A study of trapped Bose gas beyond mean-field theory

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Abstract

We study the ground-state properties of dilute Bose gas confined to both isotropic and anisotropic traps to assess the accuracy of Gross-Pitaevskii (GP) theory. To go beyond GP approximation we use Huang-Yang theory of interatomic interaction energy for hard-sphere Bose gas and use a variational method to solve the resulting modified GP equation. We also make an analytic estimate of the corrections due to the higher-order terms in the interatomic interaction energy. We find that corrections are of the order of 1%. However, there is a qualitative change in the density profile due to presence of logarithmic term in the interaction energy for large $N$ (number of atoms).

1 Introduction

The discovery of Bose-Einstein condensation (BEC) in magnetically trapped alkali atoms [1, 2, 3] and spin-polarized hydrogen atom [4] has resulted in large body of theoretical and experimental research [5] on the ground-state as well as excited state properties of trapped atomic gases. For the case of dilute atomic gas, which is the case for most of the experimental situation, the mean-field theory of GP [6] has been quite successful in explaining both static (ground-state) and dynamic (collective excitations) properties of the condensates. The interacting atomic gas is considered to be dilute when the average distance between the atoms is much larger than the range of interaction potential between the atoms [7] (mathematically this is expressed by the condition $n|a|^3 << 1$, where $n$ atomic density and $a$ is the s wave scattering length of interatomic potential). For this case the interaction between the atoms is well described by two-body collisions characterized by a single parameter obtainable from the potential namely, the s wave scattering length $a$.

In some recent experiments [4, 8, 9] BEC is achieved with number of atoms $N$ being quite high. It is possible to produce condensates of $\approx 10^7$ $^{87}$Rb atoms, $\approx 5 \times 10^7$ Na atoms and $\approx 10^9$ H atoms. The maximum density in the optical traps has been around $10^{15}$
Thus, with the increasing atomic density in the condensate it becomes necessary to test the validity of mean-field GP theory. The main aim of this paper is to investigate systematically the accuracy of the GP theory in the high density limit. We go beyond mean-field theory and evaluate the corrections using a variational formalism. We also derive an analytic estimate for the corrections in the framework of Thomas-Fermi (TF) approximation. For this purpose we use Huang-Yang \cite{10} theory for the interatomic interaction energy $\epsilon$. In this theory, $\epsilon$ is expanded in power of gas parameter $n|a|^3$ by assuming the atomic gas to be a uniform hard-sphere Bose gas. It is important to note here that the interatomic potential in Huang-Yang theory is replaced by a pseudopotential. The expression for $\epsilon$ is \cite{11, 12}

$$
\epsilon(n) = \frac{2\pi\hbar^2an}{m} \left[ 1 + \frac{128}{15\sqrt{\pi}} (na^3)^{\frac{1}{3}} + 8 \left( \frac{4\pi}{3} - \sqrt{3} \right) (na^3) \ln(na^3) + O(na^3) \right] \tag{1}
$$

In GP theory only the first term in the above expansion is considered as higher order terms are negligible for dilute gas. However, with increasing density, higher-order terms become appreciable. It is, therefore, of interest to study the effects these higher order terms on the ground-state properties of BEC.

