Application of the homotopy analysis method for the Gross–Pitaevskii equation with a harmonic trap*

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The Homotopy analysis method (HAM) is adopted to find the approximate analytical solutions of the Gross–Pitaevskii equation, a nonlinear Schrödinger equation is used in simulation of Bose–Einstein condensates trapped in a harmonic potential. Comparisons between the analytical solutions and the numerical solutions have been made. The results indicate that they fit very well with each other when the atomic interaction is weak.

Keywords: Gross–Pitaevskii equation, homotopy analysis method, analytical solution

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1. Introduction

Bose–Einstein condensates (BEC) in dilute atomic gases, which were first realized experimentally in 1995 for rubidium,[1] sodium,[2] lithium,[3,4] etc., provide unique opportunities for exploring quantum phenomena on a macroscopic scale. In experiments, the atoms were confined in magnetic traps and cooled down to extremely low temperatures. As the temperature of atoms gets very low, their de Broglie wavelength, an inherently quantum character, can become larger than the interatomic distance. At that point, bosonic atoms will condense into a unique quantum state and become indistinguishable parts of a macroscopic quantum object. This has now been achieved for all stable alkali atoms,[1−6] as well as with hydrogen,[7] metastable helium,[8,9] and for diatomic molecules.[10]

In the mean-field treatment, the order parameter, or wave function, for the condensates is governed by a nonlinear Schrödinger equation, the Gross–Pitaevskii equation (GPE)[11−13]

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t) = \Big[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{trap}}(\boldsymbol{r}) + U|\Psi(\boldsymbol{r},t)|^2\Big]\Psi(\boldsymbol{r},t), \quad (1)$$

where $\hbar$ is the reduced Planck constant, m the mass of the boson, V_{trap} a trapping potential spatially confining the condensate, $\boldsymbol{r} = (x, y, z)$ and t denote the space and time coordinates respectively, $U = 4\pi\hbar^2 a_{\mathrm{s}}/m$, a_{s} the s-wave scattering length, which varies according to the species of bosons being considered. When $a_{\mathrm{s}} > 0$, the interactions are repulsive. In contrast, when $a_{\mathrm{s}} < 0$, the interactions are attractive and a BEC tends to contract to minimize its overall energy. Some experiments on the BEC gave: $a_{\mathrm{s}} = 2.75$ nm for ^{23}Na, $a_{\mathrm{s}} = 5.77$ nm for ^{87}Rb, and $a_{\mathrm{s}} = -1.45$ nm for ^{7}Li.[13]

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

is the Laplace operator. The wave function Ψ is normalized according to $\|\Psi\|^2 = \int |\Psi|^2 \mathrm{d}\boldsymbol{r} = N$, where N is the total number of particles in the condensate. In most cases, the confinement due to the magnetic trap is well described by a harmonic oscillator potential

$$V_{\mathrm{trap}}(\boldsymbol{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$$

with ω_x, ω_y, and ω_z being the trap frequencies in the x, y, and z directions, respectively.

By introducing dimensionless variables $t' = \omega_z t$, $(x, y, z) = a_{\mathrm{ho}}(x', y', z')$, $\Psi' = \left(a_{\mathrm{ho}}^3/N\right)^{1/2}\Psi$ with $a_{\mathrm{ho}} = \sqrt{\hbar/m\omega_z}$, and dropping the prime, equation (1) becomes to

$$\mathrm{i}\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t) = \Big[-\frac{1}{2}\nabla^2 + \frac{1}{2}\left(\gamma_x^2 x^2 + \gamma_y^2 y^2 + z^2\right)$$

