Approximation for nonlinear dynamics of trapped Bose-Einstein condensates

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(Received 24 July 2001; published 30 January 2002)

We present an analytical approximation for nonlinear dynamics of trapped Bose-Einstein condensates. The 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. The approximation is useful in providing a simple and easy quantitative computational tool for the analysis of experimental data.

DOI: 10.1103/PhysRevA.65.035601 PACS number(s): 03.75.Fi, 05.30.Jp

The newly created Bose-Einstein condensates (BEC) of weakly interacting alkali-metal atoms [1] stimulated a huge 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 BEC at zero temperature.

In the limit of a large number of *N* of atoms, the determination of the condensate wave function is simplified by neglecting the kinetic-energy term. This approximation, known as the Thomas-Fermi (TF) approximation [4,5], was used quite extensively [6–13], 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 on properties of the traps.

In this Brief Report, we develop an analytical approximation that is a substantial improvement over the TF results for a 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]. The approximation is very useful since it provides a simple quantitative tool for the analysis of experimental data for trapped condensed gases.

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

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

with

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

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 Ψ is the condensate wave function normalized as $\int|\Psi|^2 d\vec{r}=1$.

We introduce auxiliary Hamiltonians

$$\tilde{H}_i=\frac{\hbar\omega_i}{2}\sqrt{\gamma_i}+\frac{m\omega_i^2}{2}(1-\gamma_i)x_i^2, \tag{3}$$

where γ_i are parameters, $0\leqslant\gamma_i<1$, and we rewrite Eq. (1) as

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

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

$$\frac{E}{N}=\sum_{i=1}^{3}\frac{\hbar\omega_i}{2}\sqrt{\gamma_i}+\frac{E_{\rm TF}(\tilde{\omega}_x,\tilde{\omega}_y,\tilde{\omega}_z)}{N}, \tag{5}$$

$$\mu=\sum_{i=1}^{3}\frac{\hbar\omega_i}{2}\sqrt{\gamma_i}+\mu_{\rm TF}(\tilde{\omega}_x,\tilde{\omega}_y,\tilde{\omega}_z), \tag{6}$$

and

$$\rho(\vec{r})=\rho^{\rm TF}(\tilde{\omega}_x,\tilde{\omega}_y,\tilde{\omega}_z,\tilde{r}), \tag{7}$$

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

$$E_{\rm TF}(\omega_x,\omega_y,\omega_z)=\tfrac{5}{14}N\left(\frac{15}{4\pi}\omega_x\omega_y\omega_z m^{3/2}gN\right)^{2/5}, \tag{8}$$

$$\mu_{\rm TF}(\omega_x,\omega_y,\omega_z)=\frac{1}{2}\left(\frac{15}{4\pi}\omega_x\omega_y\omega_z m^{3/2}gN\right)^{2/5}, \tag{9}$$

and

$$\rho^{\rm TF}(\omega_x,\omega_y,\omega_z,\vec{r})=\frac{\mu_{\rm TF}(\omega_x,\omega_y,\omega_z)}{Ng}\left[1-\sum_{i=1}^{3}\left(\frac{x_i}{R_i^{\rm TF}}\right)^2\right]\times\theta\left[1-\sum_{i=1}^{3}\left(\frac{x_i}{R_i^{\rm TF}}\right)^2\right], \tag{10}$$

where

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TABLE I. Comparison of the results of our approximation for the ground state of ^{87}Rb atoms, calculated from Eqs. (5), (6), and (13) and those obtained from numerical solutions of the GP equation [16]. Chemical potential and energy are in units of $\hbar\omega_\perp$, and length is in units of $\sqrt{\hbar/m\omega_\perp}$.

