

Analytical Solutions to the Time-Independent Gross-Pitaevskii Equation with a Harmonic Trap *

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(Received 22 May 2012)

We try to find the analytical solutions to the time-independent Gross-Pitaevskii equation, a nonlinear Schrödinger equation used in the simulation of Bose-Einstein condensates trapped in a harmonic potential. Both the homotopy analysis method and the Galerkin spectral method are applied. We investigate the one-dimensional case and obtain the approximate analytical solutions successfully. Comparison between the analytical solutions and the numerical solutions has been made. The results indicate that they agree very well with each other when the atomic interaction is not too strong.

PACS: 03.65.Ge, 03.75.Hh, 02.70.Dh

DOI: 10.1088/0256-307X/29/11/110302

The experimental realization of Bose-Einstein condensates (BEC) in dilute atomic gases^[1-4] has prompted much work on the study of the dynamics of these condensates. 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 can become greater 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. It has now been achieved for all stable alkali atoms,^[1-6] as well as with hydrogen,^[7] metastable helium,^[8,9] diatomic molecules,^[10] etc.

In the dilute limit each atom feels the effects of all surrounding atoms to the first (mean-field) approximation via an effective potential energy, which is proportional to the local density of the condensate. In addition, the depletion of the condensate due to quantum fluctuations is very small. Under these conditions the confined gas at zero temperature is fully characterized by the condensate wave function, which is determined by a nonlinear Schrödinger equation, known as the Gross-Pitaevskii equation (GPE)^[11-13]

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}(\mathbf{r}) + U|\Psi(\mathbf{r})|^2 \right] \Psi(\mathbf{r}) = \mu\Psi(\mathbf{r}) \quad (1)$$

under the normalization condition $\|\Psi\|^2 = \int |\Psi|^2 d\mathbf{r} = 1$, where $\mathbf{r} = (x, y, z)$ denotes the space coordinates; $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplace operator, \hbar the reduced Planck constant, m the mass of the boson, V_{trap} a trapping potential spatially confining the condensate, μ the chemical potential, $U = 4\pi\hbar^2 Na_s/m$, N the total number of particles in the condensate, a_s the s-wave scattering length.

When $a_s > 0$, the interactions are repulsive. In contrast, when $a_s < 0$, the interactions are attractive and a BEC tends to contract to minimize its overall energy. Some experiments on BEC give: $a_s = 2.75$ nm for ^{23}Na , $a_s = 5.77$ nm for ^{87}Rb , and $a_s = -1.45$ nm for ^7Li .^[13] By applying an ac magnetic field may induce a periodic modulation of a_s , opening a way to "Feshbach resonance management"(FRM).^[14]

The value of the energy per particle associated with the wave function $\Psi(\mathbf{r})$ is obtained according to^[11-13]

$$E(\Psi) = \int \left[\frac{\hbar^2}{2m} |\nabla\Psi|^2 + V_{\text{trap}}(\mathbf{r}) |\Psi|^2 + \frac{U}{2} |\Psi|^4 \right] d\mathbf{r}. \quad (2)$$

For repulsive interactions ($a_s > 0$) the energy functional is convex and its minimum delivers the stable ground state of the gas. For $a_s < 0$ the ground state exists only at low coupling for limited numbers of bosons in the trap, as long as the zero-point energy balances the effect of attractions and prevents collapse.^[15]

In most cases, the confinement due to the magnetic trap is well-described by a harmonic oscillator potential

$$V_{\text{trap}}(\mathbf{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \quad (3)$$

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

There are many numerical methods, such as the imaginary-time propagation (ITP) method,^[15-18]

*Supported by the National Natural Science Foundation under Grant No 11047010, and the Key Project Foundation of the Education Ministry of China under Grant No 209128

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the Galerkin spectral method,^[19,20] the time-splitting Fourier transformation method,^[21,22] and so on, for solving the GPE. Many researchers have investigated the GPEs analytically,^[23–31] but most works are 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 challenging to find the exact analytical solutions to Eq. (1) with a harmonic oscillator potential and a constant interaction coefficient. In this Letter, an analytical approach based on the homotopy analysis method (HAM)^[32–38] is adopted to find the approximate analytical solutions of Eq. (1) for the 1D case. This method can be implemented by using computer algebraic software such as Maple or Mathematica. The results indicate that the analytical solutions agree very well with the numerical results if the atomic interaction is not too strong.