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$$+ g|\Psi(\boldsymbol{r},t)|^2\Big]\Psi(\boldsymbol{r},t), \tag{2}$$

where

$$g = UN/(\hbar\omega_z a_{\rm ho}^3) = 4\pi N a_{\rm s}/a_{\rm ho},$$

$\gamma_x = \omega_x/\omega_z, \gamma_y = \omega_y/\omega_z$. The dimensionless energy functional per particle $E(\Psi)$ is defined as

$$E(\Psi) = \int \Big[\frac{1}{2}|\nabla\Psi|^2 + \frac{1}{2}(\gamma_x^2x^2 + \gamma_y^2y^2 + z^2)|\Psi|^2 + \frac{g}{2}|\Psi|^4\Big]\,{\rm d}\boldsymbol{r}. \tag{3}$$

In the disk-shaped condensates, i.e., $\omega_x \approx \omega_y$ and $\omega_z \gg \omega_x$, the three-dimensional (3D) GPE can be reduced to a 2D GPE. In the cigar-shaped condensates, i.e., $\omega_y \gg \omega_x$ and $\omega_z \gg \omega_x$, the 3D GPE can be reduced to 1D GPE. We now consider the spherical symmetry case, i.e., $\omega_x = \omega_y = \omega_z$ ($\gamma_x = \gamma_y = 1$), equation (2) can be reduced to 1D form

$$-\frac{1}{2}\frac{{\rm d}^2\psi}{{\rm d}r^2} + \frac{1}{2}r^2\psi + \frac{g}{r^2}\psi^3 = \mu\psi \tag{4}$$

with $\Psi(\boldsymbol{r},t) = [\psi(r)/r]\,{\rm e}^{-{\rm i}\mu t}$, $r^2 = x^2 + y^2 + z^2$, μ is the chemical potential. With this transformation, the order parameter $\psi(r)$ must to be an odd function of r and satisfies the normalization condition $\int_0^{+\infty}\psi^2{\rm d}r = 1/4\pi$. It is evident that the importance of the atom–atom interaction is completely fixed by the parameter $Na_{\rm s}/a_{\rm ho}$. In the first experiments with rubidium atoms at JILA[1] the ratio $|a_{\rm s}|/a_{\rm ho}$ was about 7×10^{-3}, with N in the order of a few thousands. In the experiments with ^{7}Li at Rice University[4] the same parameter is smaller than 1, since the number of particles is in the order of 1000 and $|a_{\rm s}|/a_{\rm ho} \approx 0.5\times10^{-3}$.

There are many numerical methods, such as the imaginary-time propagation (ITP) method,[14–18] the Galerkin spectral method,[19–21] the time-splitting Fourier transformation method,[22,23] and so on, for solving Eq. (1). Many researchers investigated the Gross–Pitaevskii equations analytically,[24–29] but most work has focused on the case that the trapping potential is not harmonic, or the coefficient of the atom–atom interaction is not a constant. In fact, it is a challenging task to find the exact analytical solutions of Eq. (2) with a harmonic oscillator potential and a constant interaction coefficient. In this paper, an analytical approach based on the homotopy analysis method (HAM)[30–36] is adopted to find the approximate analytical solutions for the stationary state of Eq. (4). This method can be implemented by a computer algebraic software, such as Maple or Mathematica. The results indicate that the method is effective and efficient for solving Eq. (4) when the nonlinear coefficient g is not too large.

2. Homotopy analysis method

The HAM is a rather general and powerful approach for nonlinear problems. It has been widely applied to solve different types of nonlinear problems in science and engineering. For interested readers, we refer to Refs. [30] and [31] for more details. As is done in the standard HAM, we construct a homotopy

$$(1-q)\left[\hat{H}_0\Phi(r,q) - M(q)\Phi(r,q)\right] = qc_0\left[\hat{H}_0\Phi(r,q) + \frac{g}{r^2}\Phi^3(r,q) - M(q)\Phi(r,q)\right] \tag{5}$$

with the linear operator

$$\hat{H}_0 = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{1}{2}r^2.$$

Here $q\in[0,1]$ is the embedding parameter and c_0 is an auxiliary parameter (an adjustable constant), called the convergence-control parameter. When $q = 0$, equation (5) becomes

$$-\frac{1}{2}\frac{\partial^2\Phi(r,0)}{\partial r^2} + \frac{1}{2}r^2\Phi(r,0) = M(0)\Phi(r,0). \tag{6}$$

