Ground state properties of BECs of $^{87}$Rb atoms in an isotropic magnetic trap for different total number of atoms

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Ginzburg-Pitaevskii Gross (GPG) non-linear equation for the Bose Einstein Condensate (BEC) having different number of $^{87}$Rb atoms (in the range $10^2$ to $5 \times 10^3$) in an isotropic magnetic trap, has been numerically solved to obtain its eigenvalue, the chemical potential, and the corresponding wave function, to study its various observable physical properties, such as, the correlation length, healing length, inter-particle separation in the core and the speed of sound in the condensate. These have been compared with the corresponding results computed by using the approximate expression obtained in the limiting case when the number of atoms in the condensate tends to a large value, that is, in the Thomas-Fermi approximation. Significance and inter-relationships of various physical quantities have also been discussed in the light of recent experimental results.

[Keywords: Bose-Einstein Condensation, Chemical potential, Order parameter, Correlation and healing lengths]

1 Introduction

The basic condition for the onset of Bose Einstein Condensation (BEC) in a non-interacting assembly of fixed number of bosons is $\rho \lambda_{\text{dB}}^3 \geq 2.612$, obtained by Einstein\(^1\) way back in 1925. This condition is essentially the ratio of the two lengths, the thermal deBroglie wavelength, $\lambda_{\text{dB}}$, of the bosons ($\hbar/(2\pi m k_B T)^{1/2}$ where $m$ is the mass of the boson, $T$ the temperature of the boson gas and, $k_B$ the Boltzmann constant; the energy of the boson is taken to be its most probable value) and the inter-particle separation $2r_c$ ($2r_c=\sqrt{6/(\pi\rho)}$\(^{11}\) assuming that, each atom is assigned a spherical volume of radius $r_c$, $\rho=N/V$, $N$ is the total, fixed number of atoms in the condensate confined in volume $V$). Since the inter-particle separation for a system of non-interacting particles cannot be decreased beyond a certain limit, to ensure inter-particle interaction to be zero, it is imperative to increase the thermal deBroglie wavelength, by sharply decreasing the temperature of the gas. Such a feat was accomplished for the first time, in an assembly of bosonic $^{87}$Rb atoms in 1995, at a number density of $2.5 \times 10^{12}$ atoms/cm$^3$ at 170 nK confined in a magnetic trap\(^2\).

So far, such a process of BEC has been observed in several different atomic boson assemblies\(^3\). However, in this purely quantum mechanical phase transition (because only the dynamics of free particles, massive bosons under the present consideration, and statistics are involved in the phase transition and both of them are purely quantum mechanical) the bosonic condensate is no longer non-interacting, but is weakly interacting via two-body collisions and, under the influence of magnetic trap potential. The Bose Einstein Condensate (BEC) is, therefore, described through a wave function, also referred to as the order parameter, $\psi(\hat{r})$, and the corresponding eigenvalue, $\mu$, the chemical potential, both of which have to be determined through the Ginzburg-Pitaevskii Gross (GPG) non-linear equation\(^{10}\), in which the kinetic energy of the condensate, the inter-particle interaction and the interaction of the bosonic atoms forming the condensate with the magnetic trap have to be used as inputs.

Once the wave function and the chemical potential of the condensate are known, one can determine various physical properties, such as, the speed of sound, healing length, correlation length

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\(^{1}\)Preliminary part of this work was presented at the Seventh International Conference on –Squeezed States and Uncertainty Relations (ICSSUR 2001), June 4-8, Boston University, Boston, USA.
and inter-particle separation of the core in the condensate, the mathematical expressions of which are given in Section 2. The computations have been done for all these quantities, using the wave function and the chemical potential obtained by solving the GPG non-linear equation, numerically, for $^{87}$Rb condensates, having the total number of bosonic $^{87}$Rb atoms ranging from $10^3$ to $5 \times 10^6$, in an isotropic magnetic trap. These various physical quantities have also been computed under the Thomas-Fermi Approximation (TFA), which, strictly speaking, is valid for large $N$. The results of the computations are described in Section 3 followed by a salient conclusion in Section 4. An algebraic form of the numerically evaluated wave function is also given in the appendix for future use.

