Bose-Einstein Condensates in the Large Gas Parameter Regime

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Bose-Einstein condensates of $10^4$ $^{85}$Rb atoms in a cylindrical trap are studied using a recently proposed modified Gross-Pitaevskii equation. The existence of a Feshbach resonance allows for widely tuning the scattering length of the atoms, and values of the peak gas parameter, $x_{pk}$, of the order of $10^{-2}$ can be attained. We find large differences between the results of the modified Gross-Pitaevskii and of the standard Thomas–Fermi, and Gross-Pitaevskii equations in this region. The column densities at $z = 0$ may differ by as much as $\sim 30\%$ and the half maximum radius by $\sim 20\%$. The scattering lengths estimated by fitting the half maximum radius within different approaches can differ by $\sim 40\%$.

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Bose-Einstein condensation (BEC) of magnetically trapped alkali atoms has been achieved in several experimental setups, most of them in regimes where the atomic gas is considered to be very dilute, i.e. the average interatomic distance is much larger than the range of the interaction. As a consequence, the physics is dominated by two body collisions, generally well described in terms of the $s$-wave scattering length, $a$. The crucial parameter defining the condition of diluteness is the gas parameter, $x(\mathbf{r}) = n(\mathbf{r})a^2$, where $n(\mathbf{r})$ is the local density. For low values of the average gas parameter, $x_{av} \leq 10^{-3}$, the mean field Gross-Pitaevskii (GP) equation $[1]$ is the logical tool to study the system.

The gas parameter can be brought outside the regime of validity of the GP equation by two ways: either by increasing the number of atoms, $N$, in the condensate, or by changing their effective size. Recent experiments have explored both possibilities. On one side they have reached very large $N$ values, $N \sim 10^8$; on the other the scattering lengths have been widely tuned. The second approach promises to be much more efficient to reach large $x$ regions.

In a recent experiment performed at JILA $[2]$, it was possible to confine about $10^4$ atoms of $^{85}$Rb in a cylindrical trap. By exploiting the presence of a Feshbach resonance at a magnetic field of $B \sim 155$ Gauss, the scattering length was varied from negative to very high positive values. Actually, it was suggested some time ago $[3]$ that $a$ could be modulated by taking advantage of its expected strong variation in the vicinity of a magnetic induced Feshbach resonance in collisions between cold alkali atoms. Several experiments have supported this proposal by demonstrating this type of scattering length variation for several alkali atoms, as $^{85}$Rb, Cs and Na $[4-6]$. However, only very recently the Boulder group at JILA has been succesful in producing stable $^{85}$Rb condensates where $a$ can be effectively tuned over a very wide range.

To explore with confidence such regimes of high values of the parameter $x$, a necessary task is to investigate the accuracy of the GP equation. Moreover, to quantify the limitations of the GP description is of particular relevance since the empirical estimate of the scattering length is based upon the so called Thomas–Fermi (TF) approximation to the GP equation. The TF approximation amounts to disregard the kinetic energy term in the GP equation. The TF and GP results are expected to coincide for large $N$ and/or $a$ values. In the experimental analysis, a common procedure consists in measuring the column density, given by the integral of the particle density along a direction perpendicular to the simmetry axis of the trap, $n_c(z) = \int dx \; n(x,0,z)$. The $x$ direction coincides with that of the light beam used to image the atomic cloud. Then, the scattering length is inferred by finding the value of $a$ that, in the framework of the TF equation, provides a column density with the same experimental size.

In this paper, we will use a recently proposed modified Gross Pitaevskii equation (MGP) $[8]$ to estimate the corrections to the GP results. We begin by briefly recalling the derivation of the MGP equation. Then, in the simpler case of a spherical trap we will compare different approaches in a situation where the number of atoms and the frequency of the trap are kept fixed and the scattering length is allowed to vary in a representative range of values. This study is done to ascertain the degree of reliability of the MGP results. Finally, we will consider a cylindrical trap corresponding to the experimental situation. Depending on the value of the scattering length, the corrections to the GP results can be as large as 30\% for energy, chemical potential and $\sim 40\%$ for the extracted scattering length.