Equation (6) is a linear Schrödinger equation with harmonic potential for a stationary state. Considering that it should be an odd function of r, $\Phi(r,0)$ can be choosen as $\Phi(r,0)\propto r\,{\rm e}^{-r^2/2}$ and $M(0) = 3/2$. When $q = 1$, equation (5) suggests that $\psi(r) = \Phi(r,1)$ and $\mu = M(1)$. It can be seen from Eq. (5) that as parameter q increases from 0 to 1, solution $\Phi(r,q)$ varies from $\Phi(r,0)$ to $\psi(r)$, so does the $M(q)$ from μ_0, the initial guess of μ, to μ. If this continuous variation is smooth enough, the Maclaurin's series with respect to q can be constructed for $\Phi(r,q)$ and $M(q)$ respectively, and further, if these two series are convergent at $q = 1$, we then have

$$\psi(r) = \Phi(r,q)|_{q=1} = \psi_0(r) + \sum_{k=1}^{+\infty}\psi_k(r),$$
$$\mu = M(q)|_{q=1} = \mu_0 + \sum_{k=1}^{+\infty}\mu_k, \tag{7}$$

where

$$\psi_k(r) = \frac{1}{k!}\frac{\partial^k\Phi(r,q)}{\partial q^k}\Big|_{q=0},$$
$$\mu_k = \frac{1}{k!}\frac{{\rm d}^kM(q)}{{\rm d}q^k}\Big|_{q=0}, \quad (k = 0,1,2,\ldots) \tag{8}$$

are called the k-th order deformation derivatives.

Differentiating Eq. (5) k times with respect to q then setting $q = 0$ and finally dividing them by $k!$, we gain the k-th order deformation equation for $\psi_k(r)$

$$\begin{aligned} &k = 0 : \hat{H}_0\psi_0 = \mu_0\psi_0, \\ &k = 1 : \hat{H}_0\psi_1 - \mu_0\psi_1 - \mu_1\psi_0 = \frac{c_0 g}{r^2}\psi_0^3, \\ &k > 1 : \hat{H}_0(\psi_k - \psi_{k-1}) + \sum_{j=0}^{k-1}\mu_j(\psi_{k-1-j} - \psi_{k-j}) \\ &\qquad -\mu_k\psi_0 \\ &\qquad = c_0\Bigg[\hat{H}_0\psi_{k-1} + \frac{g}{r^2}\sum_{j=0}^{k-1}\psi_j\sum_{l=0}^{k-1-j} \\ &\qquad \times\psi_l\psi_{k-1-j-l} - \textstyle\sum_{j=0}^{k-1}\mu_j\psi_{k-1-j}\Bigg]. \end{aligned} \tag{9}$$

It should be emphasized that the system of Eq. (9) is a recursive one, which means we can gain ψ_1 once ψ_0 is obtained; furthermore, we can obtain ψ_2 when ψ_0 and ψ_1 have been derived, and so on. Unfortunately, in the set of Eq. (9), only the solution of the first equation can be obtained easily although all the equations are linearized. It is rather difficult to obtain the exact solutions for ψ_k when $k > 0$. We now use the Galerkin spectral method to find the approximate analytical solutions for ψ_k of Eq. (9).

For a given k, suppose that ψ_j and μ_j ($j = 0, 1, \ldots, k-1$) are known and we will seek ψ_k and μ_k. Let us consider a basis of functions, $\{\phi_n(r)|n = 1, 2, \ldots, \mathscr{N}\}$, perhaps satisfying some set of boundary conditions over the interval $(-\infty, +\infty)$, which is complete enough for expanding the unknown function over that interval to sufficient accuracy. For simplicity we assume that these functions form an orthonormal basis for the space. We choose ϕ as the eigenfunctions of the 1D harmonic oscillator