2 Theoretical Considerations

BEC of weakly interacting gas of bosonic atoms in a magnetic trap can be described by the following well-known GPG non-linear equation:

![Graph 1](image1.png)

Fig. 1 — Variation of chemical potential, $\mu$, expressed in harmonic oscillator (HO) units with number of bosonic atoms, $N$, forming the BEC of $^{87}$Rb atoms in an isotropic magnetic trap. $\mu$ obtained by GPG Eq. (2) i.e., $\mu = \rho_{\text{SG}}$ (--- --- ---) $\mu$ under Thomas Fermi Approximation (TFA), $\mu = \rho_{\text{TFA}}$. In the inset is shown the percentage deviation of $\mu = \rho_{\text{TFA}}$ with $\mu = \rho_{\text{SG}}$, defined in the text, with $N$.

![Graph 2](image2.png)

Fig. 2 — Comparison of the wave function obtained from the Ginzburg-Pitaevskii and Gross (GPG) equation (———) and under the TFA (--- --- ---) of BEC of $^{87}$Rb atoms in an isotropic magnetic trap for $N = 100$. (----------) represents the wave function obtained from the algebraic form described in the appendix.
ground state properties of $^{87}\text{Rb}$ atoms

$$E[\psi] = \int d^3r \left[ \left( \frac{\hbar^2}{2m} \right) |\nabla \psi (\vec{r})|^2 + V_{\text{env}} (\vec{r}) |\psi (\vec{r})|^2 + \left( \frac{2\pi \hbar^2 a}{m} \right) |\psi (\vec{r})|^4 \right]$$

\[ \cdots (1) \]

Here, the inter-particle two-body interaction is taken to be repulsive, unlike the case of $^7\text{Li}$, where it is attractive, through a positive value of the $s$-wave triplet spin scattering length $a$, and $E$ is the energy functional of the condensate. In order to obtain the ground state wave function of the condensate or its order parameter, and the corresponding eigenvalue, one minimizes Eq. (1) with respect to $\psi (\vec{r})$, or $\psi (\vec{r})$, to obtain the following equation:

$$\mu \psi (\vec{r}) = \left( -\frac{\hbar^2}{2m} \right) \nabla^2 + V_{\text{env}} (\vec{r})$$

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**Fig. 3** — Same as in Fig. 2 but now $N = 10,000$

**Fig. 4** — Same as in Fig. 2 with $N = 5 \times 10^6$
the truncated equation, which is as follows:

$$
\psi(\vec{r}) = \left[ \frac{m}{8\pi \hbar^2 a} \left( 2\mu - m\omega_{ho}^2 r^2 \right) \right]^{1/2}
$$

and the chemical potential turns out to be:

$$
\mu = \frac{\hbar \omega_{ho}}{2} \left( \frac{15Na}{a_{ho}} \right)^{2/5}
$$

The form of the wave function and the chemical potential for the system are

![Graph showing variation of energy and speed of sound](image-url)
potential given by Eqs (3) and (4), respectively, are used to numerically solve Eq. (2) to obtain realistic values\(^{(12,13)}\) of \(\mu\) and \(\psi(\vec{r})\). Once these are known, one can evaluate the ground state properties of the condensate. The speed of sound, \(c\), for example, is given by the following relation:

\[
c^2 = \frac{\mu}{m}
\]

and the healing length, \(\xi\), turns out to be:

\[
\xi = \frac{\hbar}{\sqrt{2\pi} m \mu^{1/3}}
\]

The healing length of the condensate, \(\xi\), is the distance over which the wave function tends to its bulk value when subjected to a localized perturbation. It gives us the extent up to which the kinetic energy plays a dominant role along with the interaction energy term. This is different from the correlation length, \(\sqrt{\langle r^2 \rangle}\), defined below:

\[
\sqrt{\langle r^2 \rangle} = \frac{\int \psi^*(\vec{r}) r^2 \psi(\vec{r}) d\vec{r}}{\int \psi^*(\vec{r}) \psi(\vec{r}) d\vec{r}}
\]

which gives the spatial extent of the Bose Einstein Condensate\(^{(14)}\) and has recently been studied in a blob of \(^{23}\)Na BEC atoms.

