Beyond the Thomas-Fermi Approximation for Nonlinear Dynamics of Trapped Bose-Condensed Gases
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Abstract

We present an analytical approximation for nonlinear dynamics of trapped Bose-condensed gases. The new approximation is a substantial improvement over the Thomas-Fermi approximation and is shown to be applicable for systems with a rather small number of atoms $N$. The calculated aspect ratios after ballistic expansion are found to be in good agreement with those observed in recent experiments.

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The newly created Bose-Einstein condensates (BEC) of weakly interacting alkali-metal atoms [1] stimulated a large number of theoretical investigations (see recent reviews [2]). A mean-field approach, based on the time-dependent Gross-Pitaevskii (GP) equation [3], is the most widely used theory for nonlinear dynamics of trapped Bose-condensed gases at zero temperature.

In the limit of a large number of atoms \( N \), the determination of the condensate wave function is simplified by neglecting the kinetic energy term. This approximation is known as the Thomas-Fermi (TF) approximation [4,5]. It has been used quite extensively [7-13], including the explicit time evolution of the condensate (shape of profiles, aspect ratio etc.) during the expansion after switching off the trap [7,9]. We note that the validity of the TF approximation depends not only on the number of atoms \( N \), but also depends on properties of the traps.

In this letter we develop an analytical approximation which is a substantial improvement over the TF results for rather small number of atoms \( N \). The aspect ratios calculated from the new approximation method are also found to be in good agreement with those observed in recent experiments [14].

In the mean-field approximation, the ground state energy of the system is given by the Ginzburg-Pitaevskii-Gross (GPG) energy functional [3,15]

\[
\frac{E}{N} = \langle \Psi \mid \sum_{i=1}^{3} H_i \mid \Psi \rangle + \frac{gN}{2} \int | \Psi |^4 \, d\vec{r},
\]

(1)

with

\[
H_i = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{m\omega_i^2}{2} x_i^2,
\]

(2)

and \( g = 4\pi \hbar^2 a/m \), where \( a \) is the S-wave scattering length, \( N \) is the number of atoms in the BEC, and \( \Psi \) is the condensate wave function normalized as \( \int | \Psi |^2 \, d\vec{r} = 1 \).

We introduce an auxiliary Hamiltonians

\[
\tilde{H}_i = \frac{\hbar \omega_i}{2} \sqrt{\gamma_i} + \frac{m\omega_i^2}{2} (1 - \gamma_i) x_i^2,
\]

(3)

where \( \gamma_i \) are parameters, \( 0 \leq \gamma_i < 1 \), and rewrite Eq.(1) as

\[
\frac{E}{N} = \langle \Psi \mid \sum_{i=1}^{3} (H_i - \tilde{H}_i) \mid \Psi \rangle + \langle \Psi \mid \sum_{i=1}^{3} \tilde{H}_i \mid \Psi \rangle + \frac{gN}{2} \int | \Psi |^4 \, d\vec{r}.
\]

(4)
Omission of $<\Psi | \sum_{i=1}^{3} (H_i - \tilde{H}_i) | \Psi >$ in Eq.(4) yields our approximation for the ground state,

$$\frac{E}{N} = \frac{3}{N} \sum_{i=1}^{3} \frac{\hbar \omega_i}{2} \sqrt{\gamma_i} + \frac{E_{TF}(\tilde{\omega}_x, \tilde{\omega}_y, \tilde{\omega}_z)}{N},$$

(5),

$$\mu = \frac{3}{N} \sum_{i=1}^{3} \frac{\hbar \omega_i}{2} \sqrt{\gamma_i} + \mu_{TF}(\tilde{\omega}_x, \tilde{\omega}_y, \tilde{\omega}_z),$$

(6)

and

$$\rho(\vec{r}) = \rho_{TF}(\tilde{\omega}_x, \tilde{\omega}_y, \tilde{\omega}_z),$$

(7)

where $\tilde{\omega}_i = \sqrt{1 - \gamma_i \omega_i}$. $E_{TF}, \mu_{TF},$ and $\rho_{TF}$ are the Thomas-Fermi energy, chemical potential, and density, respectively, which are given by

$$E_{TF}(\omega_x, \omega_y, \omega_z) = \frac{5}{14} \frac{N}{4\pi} \frac{15}{16} \omega_x \omega_y \omega_z m^{3/2} g N^{2/5},$$

(8)

$$\mu_{TF}(\omega_x, \omega_y, \omega_z) = \frac{1}{2} \frac{15}{4\pi} \frac{3}{4} \omega_x \omega_y m^{3/2} g N^{2/5},$$