The effect of higher-order terms in the interatomic potential on the physical properties of BEC has recently been reported in the literature \cite{13, 14}. Nunes \cite{13} has used density functional theory to derive the modified GP (MGP) equation. By solving the MGP equation for a weak isotropic trap in the Thomas-Fermi (TF) approximation, he finds that the maximum change in the ground state density due to the higher order terms in Eq.(1) is only a few percent for the value of $N$ as large as $10^9$. On the other hand, the change in the ground state energy per particle has been reported to be sensitive to $N$ - for $N \leq 10^7$ both GP and MGP results are very close whereas, they differ by 33% for $N = 10^9$. This result is not in conformity with the analytic estimate \cite{5} of the correction introduced in the ground state energy by the higher order terms in Eq.(1). According to the analytic estimate, the first higher order term in Eq.(1) causes a change of only a few percent in the ground state energy even for very large value of $N$. As discussed below, the second higher order term in Eq.(1) being logarithmic gives negative correction. Therefore, this is expected to partially cancel the correction due to the first higher-order term in the interatomic interaction energy. As a result of this, the net correction remain close to a few percent when $N$ is varied from $10^7$ to $10^9$. Fabrocini and Polls \cite{14} have studied the effect of interatomic correlations within the local density approximation and the correlated basis function (CBF) theory. They have solved the resulting MGP equation and the lowest order correlated Hartree (CH$_{LO}$) equation for an isotropic trap using the steepest descent method. Both of these methods give corrections which are close to those predicted by the analytical estimates. However, the CH$_{LO}$ equation gives lower value of the ground state energy than the MGP equation. The difference between the results obtained by these two methods shows up more at higher values of $N$. It is not clear if this is due to any numerical problem or due to some physical reason. We discuss more about these results in section 4.
In this paper we employ variational approach \cite{15,16,17} to solve the MGP equation by using the variational ansatz for the density recently proposed in Ref.\cite{17}. We also perform calculations for more realistic case of axially symmetric trap ($\omega_x = \omega_y = \omega_\perp \neq \omega_z$) potential. In order to assess the accuracy of our variational results we generalize the virial relations \cite{5} for the interatomic interaction energy given by Eq.(1).

Recently, several authors \cite{5,18,19} have estimated the corrections introduced by the first higher-order term in the Eq.(1) to assess the accuracy of GP theory. These authors obtained analytical expressions for the corrections over mean-field results within the Thomas-Fermi (TF) approximation valid in the large $N$ limit. Here we extend these results by including second higher-order term of Eq.(1). Beside, providing the estimates for corrections these results also serve as a check for the accuracy of our numbers obtained by the variational calculation.

It is necessary to emphasize here that our previous and the present study clearly bring out the advantages of variational approach. This approach requires numerically less effort than the direct numerical integration method and can handle system of arbitrary number of particle. At the same time, it provides a very accurate description of the ground state properties of the system.

Rest of the paper is organized as follows: In section 2 we describe the variational approach and also derive an expression for the generalized virial relation. Section 3 contains analytical estimates for corrections in the density profile, the total energy and the chemical potential. Results are discussed in section 4 and paper is concluded in section 5.

### 2 Variational method

The energy functional for a system of $N$-bosons, each of mass $m$, confined in a trap potential $V_\text{t}(\mathbf{r})$ is given by

\[
E[\Psi] = \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla \Psi(\mathbf{r})|^2 + V_\text{t}(\mathbf{r})|\Psi(\mathbf{r})|^2 + \epsilon(n)|\Psi(\mathbf{r})|^2 \right],
\]

where $\Psi(\mathbf{r})$ is the corresponding wave function and gives density via the relation $n(\mathbf{r}) = |\Psi(\mathbf{r})|^2$. For $\epsilon(n)$ we use the local-density approximation (LDA) expression as given in Eq.(1). The energy functional associated with GP theory can be obtained from Eq.(2) by substituting only the first term of Eq.(1) for $\epsilon(n)$ in Eq.(2). In this study we go beyond GP theory by including the second and the third term of Eq.(1) to study the ground-state properties of BEC.

For our purpose we consider an axially symmetric trap characterized by two angular frequencies $\omega_\perp$ and $\omega_z$ and the corresponding potential is given by

\[
V_\text{t}(\mathbf{r}) = \frac{m \omega_\perp^2}{2} \left( x^2 + y^2 + \lambda_0^2 z^2 \right),
\]
where $\lambda_0 = \omega_\perp / \omega_0$ is the anisotropy parameter of the trapping potential.