The HAM is a rather general and powerful approach for nonlinear problems. It has been widely applied for solving different types of nonlinear problems in science and engineering. We refer interested readers to Refs. [32,33] for more details. In this study, the HAM will be employed to find the approximation analytical solutions of the GPE for the 1D case. The dimensionless version of the GPE for the 1D case can be obtained by the procedure used in Ref. [21,22,39]

$$\left[-\frac{1}{2} \frac{\partial^2}{\partial x'^2} + \frac{1}{2} x'^2 + g_{1D} |\Psi'(x')|^2 \right] \Psi'(x') = \mu' \Psi'(x') \quad (4)$$

under the normalization condition $\int |\Psi'(x')|^2 dx' = 1$, where $g_{1D} = \frac{4\pi N a_s \sqrt{\gamma_y \gamma_z}}{a_{ho} 2\pi}$, $\gamma_y = \omega_y/\omega_x$, $\gamma_z = \omega_z/\omega_x$, $\mu' = \mu/\hbar\omega_x$, $x' = x/a_{ho}$, $a_{ho} = \sqrt{\hbar/m\omega_x}$. The dimensionless energy per particle is

$$E'(\Psi') = \int_{-\infty}^{+\infty} \left[\frac{1}{2} \left| \frac{\partial \Psi'}{\partial x'} \right|^2 + \frac{1}{2} x'^2 |\Psi'|^2 + \frac{g_{1D}}{2} |\Psi'|^4 \right] dx'. \quad (5)$$

We can see from the above that all the physical parameters have been absorbed in the nonlinear parameter g_{1D} and the value of g_{1D} is proportional to the total number of particles as other parameters are fixed. Calculations with the same g_{1D} can correspond to results for different species, but under diverse experimental conditions.

For convenience, we drop the prime for all the variables and replace g_{1D} with g . Recall that if V_{trap} is continuous and goes to $+\infty$ at infinity, and if $g \geq 0$, the ground state of $E(\Psi)$ exists and is unique up to a global phase. In addition, the global phase can be chosen such that Ψ is real-valued and positive.^[20] Thus, we can only consider the case that the order parameter, or wave function, Ψ is real-valued. As carried out in the standard HAM, we construct a homotopy

$$\begin{aligned} & (1-q)[\hat{H}_0 \Phi(x,q) - M(q)\Phi(x,q)] \\ & = qc_0[\hat{H}_0 \Phi(x,q) + g\Phi^3(x,q) - M(q)\Phi(x,q)] \end{aligned} \quad (6)$$

with the linear operator $\hat{H}_0 = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} x^2$. Here $q \in [0, 1]$ is the embedding parameter and c_0 is the convergence-control parameter. When $q = 0$, Eq. (6) becomes

$$-\frac{1}{2} \frac{\partial^2 \Phi(x,0)}{\partial x^2} + \frac{1}{2} x^2 \Phi(x,0) = M(0) \Phi(x,0). \quad (7)$$

Equation (7) is a linear Schrödinger equation with harmonic potential for stationary state. Considering that we seek the ground state solutions of the 1D GPE, $\Phi(x,0)$ can be chosen as $\Phi(x,0) \propto e^{-x^2/2}$ and $M(0) = \frac{1}{2}$. When $q = 1$, Eq. (6) suggests that $\Psi(x) = \Phi(x,1)$ and $\mu = M(1)$. We now come to the conclusion from Eq. (6) that as the parameter q increases from 0 to 1, $\Phi(x,q)$ varies from $\Phi(x,0)$ to $\Psi(x)$, so does the $M(q)$ from μ_0 , the initial guess of μ , to μ . If this continuous variation is smooth enough, the Maclaurin series with respect to q can be constructed for $\Phi(x,q)$ and $M(q)$, respectively. If these two series are convergent at $q = 1$, we then have

$$\begin{aligned} \Psi(x) &= \Phi(x,q)|_{q=1} = \psi_0(x) + \sum_{k=1}^{+\infty} \psi_k(x), \\ \mu &= M(q)|_{q=1} = \mu_0 + \sum_{k=1}^{+\infty} \mu_k, \end{aligned} \quad (8)$$

where

$$\begin{aligned} \psi_k(x) &= \frac{1}{k!} \left. \frac{\partial^k \Phi(x,q)}{\partial q^k} \right|_{q=0}, \\ \mu_k &= \frac{1}{k!} \left. \frac{d^k M(q)}{dq^k} \right|_{q=0}, \quad k = 0, 1, 2, \dots \end{aligned} \quad (9)$$

are the k th order deformation derivatives.