Under TFA, one can define another length, \(2r'_c\), the inter-particle separation in the core of the condensate, which is given as follows:

\[
2r'_c = \left( \frac{2\hbar^2 a}{m^2 \mu} \right)^{1/3}
\]

3 Results and Discussion

Various ground state properties of BEC at temperature 0 K can be studied, once Eq. (2) is solved. However, as mentioned earlier, Eq. (2) has to be solved numerically, being a non-linear equation, which cannot be solved analytically. One, therefore, makes use of the Eqs (3) and (4) to generate iterated wave function and the corresponding chemical potential, until the iterated value of the order parameter lie within a stipulated accuracy. The computations have been made on the above basis and the results of the computations have been shown, for the numerically-generated chemical potential, \(\mu = \mu_{\text{NG}}\), expressed in harmonic oscillator...
(HO) units (1 HO unit = 5.1332×10^{-22} J), for different number of particles, \( N \), ranging from \( 10^2 \) to \( 5 \times 10^6 \) constituting the condensate, in Fig. 1 by continuous curve along with the results obtained under the TFA shown by a dashed curve. When \( N=100 \), the value of \( \mu_{\mathrm{TFA}} \) turns out to be nearly 1.79 in HO units, which gradually increases to 6.89 for \( N=10,000 \) beyond which the increase is sharper, rising to a value of 80.24 at \( N=5 \times 10^6 \). The computed value of \( \mu \) from Eq. (4), \( \mu_{\mathrm{TFA}} \), starts with still lower values of \( \mu=1.06 \) for \( N=100 \), where the difference between this value and the value computed accurately from Eq. (2), \( \mu_{\mathrm{SG}} \), is maximum. This difference between the two keeps on decreasing with increase in the value of \( N \) and becomes quite small when \( N \sim 10^3 \), as is evident from Fig. 1. The percentage deviation, \% deviation \( = [(\mu_{\mathrm{SG}}-\mu_{\mathrm{TFA}})/\mu_{\mathrm{SG}}] \times 100 \), between the two is also shown in the inset of Fig. 1. It may be noticed that, the effect of neglect of the kinetic energy (KE) term in Eq. (1) leads to lower and perceptibly different values of \( \mu \), as shown by the dashed curve, particularly, for lower values of \( N \). From the exercise it is also borne out that, for large \( N \), the interaction energies, both due to inter-particle interaction and that due to the interaction of the condensate with the magnetic trap, dominate the processes, as will be clearer from further discussions.

In Figs 2-4 have been plotted the variation of the computed wave function or the order parameter \( \psi(r) \), with \( r \) expressed in HO units of length (1 HO length unit = 1.22×10^{-3} m), when \( N=100, N=10,000 \) and \( N=5 \times 10^6 \), respectively. While continuous curve is from the numerically-generated solution of Eq. (2), the large dash curve corresponds to Eq. (3), which is an outcome of TFA. When \( N=100 \), there is a large difference between the two wave functions in the entire domain. While TFA yields sharper fall near \( r=1.6 \), that from Eq. (2) shows a gradual decrease with increase in \( r \), as is evident from Fig. 2. The difference in the two \( \psi(r) \) with \( r \) becoming smaller with increase in \( N \) as shown in Figs 3 and 4.

While TFA yields a sharper drop in \( \psi(r) \) near that value of \( r \) where it goes to zero, for all values of \( N \), the gradual variation in the form of a tail stays in the realistic situation, i.e. from Eq. (2). This comes about due to the presence of the KE term in Eq. (2), as ground state properties of BEC being discussed, i.e. at \( T=0 \) K. No thermal effect is, therefore, involved.