As in the GP approach, from Eqs.(1) and (2) the MGP equation can be derived by making the energy functional $E[\Psi]$ stationary with respect to the wave function $\Psi(r)$ such that the wave function remains normalized to the total number of particles $N$ given by the condition

$$\int |\Psi(r)|^2 d\mathbf{r} = N.$$

Such a variation leads to:

$$-\nabla_1^2 + \left( x_1^2 + y_1^2 + \lambda_0^2 z_1^2 \right) + 8\pi N |\psi_1(r_1)|^2 + \frac{256}{3} \left( \frac{\pi a^3 N}{3} \right)^{\frac{3}{2}} |\psi_1(r_1)|^3$$

$$+ \frac{8\pi a^4 N^2}{3} \left( \frac{4\pi}{3} - \sqrt{3} \right) |\psi_1(r_1)|^4 \left\{ 6 \ln \left( \frac{N a^3 |\psi_1(r_1)|^2}{\pi a^2} \right) + 2 \right\} \psi_1(r_1)$$

$$= 2\mu_1 \psi_1(r_1),$$

where, $\mu_1$ is the chemical potential in the units of $\hbar \omega_\perp$ corresponding to the normalization constraint given by Eq.(4). In this equation we have used the length scale rescaled variables $r_1 = r/a_{ho}, a = a/a_{ho}, \nabla_1 = a_{ho} \nabla, E_1 = E/\hbar \omega_\perp$, with $a_{ho} = (\hbar/m \omega_\perp)^{\frac{1}{2}}$ and $\Psi(r_1)$ is normalized to unity.

In Ref.[14] and [13] above equation (Eq.5) has been solved numerically for isotropic trap ($\lambda_0 = 1$). In this paper we take recourse to variational approach to solve the Eq.(5). The main advantage of this method is that with a suitable choice for the variational form of the wave function one can get quite accurate results with less computational effort. In addition, this approach may provide physical insight which generally get obscured by the complicated computational procedures. In this paper we use the variational form given by [17]

$$\psi_1(r_1) = \sqrt{\frac{p}{2\pi(G/2p)}} \lambda_1^\frac{p}{2} \left( \frac{\omega_\perp}{\omega_0^2} \right)^{\frac{p}{4}} e^{-\frac{1}{2} \left( \frac{\omega_\perp}{\omega_0^2} \right) \left( r_1^2 + \lambda z_1^2 \right)^p}$$

(6)

where $\lambda, \omega_\perp$ and $p$ are the variational parameters which are obtained by minimizing $E_1$ with respect to this parameters. This variational form has been shown to describe quite accurately the ground state of the dilute Bose gas confined in a trap for a wide range of particle numbers. When number is small it tends correctly towards Gaussian and in the opposite limit it resembles with the TF wave function. In addition to this in the intermediate region it combines the feature of both in an effective way. This variational form is also well suited for negative scattering length and is easily generalized for the vortex states. Further, using Eq.(6) the physical observables can be expressed analytically in terms of these three variational parameters. For example, energy functional $E_1$ can be written as:

$$\frac{E_1}{N} = E_{\text{kin}} + E_{ho} + E_{\text{int}}^1 + E_{\text{int}}^2 + E_{\text{int}}^3.$$
energies corresponding to the first, second and the third terms in the energy expansion in Eq. (1).

\[ E_{\text{kin}} = \frac{1}{12} \frac{\omega_{\perp}}{\omega_{\perp}^0} \left( 1 + \frac{\lambda}{2} \right) \Gamma \left( \frac{1}{2p} \right) \Gamma \left( \frac{3}{2p} \right) (1 + 2p) \]  
\[ E_{\text{ho}} = \frac{1}{3} \frac{\omega_{\perp}}{\omega_{\perp}^0} \left( 1 + \frac{\lambda^2}{2\lambda} \frac{\lambda}{\omega_{\perp}^0} \right) \Gamma \left( \frac{5}{2p} \right) \Gamma \left( \frac{3}{2p} \right) \]  
\[ E_{\text{int}}^1 = N a_{\perp} \frac{\omega_{\perp}}{\omega_{\perp}^0} \sqrt{\lambda} \frac{p}{\Gamma \left( \frac{3}{2p} \right)} \left( \frac{1}{2} \right)^{\frac{1}{2p}} \]  
\[ E_{\text{int}}^2 = \frac{128}{15\sqrt{2\pi}} \frac{a_{\perp}^2 N \frac{P}{2\lambda} \lambda^2 \sqrt{\lambda}}{\Gamma \left( \frac{3}{2p} \right)} \left( \frac{2}{5} \right)^{\frac{1}{2p}} \]  
\[ E_{\text{int}}^3 = 4\sqrt{\lambda^4 N^2 \left( \frac{4\pi}{3} - \sqrt{3} \right) \frac{p^2 \lambda}{\Gamma \left( \frac{3}{2p} \right)} \left( \frac{\omega_{\perp}^0}{\omega_{\perp}} \right)^3} \times \]  
\[ \ln \left[ N\pi^3 \left( \frac{2p}{2\pi \Gamma \left( \frac{3}{2p} \right)} \lambda^2 \frac{\omega_{\perp}}{\omega_{\perp}^0} \right) \right]^2 - \left( \frac{\omega_{\perp}}{\omega_{\perp}^0} \right)^{\frac{1}{2}} \frac{1}{2\sqrt{3}} \Gamma \left( \frac{3}{2p} + 1 \right) \]  