N	E/N	μ	$\sqrt{\overline{x^2}}$	$\sqrt{\overline{z^2}}$	$E_{\rm num}/N$	$\mu_{\rm num}$	$\sqrt{\overline{x^2_{\rm num}}}$	$\sqrt{\overline{z^2_{\rm num}}}$
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

$$(R_i^{\rm TF})^2=\frac{2\mu_{\rm TF}(\omega_x,\omega_y,\omega_z)}{m\omega_i^2}. \tag{11}$$

Projecting $|\Psi\rangle$ on the complete basis states $|n\rangle$, obtained from $h_i=-(\hbar^2/2m)(\partial^2/x_i^2)+(m\omega_i^2\gamma_i/2)x_i^2$, and $h_i|n\rangle=\epsilon_n|n\rangle$, we get

$$\langle\Psi|h_i|\Psi\rangle=\sum_n \epsilon_n|\langle\Psi|n\rangle\langle n|\Psi\rangle|\geqslant\epsilon_1=\frac{\hbar\omega_i\sqrt{\gamma_i}}{2}. \tag{12}$$

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 γ_i which maximizes the energy, Eq. (5), will yield an optimal value for the ground-state energy given by

$$\frac{E}{N}=\max_{\gamma_x,\gamma_y,\gamma_z}\left[\sum_{i=1}^{3}\frac{\hbar\omega_i}{2}\sqrt{\gamma_i}+\frac{5}{14}\times\left(\frac{15}{4\pi}gNm^{3/2}\prod_{i=1}^{3}[(1-\gamma_i)\omega_i]\right)^{2/5}\right]. \tag{13}$$

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

$$E_{\rm TF}\leqslant E\leqslant E_{\rm exact}, \tag{14}$$

where $E_{\rm exact}$ is the exact GP 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 $\omega_z/2\pi=220$ Hz, and the 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 μ, and the average transverse sizes $\sqrt{\overline{x^2}}$ and vertical sizes $\sqrt{\overline{z^2}}$, using Eqs. (5), (6), and (13). The calculated results are compared with those obtained from the numerical solutions of the GP equation, $E_{\rm num}/N$, $\mu_{\rm num}$, $\sqrt{\overline{x^2_{\rm num}}}$, and $\sqrt{\overline{z^2_{\rm num}}}$ [16] in Table I, and with those obtained in the TF approximation $E_{\rm TF}/N$, $\mu_{\rm TF}$, $\sqrt{\overline{x^2_{\rm TF}}}$, and $\sqrt{\overline{z^2_{\rm TF}}}$ in Table II. These comparisons show that our analytical approximation greatly improves the TF results for a rather small number N. For $100\leqslant N\leqslant 20\,000$, the difference between our results and those of the numerical solution of the GP equation [16] is less than 3%.

We also give in Table II values of the TF parameter $Na/a_{\rm ho}$, where $a_{\rm ho}$ is the typical length of harmonic confinement, $a_{\rm ho}=\sqrt{\hbar/(m\omega_{\rm ho})}$, with $\omega_{\rm ho}=(\omega_\perp^2\omega_z)^{1/3}$. It is conventionally assumed that this parameter needs to be large in order for the TF approximation to be valid. For $Na/a_{\rm ho}\approx 100$ ($N=20\,000$), the difference between the TF result and the exact GP calculation is about 5% for $\sqrt{\overline{x^2}/\overline{z^2}}$.

We now turn to an application of our approximation for

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

N	$E_{\rm TF}/N$	$\mu_{\rm TF}$	$\sqrt{\overline{x^2_{\rm TF}}}$	$\sqrt{\overline{z^2_{\rm TF}}}$	$Na/a_{\rm ho}$
100	1.44	1.60	0.68	0.24	0.5
200	1.51	2.11	0.78	0.27	1.0
500	2.18	3.05	0.93	0.33	2.6
2000	3.79	5.31	1.23	0.44	10
5000	5.47	7.66	1.48	0.52	26
10000	7.22	10.1	1.70	0.60	51
15000	8.49	11.9	1.84	0.65	77
20000	9.53	13.3	1.95	0.69	103

the time-dependent problems. Consider the BEC with the time-dependent harmonic potential $V_t=(m/2)\Sigma_{i=1}^{3}\omega_i^2(t)x_i^2$.