$$\begin{aligned} \phi_n(r) = {} & \mathrm{e}^{-r^2/2}\mathrm{H}_{2n-1}(r)/\sqrt{2^{2n-1}(2n-1)!\sqrt{\pi}}, \\ & n = 1, 2, \ldots, \mathscr{N}, \end{aligned} \tag{10}$$

where $\mathrm{H}_{2n-1}(r)$ is the Hermite polynomial with order $2n-1$. The basis functions $\{\phi_n|n = 1, 2, \ldots, \mathscr{N}\}$ form an orthonormal set which satisfy

$$\begin{aligned} \langle\phi_n|\phi_j\rangle = {} & \int_{-\infty}^{+\infty}\phi_n(r)\phi_j(r)\mathrm{d}r \\ = {} & 2\int_0^{+\infty}\phi_n(r)\phi_j(r)\mathrm{d}r \\ = {} & \delta_{nj} \end{aligned} \tag{11}$$

and

$$\hat{\mathrm{H}}_0\phi_n(r) = (2n - 1/2)\phi_n(r).$$

All the unknown functions ψ_k ($k = 0, 1, \ldots$) now can be expressed as the linear combination of the basis functions

$$\psi_k(r) = \sum_{n=1}^{\mathscr{N}} c_{k,n}\phi_n(r), \quad (k = 0, 1, \ldots), \tag{12}$$

where $c_{k,n}$ are expansion coefficients.

For the case of $k = 0$, we can choose $\psi_0(r) = c_{0,1}\phi_1(r)$ with $c_{0,n} = 0$ ($n > 1$) and $\mu_0 = 3/2$. The coefficient $c_{0,1}$ can be determined by the normalization condition of the order parameter $\psi(r)$. For $k = 1$, we have

$$\begin{aligned} &(2n - 1/2)c_{1,n} - \mu_0 c_{1,n} - \mu_1 c_{0,1}\langle\phi_1|\phi_n\rangle \\ &= c_0 g c_{0,1}^3\left\langle\frac{\phi_1^3}{r^2}\middle|\phi_n\right\rangle, \ (n = 1, 2, \ldots, \mathscr{N}), \end{aligned} \tag{13}$$

from which one can obtain

$$\mu_1 = -c_0 g c_{0,1}^2\left\langle\frac{\phi_1^3}{r^2}\middle|\phi_1\right\rangle = -\frac{c_0 g c_{0,1}^2}{\sqrt{2\pi}} \tag{14}$$

and

$$c_{1,n} = \frac{c_0 g c_{0,1}^3\left\langle\frac{\phi_1^3}{r^2}\middle|\phi_n\right\rangle}{2(n-1)}, \ (n = 2, 3, \ldots, \mathscr{N}). \tag{15}$$

The coefficient $c_{1,1}$ cannot be determined by now. Without loss of generality, one can adopt $c_{1,1} = 0$ because it can be combined with $c_{0,1}$ and determined by the normalization condition of $\psi(r)$. For the same reason, we take $c_{k,1} = 0$ ($k > 0$).

A similar way can be used to find ψ_k and μ_k ($k > 1$). As k and $\mathscr{N}$ increase, however, the computational quantity will increase rapidly. Fortunately, the procedure described above can be implemented easily with the aid of symbol calculation software, such as Maple or Mathematica. Finally, at the K-th order approximation we have the analytical solution

$$\begin{aligned} &\psi(r) \approx \psi^K(r) = \psi_0(r) + \sum_{k=1}^{K}\psi_k(r), \\ &\mu \approx \mu^K = \mu_0 + \sum_{k=1}^{K}\mu_k. \end{aligned} \tag{16}$$

3. Results and discussion

In the frame of HAM, the solution can be expressed as a series of basis functions. Note that the solution contains the adjustable parameter c_0, which provides us with a simple way to adjust and control the convergence of the solution series. In general, by means of the so-called c_0-curve, it is straightforward to choose an appropriate range for c_0 which ensures the

convergence of the series. In practice, we take $K = 4$ and $\mathscr{N} = 6$. Figure 1 shows the chemical potential μ versus c_0 for different values of $\alpha(= Na_{\rm s}/a_{\rm ho})$. We can see from Fig. 1 that there exists an appropriate range for c_0 to gain a convergent solution of μ. It is clear that as α increases, the interval of convergence becomes smaller and smaller. It fails to converge as α is large enough.