For particular value \( N \) the parameter \( \omega_{\perp}, \lambda \) and \( p \) are determined by minimizing the energy given above (Eq. (7)).

The virial relation among different energy components provides a way of checking the correctness of variational or numerical solutions. For example, within GP theory different energy components satisfy the virial relation [5]

\[ 2E_{\text{kin}} - 2E_{\text{ho}} + 3E_{\text{int}}^1 = 0 \]  

For our purpose we generalize the above relation (Eq. (13)) valid for the MGP theory. By using variational nature of energy and the scaling transformation \( \Psi(r_{\lambda}) \rightarrow \sqrt{\lambda}\Psi(r) \) we arrive at following expression for the virial relation corresponding to the MGP energy functional

\[ 2E_{\text{kin}} - 2E_{\text{ho}} + 3E_{\text{int}}^1 + \frac{9}{2} E_{\text{int}}^2 + 2E_{\text{int}}^3 + \int |\Psi_1(r_1)|^6 dr_1 = 0. \]  

For each term of this expansion we have checked the satisfaction of virial relation corresponding to our variational solutions. The virial relation is satisfied up to 5-th decimal place in our calculation.

Before presenting the results, we make an estimate of the corrections in the density, total energy and the chemical potential as a result of inclusion of two new terms in the interatomic energy. For this we follow the approach of Dalfovo et al. [5], which is valid for large \( N \).
3 Analytic Estimate

We use local density approximation for the chemical potential which is justified in the thermodynamic limit $N \to \infty$ where the profile of the density distribution is very smooth. In this approximation the chemical potential is given by:

$$\mu = \mu_{\text{local}}[n(r)] + V_t(r)$$  \hspace{1cm} (15)

Given the expression for $\mu_{\text{local}}(n)$ for the homogeneous Bose-gas, the density $n(r)$ can be calculated by solving Eq. (15), along with the normalization condition which fixes the parameter $\mu$ on the left hand side of the equation. From Eq. (1), it follows that

$$\mu_{\text{local}}[n(r)] = gn \left[ 1 + \frac{32}{5\sqrt{\pi}} (na^3)^{\frac{5}{2}} + 4 \left( \frac{4\pi}{3} - \sqrt{3} \right) (na^3) (3 \ln (na^3)) + O(na^3) \right] ,$$  \hspace{1cm} (16)

where,

$$g = \frac{4\pi \hbar^2 a}{m}.$$  \hspace{1cm} (17)

Considering only the first term in the expansion for $\mu_{\text{local}}$ we recover the mean-field Thomas-Fermi result

$$n(r) = \left( \frac{\mu - V_{t\text{trap}}(r)}{g} \right) = n_{TF}(r).$$  \hspace{1cm} (18)

Normalization condition implies that

$$\mu = \frac{\hbar \omega_0}{2} (15N\lambda_0 a^3)^{\frac{5}{2}} = \mu_{TF}.$$  \hspace{1cm} (19)