When the substitution [7] of

$$\Psi(\vec{r},t)=\frac{\Phi(x_1/\lambda_1,x_2/\lambda_2,x_3/\lambda_3,t)}{\sqrt{\lambda_1\lambda_2\lambda_3}}\times\exp\left(-i\beta(t)+im\sum_{i=1}^{3}\frac{x_i^2}{2\hbar}\frac{\dot{\lambda}_i}{\lambda_i}\right), \quad (15)$$

where β and λ are solutions of the equations

$$\hbar\dot{\beta}=\sum_{k=1}^{3}\frac{\hbar\omega_k\sqrt{\gamma_k}}{2\lambda_k^2}-\frac{\mu_{\rm TF}(\tilde{\omega}_x,\tilde{\omega}_y,\tilde{\omega}_z)}{\lambda_1\lambda_2\lambda_3}, \quad \beta(0)=0, \quad (16)$$

$$\ddot{\lambda}_k\lambda_k+\lambda_k^2\omega_k^2(t)-\frac{\omega_k^2\gamma_k}{\lambda_k^2}=\frac{(1-\gamma_k)\omega_k^2}{\lambda_1\lambda_2\lambda_3}, \quad \lambda_k(0)=1, \quad \dot{\lambda}_k(0)=0, \quad (17)$$

$\omega_k=\omega_k(0)$, and $\tilde{\omega}_k=\sqrt{1-\gamma_k}\omega_k$, is made into the time-dependent GP equation

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\Psi+V_t(\vec{r},t)\Psi+Ng|\Psi|^2\Psi, \quad (18)$$

Eq. (18) becomes

$$i\hbar\frac{\partial\Phi}{\partial t}=\sum_{k=1}^{3}\frac{H_k-\tilde{H}_k}{\lambda_k^2}\Phi+\frac{1}{\lambda_1\lambda_2\lambda_3}\left(-\mu_{\rm TF}(\tilde{\omega}_x,\tilde{\omega}_y,\tilde{\omega}_z)+\frac{m}{2}\sum_{k=1}^{3}x_k^2\tilde{\omega}_k^2+Ng|\Phi|^2\right)\Phi, \quad (19)$$

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

$$-\frac{\hbar^2}{2m}\Delta\Psi(\vec{r},0)+V_t(\vec{r},0)\Psi(\vec{r},0)+Ng|\Psi(\vec{r},0)|^2\Psi(\vec{r},0)=\mu\Psi(\vec{r},0). \quad (20)$$

Equations (15)–(17) generalize the anzatz of Ref. [7] for the case of $\gamma_k\neq 0$.

By neglecting $\Sigma_{k=1}^{3}[(H_k-\tilde{H}_k)/\lambda_k^2]$ in Eq. (19), we obtain a generalization of our approximation, Eqs. (5)–(7) and (13) to the time-dependent problem

$$|\Psi(\vec{r},t)|^2=\frac{\rho_{\rm TF}(\tilde{\omega}_x,\tilde{\omega}_y,\tilde{\omega}_z,x_1/\lambda_1(t),x_2/\lambda_2(t),x_3/\lambda_3(t))}{\lambda_1(t)\lambda_2(t)\lambda_3(t)}, \quad (21)$$

where all the dynamics is in the evolution of the scaling parameters λ_k, Eq. (17).

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

TABLE III. Calculated aspect ratio of the ^{23}Na atoms cloud, $R(t)$, using Eq. (22), after a ballistic expansion of $t=4$ ms, as a function of N. N is in units of 10^5 and $\Delta=[R(t)-R_{\rm TF}(t)]/R(t)$.