(9)

and

$$\rho_{TF}(\omega_x, \omega_y, \omega_z, \vec{r}) = \frac{\mu_{TF}(\omega_x, \omega_y, \omega_z)}{Ng} \left(1 - \sum_{i=1}^{3} \left(\frac{x_i}{R_{TF}^i}\right)^2\right) \theta \left(1 - \sum_{i=1}^{3} \left(\frac{x_i}{R_{TF}^i}\right)^2\right),$$

(10)

where

$$\left(R_{TF}^i\right)^2 = \frac{2\mu_{TF}(\omega_x, \omega_y, \omega_z)}{m \omega_i^2}. $$

(11)

Projecting $| \Psi >$ on the complete basis states $| n >$, obtained from $h_i = -\frac{\hbar^2}{2m x_i^2} + \frac{m \omega_i^2}{2} x_i^2$, and $h_i | n > = \epsilon_n | n >$, we get

$$< \Psi | h_i | \Psi >= \sum_n \epsilon_n < \Psi | n > | n >= \sum_n |\Psi > | n > > \epsilon_1 = \frac{\hbar \omega_i \sqrt{\gamma_i}}{2}. $$

(12)

Therefore, we conclude that our approximation for energy, given by Eq.(5), is a lower bound to the ground state energy, Eq.(4). Therefore a set of the optimal values of parameters $\gamma_i$ which maximizes the energy, Eq.(5), will yield an optimal value for the ground-state energy given by

$$\frac{E}{N} = \max_{\gamma_x, \gamma_y, \gamma_z} \left[ \sum_{i=1}^{3} \frac{\hbar \omega_i}{2} \sqrt{\gamma_i} + \frac{5}{14} \frac{15}{4\pi} g N m^{3/2} \prod_{i=1}^{3} ((1 - \gamma_i \omega_i))^{2/5} \right]. $$

(13)

Since the TF approximation corresponds to the case of $\gamma_i = 0$, we have

$$E_{TF} \leq E \leq E_{exact},$$

(14)

where $E_{exact}$ is the exact mean-field energy.
To study the validity of our approximation, we consider an example of the ground state of $^{87}$Rb atoms in a harmonic trap, as investigated in Ref.[16] with the S-wave triplet-spin scattering length $a = 100a_B$, where $a_B$ is the Bohr radius, the axial frequency $\omega_z/2\pi = 220\text{Hz}$, and asymmetry parameter $\lambda = \omega_z/\omega_\perp = \sqrt{8}$, where $\omega_x = \omega_y = \omega_\perp$.

Using our approximation, we calculate the energy per particle, $E/N$, the chemical potential $\mu$, and the average transverse sizes $\sqrt{x^2}$ and vertical sizes $\sqrt{z^2}$, using Eqs. (5-6,13). The calculated results are compared with those obtained from the numerical solutions of the GP equation, $E_{num}/N$, $\mu_{num}$, $\sqrt{x^2}_{num}$ and $\sqrt{z^2}_{num}$ [16] in Table I, and with those obtained in the TF approximation $E_{TF}/N$, $\mu_{TF}$, $\sqrt{x^2}_{TF}$ and $\sqrt{z^2}_{TF}$ in Table II. These comparisons show that our analytical approximation greatly improves the TF results for a rather small number $N$. For $100 \leq N \leq 20000$, the difference between our results and those of the numerical solution of the GP equation [16] are less than 3%.

Let us now turn to application of our approximation for the time-dependent problems. Consider the BEC with the time-dependent harmonic potential $V_t = (m/2) \sum_{i=1}^{3} \omega_i^2(t)x_i^2$. In Ref.[7] the following anzatz

$$\Psi(\vec{r}, t) = \Phi(x_1/\lambda_1, x_2/\lambda_2, x_3/\lambda_3, t) \sqrt{\lambda_1\lambda_2\lambda_3} \exp[-i\beta(t) + im \sum_{i=1}^{3} x_i^2 \lambda_i/2\hbar \lambda_i]$$

(15)

has been used for the solution of the time-dependent GP equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi + V_t(\vec{r}, t)\Psi + Ng |\Psi|^2 \Psi \quad (16)$$

(a similar treatment for isotropic traps has been developed in Ref.[17]). We choose $\beta$ and $\lambda$ satisfying the following equations

$$\hbar \dot{\beta} = \sum_{k=1}^{3} \hbar \omega_k \sqrt{1 - \gamma_k} \left( \frac{\mu_{TF} \tilde{\omega}_x \tilde{\omega}_y \tilde{\omega}_z}{\lambda_1 \lambda_2 \lambda_3} \right), \quad \beta(0) = 0,$$