Differentiating Eq. (6) 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 $\psi_k(x)$,

$$\begin{aligned} k=0: & \hat{H}_0 \psi_0 = \mu_0 \psi_0, \\ k=1: & \hat{H}_0 \psi_1 - \mu_0 \psi_1 - \mu_1 \psi_0 = c_0 g \psi_0^3, \\ k>1: & \hat{H}_0 (\psi_k - \psi_{k-1}) + \sum_{j=0}^{k-1} \mu_j (\psi_{k-1-j} - \psi_{k-j}) \\ & - \mu_k \psi_0 = c_0 [\hat{H}_0 \psi_{k-1} + g \sum_{j=0}^{k-1} \psi_j \\ & \cdot \sum_{l=0}^{k-1-j} \psi_l \psi_{k-1-j-l} - \sum_{j=0}^{k-1} \mu_j \psi_{k-1-j}]. \end{aligned} \quad (10)$$

The set of Eq. (10) is composed of a series of linearized equations. It is worth remarking that the system of Eq. (10) is a recursive one, which means that one can get ψ_1 once ψ_0 is obtained; furthermore, ψ_2 can be derived when ψ_0 and ψ_1 have been derived, and so on. Unfortunately, in the set of Eq. (10), only the solution

of the first equation ($k = 0$) 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. (10).

For a given k , suppose that ψ_j and μ_j ($j = 0, 1, \dots, k-1$) are known and we will seek ψ_k and μ_k . Let us consider a basis set of functions, $\{\phi_n(x)|n = 0, 1, \dots, \mathcal{N}\}$, 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. Hermite polynomials are a natural choice for this problem, as they are the eigenfunctions of the linearized GPE in harmonic traps and consequently satisfy the proper boundary conditions by construction. Thus, we take

$$\phi_n(x) = e^{-x^2/2} H_n(x) / \sqrt{2^n n! \sqrt{\pi}}, \quad n = 0, 1, \dots, \mathcal{N}, \quad (11)$$

where $H_n(x)$ is the Hermite polynomial with order n

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \quad (12)$$

The basis functions $\{\phi_n|n = 0, 1, \dots, \mathcal{N}\}$ form an orthonormal set which satisfies

$$\langle \phi_n | \phi_j \rangle = \int_{-\infty}^{+\infty} \phi_n(x) \phi_j(x) dx = \delta_{nj}, \quad (13)$$

$$\hat{H}_0 \phi_n(x) = (n + 1/2) \phi_n(x). \quad (14)$$

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

$$\psi_k(x) = \sum_{n=0}^{\mathcal{N}} c_{kn} \phi_n(x), \quad (k = 0, 1, \dots) \quad (15)$$

where c_{kn} are expansion coefficients.

For the case of $k = 0$, we can choose $\psi_0(x) = c_{00} \phi_0(x)$ with $c_{0n} = 0$ ($n > 1$) and $\mu_0 = 1/2$. The coefficient c_{00} can be determined by the normalization condition of the order parameter $\Psi(x)$. For $k = 1$, we have

$$(n + 1/2)c_{1n} - \mu_0 c_{1n} - \mu_1 c_{00} \langle \phi_0 | \phi_n \rangle = c_{0g} c_{00}^3 \langle \phi_0^3 | \phi_n \rangle, \quad (n = 0, 1, \dots, \mathcal{N}) \quad (16)$$

from which one can obtain

$$\mu_1 = -c_{0g} c_{00}^2 \langle \phi_0^3 | \phi_0 \rangle = -\frac{c_{0g} c_{00}^2}{\sqrt{2\pi}}, \quad (17)$$

and

$$c_{1n} = \frac{c_{0g} c_{00}^3}{n} \langle \phi_0^3 | \phi_n \rangle = \begin{cases} 0, & n \text{ is odd,} \\ \frac{c_{0g} c_{00}^3}{\sqrt{2\pi}} \frac{(-1)^{n/2} (n-1)!!}{n \sqrt{2^n n!}}, & n \text{ is even,} \end{cases} \quad n = 1, 2, \dots, \mathcal{N}. \quad (18)$$

The coefficient c_{10} can not be determined now. Without loss of generality, one can adopt $c_{10} = 0$ because it can be combined with c_{00} and determined by the normalization condition of $\Psi(x)$. For the same reason, we take $c_{k0} = 0$ ($k > 0$).