Making use of the numerically-generated wave function \( \psi(r) \), the total energy, \( E \), of the condensate has been computed, using Eq. (1), for various values of \( N \). The result of this computed value of energy expressed in HO units has been shown by continuous curve for different values of \( N \) ranging from \( 10^2 \) to \( 5 \times 10^6 \) in Fig. 5. The individual contribution of the KE term, the potential energy due to the magnetic trap and the inter-particle...
interaction in the condensate have also been shown by dash-dot-dash, large dash and small dash curves, respectively. The KE term is larger (~40 % of the total energy) than the corresponding inter-particle interaction energy term contribution (~8 % of the total energy) for \( \mathcal{N} = 10^5 \); the KE contribution keeps slowly decreasing with increase in the value of \( \mathcal{N} \), while the contribution of the inter-particle interaction energy term keeps increasing. Both become nearly equal for \( \mathcal{N} \approx 800 \). This is clearer from the inset of the figure. The KE term keeps decreasing with increase in the value of \( \mathcal{N} \), while the contribution of the inter-particle interaction energy term keeps increasing, reaching a value of ~40 % of the total energy at \( \mathcal{N} = 5 \times 10^6 \). It may be noted that, the interaction of the condensate with the magnetic trap is larger (~50-60 % of the total energy) than either of the two contributions throughout the range of \( \mathcal{N} \) considered. It is also noteworthy that, for large values of \( \mathcal{N} \), the KE contribution to the total energy is negligible ~0.06 % for \( \mathcal{N} = 5 \times 10^6 \); making TFA a very good approximation indeed.

The computed values of the speed of sound in the BEC of different number of atoms have been plotted in Fig. 6, when \( \mu \) given by Eq. 2 and that given by Eq. 4, are shown by continuous curve and dash curve, respectively. As is to be expected, the difference between the speeds of sound for the two cases are different for small values of \( \mathcal{N} \), which decrease when \( \mathcal{N} \) becomes larger. The percentage deviation between the two with \( \mathcal{N} \), as in the case of \( \mu \), has been plotted in the inset of Fig. 6.

In Fig. 7 have been shown the variation of the healing length, \( \xi \), with \( \mathcal{N} \) using Eq. (6), when \( \mu = \mu_{\text{NG}} \) and \( \mu = \mu_{\text{TFA}} \), by continuous curve and dash curve, respectively. Here, the trend of absolute values get reversed: \( \xi \) under TFA is higher than that given by the numerically-generated one. The percentage deviation for different \( \mathcal{N} \) values turn out to be negative and are shown in the inset of Fig. 7.

Making use of the numerically-generated wave function from Eq. (2) and that computed by using Eq. (3), the variation of the correlation length with \( \mathcal{N} \) for the two cases using Eq. (7) have been computed and plotted in Fig. 8 and are shown by continuous and dashed curves, respectively. As the number of particles in the condensate increases, the value of the correlation length also increases as is evident from Fig. 8. The percentage deviation in the computed values of the correlation length has been shown in the inset of Fig. 8. It may be pointed out that, the correlation length represents the extent of the condensate consisting of different number of bosonic atoms. One may note that, the BEC when forced to rotate gives rise to the formation of quantized vortices\(^{15} \). Further, unlike super-
conductivity, the radius of a vortex thus formed in a BEC corresponds to the healing length and not to the correlation length defined here. However, like in high temperature superconductivity, where the coherence length covers few particles, here too, the healing length spans two to three inter-particle separations only. One may note that, if one compares the extent of the condensate given by the correlation length with the healing length and the inter-vortices separation, one finds that there are not many vortices that can be formed. This is also borne out by the recent experimental results in $^{23}$Na Bose Einstein Condensate\textsuperscript{\textcopyright}. Further, the inter-particle separation in the condensate, $2r_c$, is comparable with the healing length.