In the spherical case, the energy functional associated with the MGP equation:

$$E_{MGP}[\psi] = \int d r \left[ \frac{\hbar^2}{2m} | \nabla \psi(r) |^2 + \frac{m}{2} \omega^2 r^2 | \psi |^2 + \frac{2\pi \hbar^2 a}{m} | \psi |^4 + \frac{256\hbar^2}{15m} \sqrt{a^3} \pi | \psi | \right],$$  \hspace{1cm} (1)
is obtained in the local–density approximation by keeping the first two terms in the low density expansion for the energy density of a homogeneous system of hard-spheres, whose diameter coincides with the scattering length \[3\]:

\[
E = \frac{2\pi n^2 a^2 \hbar^2}{m} \left[ 1 + \frac{128}{15} \left( \frac{na^3}{\pi} \right)^{1/2} + 8 \left( \frac{4}{3} \pi - \sqrt{3} \right) (na^3) \ln(na^3) + O(na^3) \right].
\]

(2)

Up to this order of the expansion, the details of the potential do not show up, and any potential with the same scattering length would give identical results. This universal behavior has recently been checked by a diffusion Monte Carlo calculation (DMC) \[14\], providing the exact solution of the many–body Schrödinger equation. In Refs. \[3,10,11\], it was shown that, for a uniform system, the first term of the expansion is accurate only at very low values of \(x\), while the addition of the second term gives a good representation of the exact DMC results up to \(x = 10^{-2}\). The inclusion of the logarithmic term severely spoils the agreement already at intermediate \(x\)-values and therefore it has not been incorporated into the functional energy, \(E_{MGP}[\psi]\). In the same references it was also shown that the energy functional computed in hypernetted chain (HNC) theory, explicitly taking into account the interatomic correlations induced by the potential, provided a description very close to the MGP one.

It is convenient to simplify the notation by expressing lengths and energies in harmonic oscillator (HO) units. The spatial coordinates, the energy, and the wave functions are rescaled as \(r = a_{HO} r, E = \hbar \omega E_1, \) and \(\Psi(r) = (N/a_{HO}^3)^{1/2} \Psi_1(r_1), \) where \(\Psi_1(r_1)\) is normalized to unity and \(a_{HO} = (\hbar/m\omega)^{1/2}. \) Using these new variables and performing a functional variation of \(E_{MGP}[\psi]\), one gets the modified Gross–Pitaevskii equation,

\[
\left[ -\frac{1}{2} \nabla^2 - \frac{1}{2} \frac{1}{\omega_0^2} + 4\pi a_1 N \left| \psi_1(r_1) \right|^2 + \sqrt{\pi a_1^2 N^3} \frac{128}{3} \left| \psi_1(r_1) \right|^3 \right] \psi_1(r_1) = \mu_1 \psi_1(r_1),
\]

(3)

where \(a_1 = a/a_{HO}\) and \(\mu_1\) is the chemical potential in HO units. The GP approximation is recovered by dropping the \(\left| \psi_1(r_1) \right|^3\) term.

Table \[5\] gives some results for \(N = 10^4 85\) Rb atoms confined in a spherical trap with an oscillator angular frequency \(\omega_{HO}/2\pi = (\omega_0^2 \omega_r)^{1/2}/2\pi = 12.77\) Hz, where \(\omega_0/2\pi = 17.5\) Hz and \(\omega_r/2\pi = 6.9\) Hz are the radial and axial frequencies associated with the external potential of the cylindrical trap used in Ref. \[3\]. In the table we study the dependence of the energy per particle and of the chemical potential on the scattering length, given in units of the Bohr radius of the Hydrogen atom, \(a_0\). For this trap, \(a_{HO} = 57657 a_0\). We also show the TF results. In this approximation it is often possible to derive simple analytical expressions \[12\], useful to get quick estimates of several quantities. For instance, \(\mu_1^{TF} = 1/2 (15a_1 N)^{2/5}\). Also reported are the peak values of the gas parameter, \(x_{pk} = n(0) a^3 = Na_1^3 \left| \psi_1(0) \right|^2\), whose TF estimate is \(x_{pk}^{TF} = (15^2 a_1^2 N^2)^{1/5}/(8\pi)\).