(17)

and

$$\lambda_k \dot{\lambda}_k + \lambda_k^2 \omega_k^2(t) - \frac{\omega_k^2 \gamma_k}{\lambda_k^2} = \frac{1 - \gamma_k}{\lambda_1 \lambda_2 \lambda_3} \omega_k^2, \quad \lambda_k(0) = 1, \quad \dot{\lambda}_k(0) = 0,$$

(18)

with $\omega_k = \omega_k(0)$, and $\tilde{\omega}_k = \sqrt{1 - \gamma_k \omega_k}$. For a special case of $\gamma_k = 0$, the above choices of $\beta$ and $\lambda_k$ reduce to those of Ref.[7]. With substitutions of Eqs.(15,17-18), Eq.(16) becomes

$$i\hbar \frac{\partial \Phi}{\partial t} = \sum_{k=1}^{3} \frac{H_k - \tilde{H}_k}{\lambda_k^2} \Phi + \frac{1}{\lambda_1 \lambda_2 \lambda_3} \left[ -\mu_{TF} (\tilde{\omega}_x \tilde{\omega}_y \tilde{\omega}_z) + \frac{m}{2} \sum_{k=1}^{3} x_k^2 \tilde{\omega}_k^2 + Ng |\Phi|^2 \right] \Phi,$$

(19)
with the initial condition \( \Phi(\vec{r}, 0) = \Psi(\vec{r}, 0) \), where \( \Psi(\vec{r}, 0) \) is a solution of the time-independent mean-field equation

\[
-\frac{\hbar^2}{2m} \Delta \Psi(\vec{r}, 0) + V_\ell(\vec{r}, 0) \Psi(\vec{r}, 0) + Ng \mid \Psi(\vec{r}, 0) \mid^2 \Psi(\vec{r}, 0) = \mu \Psi(\vec{r}, 0). \tag{20}
\]

By neglecting \( \sum_{k=1}^{3} \frac{H_k - \tilde{H}_k}{\lambda_k} \) in Eq. (19), we obtain a generalization of our approximation, Eqs.(5-7,13) to the time-dependent problem

\[
\mid \Psi(\vec{r}, t) \mid^2 = \frac{\rho_T F(\tilde{\omega}_x, \tilde{\omega}_y, \tilde{\omega}_z, x_1/\lambda_1(t), x_2/\lambda_2(t), x_3/\lambda_3(t))}{\lambda_1(t) \lambda_2(t) \lambda_3(t)}, \tag{21}
\]

where all the dynamics is in the evolution of the scaling parameters \( \lambda_k \), Eq.(18).

For the case \( \omega_x = \omega_y = \omega_\perp \) and \( \lambda_1 = \lambda_2 = \lambda_\perp \), the aspect ratio of the cloud in our approximation is given by

\[
R(t) = \frac{\sqrt{x^2(t)}}{z^2(t)} = \frac{\omega_\perp \lambda_\perp(t) \sqrt{1 - \gamma_\perp}}{\omega_\perp \lambda_\perp(t) \sqrt{1 - \gamma_\perp}}. \tag{22}
\]

As an example, we consider application of the above results to the experimental data with \(^{23}\text{Na}\) atoms obtained in the Ioffe-Pritchard type magnetic trap with radial and axial trapping frequencies of \( \omega_\perp/(2\pi) = 360 \text{ Hz} \) and \( \omega_z/(2\pi) = 3.5 \text{ Hz} \) [14], respectively. In our analysis we use \( a = 2.75 \text{nm}, t = 4 \text{ ms}, \) and \( a/a_\perp = 2.488 \times 10^{-3} \), where \( a_\perp = \sqrt{\hbar/m \omega_\perp} \). As in Ref. [7] we consider a sudden and total opening of the trap at \( t = 0 \). For this case Eq. (17) becomes

\[
\frac{d^2 \lambda_\perp}{d\tau^2} = \frac{\gamma_\perp}{\lambda_\perp^3} + \frac{1 - \gamma_\perp}{\lambda_\perp^3 \lambda_z}, \tag{23}
\]

\[
\frac{d^2 \lambda_z}{d\tau^2} = \left( \frac{\gamma_z}{\lambda_z^2} + \frac{1 - \gamma_z}{\lambda_\perp \lambda_z} \right) \epsilon^2, \tag{24}
\]

where \( \tau = \omega_\perp t \) and \( \epsilon = \omega_z/\omega_\perp \ll 1 \).

To the zero-th order in \( \epsilon \), we have \( \lambda_z = 1 \) and \( \lambda_\perp = \sqrt{1 + \tau^2} \). For the experimental conditions [14], the terms in \( \epsilon^2 \) are negligible.