A similar way can be used to find ψ_k and μ_k ($k > 1$). As k and \mathcal{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

$$\Psi(x) \approx \Psi^K(x) = \psi_0(x) + \sum_{k=1}^K \psi_k(x), \quad \mu \approx \mu^K = \mu_0 + \sum_{k=1}^K \mu_k. \quad (19)$$

The zeroth-order approximation for $\Psi(x)$ is

$$\Psi(x) \approx \Psi^0(x) = c_{00} \phi_0(x) = \frac{1}{\sqrt{4/\pi}} e^{-x^2/2}, \quad \mu \approx \mu_0 = 0.5. \quad (20)$$

This is just the Gaussian profile, which can be regarded as an approximate solution to Eq. (4) only for the case that the atom-atom interaction is rather weakly, i.e., the value of g is very small.

The first-order approximation for $\Psi(x)$ is

$$\Psi(x) \approx \Psi^1(x) = c_{00} \phi_0(x) + \frac{c_{0g} c_{00}^3}{\sqrt{2\pi}} \sum_{n=1}^{[\mathcal{N}/2]} \frac{(-1)^n (2n-1)!!}{2n \sqrt{2^{2n} (2n)!}} \phi_{2n}(x) \quad (21)$$

with $\mu \approx \mu_0 + \mu_1 = \frac{1}{2} - \frac{c_{0g} c_{00}^2}{\sqrt{2\pi}}$, where $[\mathcal{N}/2]$ denotes the integer part of $\mathcal{N}/2$, c_{00} should be determined by the normalization condition. We will discuss how to determine the adjustable parameter c_0 later. It is worth noting that the Gauss-Hermite quadrature, employed in Refs. [19,20], is also used, which makes our method more efficient to implement using computer algebraic software.

Using ^{23}Na as an example, $m \approx 3.8194 \times 10^{-26}$ kg, $\hbar \approx 1.05457 \times 10^{-34}$ J·s, $a_s = 10a_B \approx 0.52917$ nm, where $a_B \approx 0.052917$ nm is the Bohr radius. The frequencies of the external magnetic potential are adopted as $\omega_x = 2\pi \times 40$ Hz, $\omega_y = \omega_z = 2\pi \times 130$ Hz.^[40] Then we have $g \approx 1.04 \times 10^{-3}$ N. The value of g is about 1 when $N = 10^3$ and it is about 10 as $N = 10^4$. Obviously, the atom-atom interaction increases as the total number of particles increases. If we take the ^7Li as an example, $m \approx 1.1624 \times 10^{-26}$ kg,

$a_s = -18a_B \approx -0.9525$ nm, then $g \approx -1$ when $N = 10^3$.

In the framework of the HAM, the solution is expressed as a series of basis functions. Note that the solution contains the adjustable parameter c_0 , which provides us with a simply 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 $K = 10$ and $\mathcal{N} = 8$. Figure 1 shows the chemical potential μ versus c_0 for different values of g . We can see from Fig. 1 that there exists an appropriate range for c_0 to get convergent solution of μ . It is clear that as g increases, the interval of convergence becomes smaller and smaller. It fails to converge as g is large enough.

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

g	μ_n	μ_a	E_n	E_a	e_a	$\ \epsilon\ ^2$	c_0
0.0	0.5	0.5	0.5	0.5	0	0	
1.0	0.869940	0.869944	0.689486	0.689487	-2×10^{-6}	5×10^{-7}	-0.90
2.0	1.194849	1.194859	0.862485	0.862487	-1×10^{-5}	2×10^{-5}	-0.85
4.0	1.758700	1.758664	1.173482	1.173484	-1×10^{-4}	2×10^{-5}	-0.75
6.0	2.250211	2.250073	1.452032	1.452036	-4×10^{-4}	5×10^{-5}	-0.60
8.0	2.695244	2.693612	1.708006	1.708026	-3×10^{-3}	2×10^{-4}	-0.55
10.0	3.107240	3.100232	1.947127	1.947176	-1×10^{-2}	3×10^{-4}	-0.50
-0.5	0.291641	0.291657	0.397353	0.397358	-7×10^{-5}	5×10^{-5}	-1.00
-1.0	0.062754	0.062979	0.288220	0.288270	-6×10^{-4}	5×10^{-4}	-1.05