At low values of the scattering length, MGP corrections are small and the TF approach to the GP equation is not fully satisfactory. As expected, the TF and GP results are much closer when \(a\) increases and the MGP corrections become important and of the order of 30\% at the largest value of \(a = 10000 a_0\). \(x_{pk}\) increases with \(a\). The MGP density distribution gets wider and \(\lambda_{pk}^{MGP}\) is depressed with respect to both TF and GP because of the repulsive character of the extra term in the MGP equation. The HNC results are comfortably close to the MGP ones, supporting the use of only the latter approach in the remaining of the paper.

An analogous behavior is found in the anisotropic case. The results for the cylindrical trap used in the experiments are given in Table \[11\]. Most of the TF results are again analytical. The HO units in the cylindric case are: \(r = a_{c,HO} R, E = \hbar \omega E_1, \Psi(r) = (N/a_{c,HO}^3)^{1/2} \Psi_1(r_1), \) and \(a_{c,HO} = (\hbar/m\omega_c)^{1/2}. \) The trap deformation parameter is \(\lambda = \omega_r/\omega_c = 0.39\).

An accessible experimental quantity connected to the density profile is the already defined column density. Its TF expression is

\[
n^{-1}_c^{TF}(z_1) = \frac{2}{12 \pi a_{c} N} \left[ 2(\mu_1^{TF} - \frac{1}{2} \lambda^2 z_1^2) \right]^{3/2}.
\]

(4)

A measure of the extension of the condensate is the half maximum radius of the column density, \(R_{1/2}\), defined as the \(z_1\) value where \(n_c(z_1 = R_{1/2}) = \frac{1}{2} n_c(0)\). Also interesting is the full strength at half maximum, FSHM, given by the integrated strength of the column between the \(\pm R_{1/2}\) values.

In Fig. \[5\] we show the column densities in different approaches, for the same set of scattering lengths reported in the Tables. The solid and dashed lines correspond to the MGP and TF results, respectively; stars are the GP densities; the triangles in the two upper panels give \(n_c(z_1)\) evaluated in MGP, but changing the scattering length to reproduce \(R_{1/2,TF}\), supposedly corresponding to the measured radius. The two values are \(a/a_0 = 5920\) for \(R_{1/2,TF}=10.20\) and \(a/a_0 = 4940\) for \(R_{1/2,TF}=9.75\) and the related MGP columns are practically identical to the TF ones.
The GP and TF results almost coincide and the MGP corrections are more sizeable at the two largest values of $a$, where $x_{pk}$ becomes of the order of $10^{-2}$. Because of the repulsive nature of the MGP extra term, $R_{1/2, MGP}$ is larger than $R_{1/2, TF}$, while FSHM$_{MGP}$ is smaller than FSHM$_{TF}$, and for low $z_1$-values $n_c^{MGP}(z_1)$ lies below $n_c^{TF}(z_1)$. A smaller scattering length is required to reproduce $R_{1/2, TF}$ and FSHM$_{TF}$ in the MGP approach in the high $x_{pk}$ region. In fact, we find a reduction of $\sim 40\%$ of $a/a_0$. This analysis shows that using the TF column density to extract the scattering length in the large gas parameter regime could lead to severe overestimates in this kind of trap geometry.

The lower panels of the figure roughly correspond to $x_{pk} \sim 10^{-3} - 10^{-4}$. As expected, the MGP corrections are smaller and the computed $R_{1/2}$ values become closer when $a/a_0$ decreases.

Fig. 3 shows the scattering length as a function of FSHM and $R_{1/2}$ for the cylindrical trap within the three methods we have analyzed. The figure stresses that, depending on the FSHM and $R_{1/2}$ values and on the approach, the estimates of $a$ can differ by up to 40%.

In conclusion, we find that the MGP equation induces corrections of 30% in the ground state properties of the condensate, when the conditions of the JILA experiments for $^{85}$Rb are considered. Comparable corrections are obtained for the column densities, where large differences between the MGP and the standard TF and GP results may be found. These differences appear to be relevant for the extraction of the scattering length when large values of the gas parameter come into play. MGP is still a mean field theory, since it tries to incorporate correlation effects into the average single particle potential. However, we believe that its predictions are probably indicative at those regimes attained in recent experiments.