Using the relation $\mu = \partial E/\partial N$ we get the corresponding expression for the ground state energy as

$$E = \frac{5}{4} N \mu = E_{TF}.$$  \hspace{1cm} (20)

When the higher order terms in the expansion for $\mu_{\text{local}}$ are considered the standard procedure to solve Eq. (15) is by iteration. On following such procedure we get

$$n(r) = \left( \frac{\mu - V_t(r)}{g} \right) - \frac{4m^{3/2}}{3\pi^2 \hbar^3} (\mu - V_t(r))^{3/2}$$

$$- 3 \left( \frac{4\pi}{3} - \sqrt{3} \right) \frac{m^2 a^4}{4\pi^2 \hbar^4} (\mu - V_t(r))^2 \ln \left( \frac{ma^2}{4\pi \hbar^2} (\mu - V_t(r)) \right) + O(na^3).$$  \hspace{1cm} (21)

Now imposing the normalization condition and neglecting the terms of order $O(na^3)$ and higher, we obtain

$$\mu = \mu_{TF} \left[ 1 + \sqrt{\pi a^3 n(0)} + \frac{96}{35} \left( \frac{4\pi}{3} - \sqrt{3} \right) (n(0)a^3) \ln (n(0)a^3) \right],$$  \hspace{1cm} (22)
and consequently
\[
E = \frac{5}{7}N\mu_{TF} \left[ 1 + \frac{7}{8}\sqrt{\pi a^3 n(0)} + \frac{32}{15} \left( \frac{4\pi}{3} - \sqrt{3} \right) (n(0)a^3) \ln(n(0)a^3) \right]
\]  (23)

The parameter \(a^3 n(0)\) appearing in the above equations can be written as
\[
a^3 n(0) = \frac{15\frac{\pi}{8}}{8\pi} \left( \frac{N^{\frac{1}{2}} \lambda_{0}\frac{1}{2\pi}}{\bar{\sigma}} \right)^{\frac{1}{2}}
\]  (24)

Thus by using Eqs. (21), (22) and (23) we estimate the correction over the corresponding TF results. For example a BEC with \(N = 10^7\) particles and \(\bar{\sigma} = 4.33 \times 10^{-3}\), the second terms in Eq. (22) and (23) result in 2.2% and 1.9% corrections in the chemical potential and the total energy, respectively, over the corresponding TF values. Third terms, however, lead to negative corrections and these are 0.93% in the chemical potential and 0.72% in the total energy. Due to the cancellation the net corrections are approximately of order 1.2% for both chemical potential and total energy over their corresponding TF values. Thus the third term which is logarithmic in nature compensates for the correction due to the second term in both chemical potential and energy.

In the next section we present results of our variational calculation along with the numbers obtained from these expressions as a further check for our numerical results.

4 Results and Discussion

In this section we first report calculations on \(^{87}\text{Rb}\) atoms confined in an isotropic (\(\lambda_0 = 1\)) trap. The choice of isotropic trap is motivated only for the sake of comparison with the existing studies [14]. As pointed out earlier, our variational approach is capable of dealing with asymmetric traps with cylindrical symmetry or even fully symmetric traps. For the symmetric trap we choose trap frequency \(\omega_0/2\pi\) and scaled s wave scattering length \(\bar{\sigma}\) to be 77.78Hz and 4.33 \times 10^{-3}, respectively. In Table 1 we show chemical potentials, total energy and mean radius \(<r^2>\) for particle numbers ranging from \(10^3\) to \(10^9\) for both GP and MGP cases. For comparison we also show the corresponding MGP results of Ref.[14] in parenthesis. It clearly shows that the difference between GP and MGP results grow with the increase in particle number. For example, corresponding to \(N = 10^4\) the GP numbers are lower than the MGP values by 0.4%. On the other hand for \(N = 10^8\) the difference is of the order of 1.4%. This is consistent with our estimation of the corrections given by Eq. (22) and (23). Moreover, at this point we also note that numbers obtained by us for total energy are systematically lower than the corresponding MGP results of Ref.[14]. The difference between our results and that of Ref.[14] increases with the number of particles. For example the difference is of the order 2% at \(N = 10^7\). A similar trend is observed for both chemical potential and mean radius. At this point it is worth mentioning that our method, being variational, provides an upper bound to the ground state energy. It is expected that the numerical value of the ground state
Table 1: Results for the ground-state of $^{87}$Rb atoms confined in an isotropic trap with $\omega_0^2/2\pi = 77.78$ Hz. Chemical potentials and energies are in units of $\hbar \omega_0^2$ and length is in units of $a_{ho}$. Numbers in the brackets correspond to the results of reference \[14\]