N	$R(t)$	$\gamma_\perp$	γ_z	$Na/a_{\rm ho}$	Δ (%)
1.2	0.110	0.354	0.0	138	20
0.8	0.117	0.426	0.0	92	25
0.4	0.132	0.551	0.0	46	33
0.1	0.183	0.766	0.0	11	52

$$R(t)=\left(\frac{\overline{x^2}(t)}{\overline{z^2}(t)}\right)^{1/2}=\frac{\omega_z\lambda_\perp(t)\sqrt{1-\gamma_z}}{\omega_\perp\lambda_z(t)\sqrt{1-\gamma_\perp}}. \quad (22)$$

As an example, we consider application of the above results to the experimental data with ^{23}Na atoms obtained in the Ioffe-Pritchard-type magnetic trap with radial and axial trapping frequencies of $\omega_\perp/(2\pi)=360$ Hz and $\omega_z/(2\pi)=3.5$ Hz [14], respectively. In our analysis, we use $a=2.75$ nm, $t=4$ ms, and $a/a_\perp=2.488\times10^{-3}$, 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

$$\frac{d^2\lambda_\perp}{d\tau^2}=\frac{\gamma_\perp}{\lambda_\perp^3}+\frac{1-\gamma_\perp}{\lambda_\perp^3\lambda_z}, \quad (23)$$

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

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

To zeroth order in ϵ, we have $\lambda_z=1$ and $\lambda_\perp=\sqrt{1+\tau^2}$. For the experimental conditions [14], the terms in ϵ^2 are negligible.

In Table III, we give the calculated values of the aspect

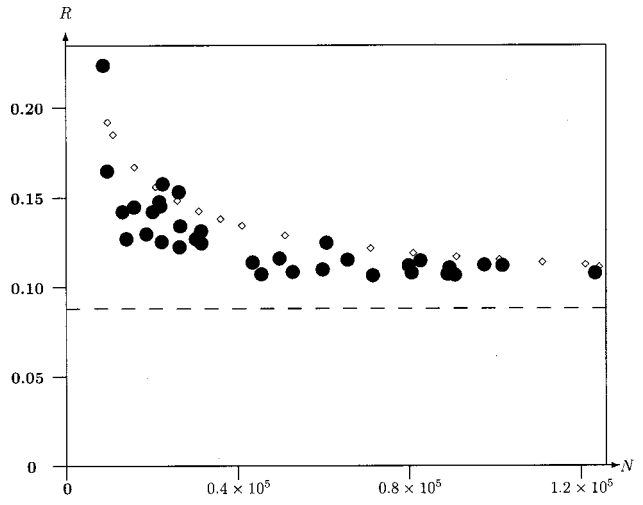

FIG. 1. Aspect ratio R of the ^{23}Na atom cloud after a ballistic expansion of $t=4$ ms, as a function of the number of atoms N, with $\omega_\perp(0)=2\pi\times360$ Hz and $\omega_z(0)=2\pi\times3.5$ Hz. Diamonds, dashed line, and circular dots represent the results of theoretical calculations using Eq. (22), the TF approximation, and experimental data from the MIT group [14], respectively.

ratio $R(t)$ of the ^{23}Na atoms cloud, after ballistic expansion of $t=4$ ms, and the calculated values of parameters $\gamma_\perp$ and γ_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 was noted already in Ref. [17]. We also note that even for the relatively large TF parameter, $Na/a_{\rm ho}\approx 100$, the relative error of the TF approximation, $\Delta=(R-R_{\rm TF})/R$, is larger than 20%. It demonstrates that the validity of the TF approximation depends not only on the TF parameter, but also on properties of the trap.

Our calculated results for $R(t)$ are compared with the recent experimental data [14] in Fig. 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-Einstein condensates for a rather small number of atoms N. The approximation is very useful since it provides an easy and simple quantitative computational tool for the analysis of experimental data for trapped condensed gases, without relying on complex and extensive computations.

We are grateful to the group at MIT for providing us with the experimental data.

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