ a negative constant. The wave function in the center-of-mass system at $R^-$ is $R^{-1} \sin[(-mU/\hbar^2)^{1/2} R]$. The argument of sine approaches infinity as $R \to 0$. To prove the second statement we do the same calculation and find all phase shifts to be zero.

(c) Although (16) is strictly meaningless, the perturbation calculations based on (15) and (16) in Refs. [5,6] give the same result to the order $a^1$, and is meaningful to that order. The considerations of the present paper are based on these results to order $a$ and are thus meaningful.

How about higher orders? This is a matter of some subtlety. It was found in Ref. [5] that to the second order in $a$, (16) gives infinity, confirming its sickness, but that (15) gives a meaningful answer, which is proportional to $a^2/L$ where $L$ is the size of the box. To order $a^3$ (15) gives an energy containing a term equal to const$\times N^3 a^3/L^5$, which approaches infinity as $L \to \infty$ while $\rho = N/L^3 = $ const. This divergence was later removed [8] by a method of summation over most divergent terms in a perturbation expansion: A summation starting with this divergent term leads to the convergent expression $(4\pi a N \rho)(128/15)(a^3 \rho/\pi)^{1/2}$ for the ground-state energy. This result was later confirmed by several authors who extended it to even higher orders.

The method of Ref. [8] was further extended to cover finite temperatures [9]. These and related developments had been summarized in Ref. [10].

(d) It is tempting to interpret (5) and (6) as indicating an additional effective potential $V_a = kT4a\lambda^2\rho = 8\pi a \rho \hbar^2/m$, and to interpret (14′) as indicating an additional potential of $V_a = 4\pi a \rho \hbar^2/m$. Such interpretations must be used with care. In particular, it is not correct to assert that the condensate is in the ground state of $V + V_a$.

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