Finally, in Fig. 9 have been plotted the variation of inter-particle separation in the core of the condensate, $2r'_c$, for the two cases: that is when $\mu=\mu_{\text{TFA}}$ and $\mu=\mu_{\text{SEC}}$, with percentage deviation plotted in the inset. The expression for the density of the condensate in the core, $\rho_0$, is taken to be that given in the TFA i.e. $\rho_0 = \frac{\mu A}{4\pi r_a^2}$. Unlike the inter-particle separation referred to as $2r_c$ described in the beginning of the introduction, which depends only on the number density of the atoms in the condensate, inter-particle separation in the core of the condensate is dependent upon the chemical potential, which is a characteristic of the Bose Einstein Condensate.

**Conclusion**

One may conclude that, the various ground state properties of BEC having different total number of bosonic atoms are quantitatively different when full GPG non-linear equation is solved numerically and when one uses TFA. This difference is significant when the number of bosonic atoms in the condensate is small. While the relative contribution of the inter-particle interaction energy in the condensate and the interaction energy of the condensate atoms due to the magnetic trap keep increasing with $N$, the KE contribution keeps decreasing and is negligible for large $N$. The correlation length in the condensate corresponds to the extent of the condensate and is not same as the extent of the wave function.

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**References**


Appendix

As has been emphasized earlier, the wave function or the order parameter of BEC has to be obtained for a fixed number of bosons in the condensate by solving the non-linear GPG equation. The wave function thus obtained are quite different from one another in its form and extension for condensates having different number of bosonic atoms as is evident from Figs 2-4, for $N=10^5$, $10,000$ and $5\times10^5$ particles, respectively. Thus, strictly speaking, one must resort to the numerical evaluation of Eq. (2). However, it is worthwhile to suggest an algebraic form of the wave function, which can mimic the wave function obtained numerically, so that one can use it to study other properties of the condensate, analytically. The following algebraic form of the condensate wave function is, therefore, suggested:

$$\psi(\vec{r}) = \frac{n}{\sqrt{2\pi \Gamma}} \sum_i \exp\left(\frac{-r_i^2}{2\Gamma}\right) + a_i \sin((r_i - b_i)c_i)$$

where $N$ is the total number of bosons in the condensate. In Eq. (A1), while $\Gamma$ represents the width of the wave function at half of its value at $r=0$, $a_i$, $b_i$, and $c_i$ are the constants dependent upon $i$, which represent certain regions of the wave function, and $n$ is the normalization constant and is given as:

$$n = \frac{N\Gamma^2}{\sum_i \{X_1i + X_2i + X_3i\}}$$

where $X_1i$ is given by:

$$X_1i = \int_{R_{i,\text{min}}}^{R_{i,\text{max}}} \exp\left(\frac{-r_i^2}{2\Gamma}\right) dr_i$$

$X_2i$ is given as:

$$X_2i = \int_{R_{i,\text{min}}}^{R_{i,\text{max}}} a_i^2 \sin\left((r_i - b_i)c_i\right) dr_i$$

and $X_3i$ is given by:

$$X_3i = \int_{R_{i,\text{min}}}^{R_{i,\text{max}}} 2a_i \exp\left(\frac{-r_i^2}{2\Gamma}\right) \sin((r_i - b_i)c_i) dr_i$$

It is possible to reproduce the numerically obtained wave function of the condensate consisting of different number of bosonic atoms by varying the subscript $i$ and by using the appropriate value of $a_i$, $b_i$, and $c_i$ occurring in Eqs A1, A5-A6. In the case of $^{87}$Rb condensate, $i$ has values lying between 4 and 7, when $N$ varies from $10^5$ to $5\times10^6$. The computations of $\psi(\vec{r})$ based on the above algebraic form have been shown in Figs 2-4 by small dashed curve, for $N=100$, $N=10,000$ and $N=5\times10^5$, respectively. Except for small variations in some regions of $r$, the present wave function turns out to be quite close to the one obtained numerically.