In Table III, we give the calculated values of the aspect ratio \( R(t) \) of the \(^{23}\text{Na}\) atoms cloud, after ballistic expansion of \( t = 4 \) ms, and the calculated values of parameters \( \gamma_\perp \) and \( \gamma_z \) which we fix from Eq.(13) , with \( \omega_i = \omega_i(0) \). One can easily see that the TF approximation is valid \( (\gamma_z \approx 0) \) along the long axis of the cloud, but not in the radial direction \( (\gamma_\perp \neq 0) \), as has been noted already in Ref. [18].
Our calculated results for $R(t)$ are compared with the recent experimental data [14] in Figure 1. This comparison shows that our predictions for the aspect ratio $R(t)$ are in good agreement with experimental data obtained by the MIT group [14].

In conclusion, we have developed an analytical approximation which provides a substantial improvement over the TF approximation for nonlinear dynamics of trapped Bose-condensed gases for a rather small number of atoms $N$. The approximation is very useful since it provides an easy quantitative tool for the analysis of experiments on trapped condensed gases.

We are grateful to the group at MIT for providing us with the experimental data.
Table I. Comparison of the results of our approximation for the ground state of $^{87}$Rb atoms, calculated from Eqs.(5-6,13) and those obtained from the numerical solutions of the GP equation [16]. Chemical potential and energy are in units of $\hbar\omega\bot$, and length is in units of $\sqrt{\hbar/m\omega\bot}$.

| $N$ | $E/N$ | $\mu$ | $\sqrt{x^2}$ | $\sqrt{z^2}$ | $E_{num}/N$ | $\mu_{num}$ | $\sqrt{x^2}_{num}$ | $\sqrt{z^2}_{num}$ |
|-----|-------|-------|---------------|---------------|--------------|--------------|-------------------|-------------------|
| 100 | 2.63  | 2.82  | 0.78          | 0.43          | 2.66         | 2.88         | 0.79              | 0.44              |
| 200 | 2.80  | 3.13  | 0.83          | 0.45          | 2.86         | 3.21         | 0.85              | 0.45              |
| 500 | 3.22  | 3.82  | 0.94          | 0.47          | 3.30         | 3.94         | 0.96              | 0.47              |
| 2000| 4.49  | 5.49  | 1.21          | 0.53          | 4.61         | 5.93         | 1.23              | 0.53              |
| 5000| 5.99  | 8.00  | 1.46          | 0.59          | 6.12         | 8.14         | 1.47              | 0.59              |
| 10000| 7.63 | 10.4  | 1.68          | 0.65          | 7.76         | 10.5         | 1.69              | 0.65              |
| 15000| 8.84 | 12.1  | 1.83          | 0.69          | 8.98         | 12.2         | 1.84              | 0.70              |
| 20000| 9.84 | 13.5  | 1.94          | 0.72          | 9.98         | 13.7         | 1.94              | 0.73              |

Table II. Results of the TF approximation for the same case as Table I.

| $N$ | $E_{TF}/N$ | $\mu_{TF}$ | $\sqrt{x^2}_{TF}$ | $\sqrt{z^2}_{TF}$ |
|-----|------------|-------------|-------------------|-------------------|
| 100 | 1.44       | 1.60        | 0.68              | 0.24              |
| 200 | 1.51       | 2.11        | 0.78              | 0.27              |
| 500 | 2.18       | 3.05        | 0.93              | 0.33              |
| 2000| 3.79       | 5.31        | 1.23              | 0.44              |
| 5000| 5.47       | 7.66        | 1.48              | 0.52              |
| 10000| 7.22 | 10.1        | 1.70              | 0.60              |
| 15000| 8.49 | 11.9        | 1.84              | 0.65              |
| 20000| 9.53 | 13.3        | 1.95              | 0.69              |
Table III. Calculated aspect ratio of the $^{23}Na$ atoms cloud, using Eq.(22), after a ballistic expansion of $t = 4$ ms, as a function of $N$. $N$ is in units of $10^5$.

| $N$  | $R(t)$ | $\gamma_\perp$ | $\gamma_z$ |
|------|--------|----------------|-----------|
| 1.2  | 0.110  | 0.354          | 0.0       |
| 0.8  | 0.117  | 0.426          | 0.0       |
| 0.4  | 0.132  | 0.551          | 0.0       |
| 0.1  | 0.183  | 0.766          | 0.0       |
FIG. 1. Aspect ratio $R$ of the $^{23}\text{Na}$ atom cloud after a ballistic expansion of $t = 4\text{ms}$, as a function of the number of atoms $N$, with $\omega_{\perp}(0) = 2\pi \times 360\text{Hz}$, $\omega_{\parallel}(0) = 2\pi \times 3.5 \text{ Hz}$. Diamonds, dashed line, and circular dots represent the results of theoretical calculations using Eq.(22), the TF approximation, and experimental data from MIT group [14], respectively.
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