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TABLE I. Ground state properties of $N = 10^4{^{85}}$Rb atoms confined in a spherical trap ($\omega/2\pi=12.77$ Hz) in different approaches. $\mu_1=$chemical potential, $E_1/N=$energy per atom, $x_{pk}=$peak gas parameter. Energies in HO units.

| $a/a_0$ | 1400 | 3000 | 8000 | 10000 |
|---|---|---|---|---|
| $\mu_1^{TF}$ | 13.29 | 18.02 | 26.00 | 29.18 |
| $\mu_1^{GP}$ | 13.41 | 18.12 | 26.75 | 29.24 |
| $\mu_1^{MGP}$ | 13.95 | 19.82 | 33.34 | 38.01 |
| $\mu_1^{HNC}$ | 13.90 | 19.66 | 33.33 | 38.41 |
| $E_1^{TF}/N$ | 9.50 | 12.87 | 18.57 | 20.84 |
| $E_1^{GP}/N$ | 9.66 | 13.01 | 19.16 | 20.93 |
| $E_1^{MGP}/N$ | 10.00 | 14.09 | 23.40 | 26.60 |
| $E_1^{HNC}/N$ | 9.97 | 13.98 | 23.24 | 26.59 |
| $x_{pk}^{TF}$ | $6.23 \times 10^{-4}$ | $3.88 \times 10^{-3}$ | $4.09 \times 10^{-2}$ | $6.98 \times 10^{-2}$ |
| $x_{pk}^{GP}$ | $6.26 \times 10^{-4}$ | $3.89 \times 10^{-3}$ | $4.09 \times 10^{-2}$ | $6.99 \times 10^{-2}$ |
| $x_{pk}^{MGP}$ | $5.70 \times 10^{-4}$ | $3.18 \times 10^{-3}$ | $2.59 \times 10^{-2}$ | $4.10 \times 10^{-2}$ |
| $x_{pk}^{HNC}$ | $5.75 \times 10^{-4}$ | $3.24 \times 10^{-3}$ | $2.52 \times 10^{-2}$ | $3.85 \times 10^{-2}$ |

TABLE II. Ground state properties of $N = 10^4{^{85}}$Rb atoms in the cylindrical trap described in the paper. Energies in HO units.

| $a/a_0$ | 1400 | 3000 | 8000 | 10000 |
|---|---|---|---|---|
| $\mu_1^{TF}$ | 9.70 | 13.15 | 19.47 | 21.29 |
| $\mu_1^{GP}$ | 9.82 | 13.25 | 19.55 | 21.36 |
| $\mu_1^{MGP}$ | 10.22 | 14.51 | 24.38 | 27.79 |
| $E_1^{TF}/N$ | 6.93 | 9.39 | 13.91 | 15.21 |
| $E_1^{GP}/N$ | 7.08 | 9.52 | 14.00 | 15.29 |
| $E_1^{MGP}/N$ | 7.33 | 10.31 | 17.09 | 19.43 |
| $x_{pk}^{TF}$ | $6.23 \times 10^{-4}$ | $3.88 \times 10^{-3}$ | $4.09 \times 10^{-2}$ | $6.98 \times 10^{-2}$ |
| $x_{pk}^{GP}$ | $6.28 \times 10^{-4}$ | $3.90 \times 10^{-3}$ | $4.10 \times 10^{-2}$ | $7.00 \times 10^{-2}$ |
| $x_{pk}^{MGP}$ | $5.72 \times 10^{-4}$ | $3.19 \times 10^{-3}$ | $2.60 \times 10^{-2}$ | $4.10 \times 10^{-2}$ |
FIG. 1. Column densities at four values of the scattering length for the cylindrical trap. Dashed lines= TF, stars= GP, solid lines= MGP. The triangles in the first (second) upper panel give the MGP column density at $a/a_0=5920$ (4940).
FIG. 2. Scattering length as a function of the full strength at half maximum (left) and of the half maximum radius (right) in the cylindrical trap. Circles, stars and triangles correspond to the TF, GP and MGP results, respectively. Lines are a guide to the eyes.