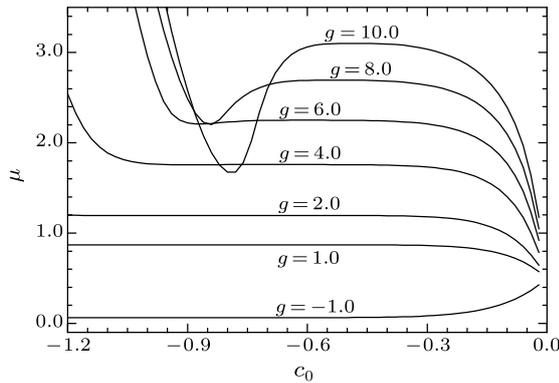


Fig. 1. The chemical potential μ versus c_0 for different value of g .

We can define the residual error

$$\epsilon(x) = \hat{H}_0 \Psi^K(x) + g(\Psi^K(x))^3 - \mu^K \Psi^K(x) \quad (22)$$

to measure the accuracy of the K th-order approximate solution we derived. The squared norm of ϵ can be defined as

$$\|\epsilon\|^2 = \int_{-\infty}^{+\infty} \epsilon(x)^2 dx. \quad (23)$$

Obviously, $\Psi(x) = \Psi^K(x)$ is an exact solution for Eq. (4) when $\|\epsilon\| = 0$. In general, the fact is that $\|\epsilon\| \neq 0$. We think that the smaller the value of $\|\epsilon\|^2$, the more precise the solution is. This implies another way to determine the value of c_0 is by minimizing the squared norm of $\|\epsilon\|^2$ theoretically. However, it is rather complicated to perform such a computation in practice. We still prefer the former method, via observing the so-called c_0 curve, to select an appropriated value for c_0 .

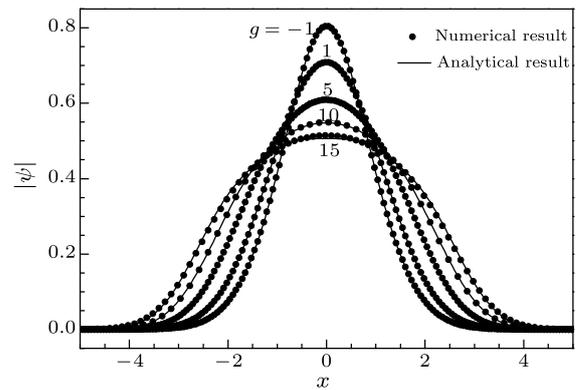


Fig. 2. Profile of wave function $|\Psi|$ for different values of g .

Table 1 lists the numerical values 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 previously, for different values of g . The value of c_0 we choose can ensure that the series are convergent. In Table 1, $e_a = 2E_{\text{kin}} - 2E_{\text{pot}} + E_{\text{int}}$, where E_{kin} , E_{pot} , E_{int} are the dimensionless kinetic energy, potential energy and interaction energy, respectively. From the Virial theorem we know that $2E_{\text{kin}} - 2E_{\text{pot}} + E_{\text{int}} = 0$ for the steady state of the BEC system we are considering. Differences between the E_n (numerical result) and E_a (analytical result) are very small ($\sim 10^{-6}$), which means that the corresponding wave function we derived is a good approximation for the ground state of the BEC system. It is clear that the analytical results agree very well with the numerical results as $|g|$ is not too large. It also can be seen that the error increases as the value of $|g|$ increases. Although we can decrease the error by increasing K or \mathcal{N} , but the computational quantity will increase rapidly, which indicates that our method is

suitable for solving GPE that the atomic interaction is not too strong. In practice, we prefer to increasing the value of K rather than \mathcal{N} to decreasing the error when \mathcal{N} is large enough.

The wave functions $\Psi(x)$ given by our method and the corresponding numerical results, derived by ITP, are shown in Fig. 2 for different values of g . Note that the atom-atom interaction is repulsive when $g > 0$, while it is attractive as $g < 0$. The results show that the HAM can deal with both cases. It is also clear that the analytical results are in good agreement with the numerical results and the error increases as g increases. Figure 2 shows the most important effect of interaction: the attractive interaction sharpens the condensate cloud, while the repulsive interaction broadens it. The density at the center of the trap is lower for larger values of g , which is expected because of the corresponding higher inter-particle repulsion.

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