| N     | GP    | MGP    |       | GP    | MGP    |       |
|-------|-------|--------|-------|-------|--------|-------|
|       | $\mu_1$ | $E_1$ | $<r>_{max}$ | $\mu_1$ | $E_1$ | $<r>_{max}$ |
| $10^3$ | 3.05  | 2.43   | 1.65  | (3.06) | (2.43) | (1.66) |
| $10^4$ | 6.87  | 5.05   | 2.44  | 6.91   | 5.07   | 2.45   |
| $10^5$ | 16.90 | 12.13  | 3.81  | 17.02  | 12.21  | 3.83   |
| $10^6$ | 42.30 | 30.24  | 6.02  | 42.71  | 30.51  | 6.06   |
| $10^7$ | 106.18| 75.86  | 9.54  | 107.53 | 76.75  | 9.61   |
| $10^8$ | 266.70| 190.50 | 15.12 | 270.42 | 193.13 | 15.23  |
| $10^9$ | 669.90| 478.50 | 23.96 | 675.77 | 483.81 | 24.00  |

energy obtained variationally will be typically higher than those obtained by solving the MGP equation directly by standard numerical procedures. It is therefore surprising that the results obtained by solving the MGP equation numerically in Ref. \[14\] gives higher value of the ground state energy than that obtained by us. On the other hand, numbers obtained by the correlated wave function approach in Ref.\[14\] are very close to our results for $N \leq 10^6$. For higher values of $N$, however, the trend is similar to the MGP results.

Next we compare results obtained by us with those of Ref.\[13\]. To do this we consider BEC of $^{87}$Rb atoms in a trap with angular frequency of 20Hz and $a = 7$nm. We do calculation for $N = 10^9$ as for this value of $N$ quite a drastic energy change is reported in Ref.\[13\]. We find that for above parameters the energy per particle corresponding to the GP case is lower than the MGP value by 1.38%. This is also consistent with the analytical estimate given by Eq.(23). The corresponding number reported in Ref.\[13\] is 33%. We feel that this is a gross overestimate of the energy correction since the first higher-order term in the Eq.(23) leads to the correction of around 3% over the TF value. But as mentioned before the second higher-order term in the Eq.(23) being logarithmic, results in a negative correction and for above parameters it is 1.6% of TF value. Consequently the net correction in energy per particle due to higher-order terms is only 1.4% over the TF number. We point out that this number compares well with the result obtained by variational calculation.

In Table 2 we present the numbers for chemical potential and total energies obtained
Table 2: Analytical estimates for the chemical potential and the ground-state energy of $^{87}\text{Rb}$ atoms confined in an isotropic trap with $\omega^0_0/2\pi = 77.78$ Hz. Chemical potentials and energies are in units of $\hbar\omega_0$ and length is in units of $a_0$. TF represents results within Thomas-Fermi approximation (Eqs. (19) and (20)) and MTF corresponds to those obtained by modified TF expressions (Eqs. (22) and (23)) via Eq. (22) and (23), respectively for several values of N. These numbers serve as an additional check for correctness of our numerical results especially for large N. This is clearly the case as MGP numbers in Table 1 are quite close to the corresponding numbers in Table 2 for large N. Furthermore, comparison of Table 1 and II also shows that our variational results are closer to the analytical estimates than those reported in Ref. [14].