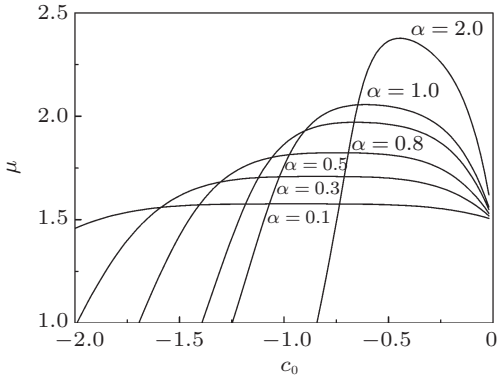


Fig. 1. The chemical potential μ versus c_0 for different value of α ($\alpha = Na_{\rm s}/a_{\rm ho}$).

To measure the accuracy of the approximate solution we derived, we define the residual error

$$\epsilon(r) = \hat{\rm H}_0\psi^K + \frac{g}{r^2}(\psi^K)^3 - \mu^K\psi^K(r). \tag{17}$$

The squared norm of ϵ can be defined as

$$\|\epsilon\|^2 = \int_0^{+\infty} \epsilon(r)^2 \,{\rm d}r.$$

Obviously, ψ^K is the exact solution of Eq. (4) when $\|\epsilon\| = 0$. We think that the smaller the value of $\|\epsilon\|^2$, the more precise the solution is. Table 1 lists the numerical value of the chemical potential μ and the energy E per particle given by the ITP method and the analytical results obtained by the HAM described above. The value c_0 we chose can ensure that the series are convergent. The wave functions $\Psi(r)(= \psi(r)/r)$ given by our method and the corresponding numerical results, derived by the ITP, are shown in Fig. 2 for different values of α. Figure 2 only shows the wave profile for $r \in [0, 1]$ because we find that the difference between the analytical solution and numerical solution goes to zero as r increases and the maximum error occurs near the point $r = 0$. The atom–atom interaction is repulsive when $\alpha > 0$, while it is attractive as $\alpha < 0$. We find that the HAM can deal with both of these two cases.

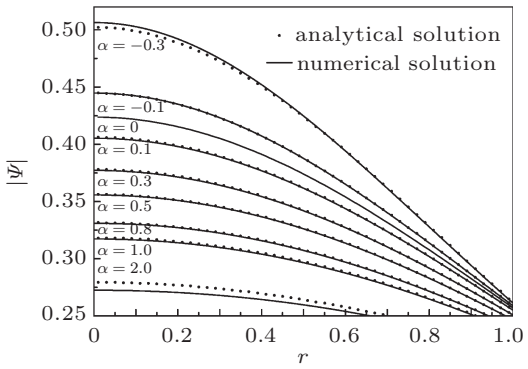


Fig. 2. Profile of wave function $|\Psi|$ for different values of α ($\alpha = Na_{\rm s}/a_{\rm ho}$).

In Table 1, $e_{\rm a} = 2E_{\rm kin} - 2E_{\rm pot} + 3E_{\rm int}$, where $E_{\rm kin}$, $E_{\rm pot}$, $E_{\rm int}$ are the dimensionless kinetic energy, potential energy, and interaction energy, respectively. From the Virial theorem we know that $2E_{\rm kin} - 2E_{\rm pot} + 3E_{\rm int} = 0$ for the steady state of the BEC system we considering. Note that $e_{\rm a}$ and $||\epsilon||^2$ are nearly zero as $|\alpha| = 0.1$, which means that the corresponding wave function we derived is a good approximation for the steady state of Eq. (2) when the trapping potential has spherical symmetry. It can be seen from Table 1 and Fig. 2 that the analytical results agree very well with the numerical results as $|\alpha|$ is not too large. It is also shown that the error increases as the value of $|\alpha|$ increases. Although we can reduce the error by increasing K and $\mathscr{N}$, the computational quantity will increase rapidly, which implies that our method is suitable for solving GPE that has a weak interaction.