Next to study the density profile we plot the ground-state wave function along x-axis in Fig. 1 corresponding to both MGP (solid line) and GP (dotted line) cases for three different values of N: $N = 10^7$, $10^8$, and $10^9$. It clearly shows that for all N the difference between the GP and the MGP wave functions arises at the region where it reaches maximum, that is at the bottom of the potential well. Moreover, for $N = 10^7$ (Fig. 1a) and $10^8$ (Fig. 1b) the value of wave function near origin corresponding to the GP case is higher than that of MGP case. The difference is of the order 1% only. However, the situation becomes just opposite for the case of $N = 10^9$ (Fig. 1c). The reason for such change in wave function profile is the contribution of logarithmic term in the interatomic energy becoming appreciable at this N. As is already discussed that this term introduces negative correction to the interatomic energy and potential. Thus the logarithmic term gives rise to an attractive potential for the atoms in BEC at large N. Consequently, inclusion of this term in the interatomic energy (potential) brings atoms closer to the bottom of potential leading to the fact that more atoms are being found near origin than the GP case. Finally it is important to note here that the tail region of the wave function is not affected by the higher-order terms in the interatomic potential.

After having discussed results for isotropic trap we now describe the results for anisotropic trap which is more relevant from experimental point of view. For this calculation we employ the numbers for the asymmetry parameter and the axial frequency corresponding to the experiment of Anderson et al. [1]. Accordingly, $\lambda_0 = \sqrt{8}$ and
Table 3: Results for the ground-state of $^{87}$Rb atoms confined in anisotropic trap with $ \lambda_0 = \sqrt{8} $ and $ \omega_0^z/2\pi = 77.78 $ Hz. Chemical potentials and energies are in units of $ \hbar \omega_0^z $ and length is in units of $ a_{ho} $.

$$ \omega_0^z/2\pi = 220\,Hz. $$

The value of s-wave scattering length is same as that of isotropic case considered earlier. We present these results in Table 3. In this Table we compare the MGP results with the corresponding GP numbers. Similar to the isotropic case here also the virial relation Eq.(14) is satisfied up to 5-th decimal place. The trend in both chemical potential and total energy with increase in the number of particles is similar to that of isotropic case. The difference between the MGP and GP numbers are of the same order as that of isotropic case. Moreover, in the axially symmetric case also we find that our variational numbers are quite close to the numbers obtained via Eq.(22) and (23) especially for $ N > 10^6 $.

Thus we conclude that the variational results obtained for anisotropic trap are also quite accurate. Therefore, we demonstrate that by using variational approach described in this paper along with a judicious choice of ansatz for the ground-state wave function it is possible to obtain reasonably accurate results for the properties of BEC, even beyond mean-field approach, without much of a computational effort.

### 5 Conclusion

In this paper we have studied the properties of Bose gas confined in both isotropic and axially symmetric potential going beyond GP or mean-field approximation by taking higher-order terms in the interatomic interaction energy. We have used the variational approach to solve the MGP equation for wide range of particle numbers. We have verified our results using the generalized virial relation as well as by making analytic estimate of the corrections introduced by higher-order terms. These higher-order terms lead to correction in the total energy, chemical potential and other physical properties of BEC. The magnitudes of these corrections are of the order of $ 1\% - 2\% $ even for very large $ N $. However, there is qualitative change in the density profile of the condensate due to presence of the logarithimic term in the interaction energy. We also critically examine the
results in the literature and compare them with our numbers. Here we emphasize that the variational method employed by us gives quite accurate results with considerable computational ease.

It is well known that, corrections of this order are difficult to detect in the experimental situation. However, these small changes are also reflected in the collective excitation frequencies of BEC and these quantities can be measured with greater accuracy. Motivated by this we are now applying the variational approach and sum rule method of response theory of many-body systems [20, 21] to calculate collective excitation frequencies. These results will be presented in our future publication.
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Figure 1: Plot of the wavefunction along transverse direction for different values of $N$: (a) $N = 10^7$, (b) $N = 10^8$ and (c) $N = 10^9$. The solid and dashed curves correspond to solutions of GP and MGP equations respectively. The numbers along Y-axis are multiplied with a scaling factor of 1000.