For convenience, the wave functions $\Psi = \psi(r)/r$, which are very close to the exact solutions of Eq. (4), for $\alpha = 0.1$, 0.3, -0.1 are listed below

$$\begin{aligned}
\alpha = 0.1 : \Psi \;&= (0.406162 + 1.72293 \times 10^{-2}\; r^2 \\
&\quad - 3.28600 \times 10^{-3}\; r^4 \\
&\quad + 4.01610 \times 10^{-4}\; r^6 \\
&\quad - 2.53853 \times 10^{-5}\; r^8 \\
&\quad + 6.16108 \times 10^{-7}\; r^{10})\, {\rm e}^{-r^2/2}, \\
\alpha = 0.3 : \Psi \;&= (0.378032 + 4.13232 \times 10^{-2}\; r^2 \\
&\quad - 6.35041 \times 10^{-3}\; r^4 \\
&\quad + 6.50380 \times 10^{-4}\; r^6 \\
&\quad - 3.57030 \times 10^{-5}\; r^8 \\
&\quad + 7.77009 \times 10^{-7}\; r^{10})\, {\rm e}^{-r^2/2}, \\
\alpha = -0.1 : \Psi \;&= (0.444731 - 2.23597 \times 10^{-2}\; r^2 \\
&\quad + 5.13803 \times 10^{-3}\; r^4 \\
&\quad - 7.08633 \times 10^{-4}\; r^6 \\
&\quad + 4.84964 \times 10^{-5}\; r^8 \\
&\quad - 1.24120 \times 10^{-6}\; r^{10})\, {\rm e}^{-r^2/2}.
\end{aligned}$$

Table 1. Comparison of the analytical results with the numerical results of chemical potential μ and energy E for different values of α. The subscripts n and a denote the numerical result and analytical result, respectively.

α	$\mu_{\rm n}$	$\mu_{\rm a}$	$E_{\rm n}$	$E_{\rm a}$	$e_{\rm a}$	$\|\epsilon\|^2$	c_0
0.0	1.5	1.5	1.5	1.5	0	0	
0.1	1.576506	1.575873	1.539192	1.538561	−0.000003	2×10^{-7}	−0.95
0.3	1.709612	1.708808	1.609556	1.609009	0.000364	1×10^{-7}	−0.90
0.5	1.825181	1.823849	1.673127	1.672641	0.001140	4×10^{-7}	−0.75
0.8	1.976196	1.971335	1.759112	1.758697	0.006260	5×10^{-6}	−0.65
1.0	2.066030	2.056094	1.811605	1.811234	0.014062	2×10^{-5}	−0.58
2.0	2.435156	2.377346	2.035531	2.035746	0.092110	5×10^{-4}	−0.44
−0.1	1.416234	1.415482	1.459327	1.458569	−0.000027	1×10^{-6}	−1.10
−0.3	1.205991	1.206439	1.364610	1.363699	−0.001997	7×10^{-5}	−1.25
−0.5	0.851339	0.904899	1.239936	1.240447	−0.041080	1×10^{-3}	−1.45

4. Conclusion

In summary, an analytical approach based on homotopy analysis and the Galerkin method is adopted to find the approximate analytical solutions of the Gross–Pitaevskii equation, which is used to describe the BEC in a harmonic potential. Comparisons between the analytical solutions we calculated and the numerical results, obtained by the ITP, have been made. The results indicate that our results agree very well with the numerical results if the atomic interaction is weak. When the atomic interaction becomes strong, a new approach should be presented. We will study this case in the future.

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