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Numerical solution for the Gross–Pitaevskii equation

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We solve the time-independent Gross–Pitaevskii (GP) equation which describes the dilute Bose-condensed atoms in harmonic trap at zero temperature by symplectic shooting method (SSM). Both the repulsive nonlinearity and the attractive nonlinearity cases are studied, and the bound state eigenvalues as well as the corresponding wavefunctions are evaluated. We also present the numerical results by studying the time-dependent GP equation, and comparisons are made between the results obtained by the time-independent approach and the time-dependent approach.

KEY WORDS: Gross–Pitaevskii equation, stationary solution, Bose–Einstein Condensate

1. Introduction

Bose–Einstein condensate, which was predicted by Bose and Einstein in 1924, was realized experimentally for the first time in 1995. Its realization in laboratory made profound impact in the theoretical research. At zero or sufficiently low temperature, Bose–Einstein condensate can be described by a self-consistent mean field equation, known as the Gross–Pitaevskii (GP) equation. This equation has a form similar to the nonlinear Schrödinger equation (NSE) [1], which incorporates the external potential as well as the interaction between atoms properly. In order to assist laboratory research, many numerical tests have been done, and good results are often reported. A simple and commonly studied case is the 3D GP equation, which incorporates the interaction between atoms and the spherically symmetric harmonic potential [2–4].

In section 2, we study the time-independent GP equation. This equation can be transformed into Hamiltonian formalism, and then an effective method to solve it is the structure-preserving method [5]. We transform the GP equation into its dimensionless form [3], and apply the symplectic shooting method (SSM) that combines the structure-preserving method and the shooting method to this problem. The bound state eigenvalues and the corresponding wavefunctions for both the repulsive nonlinearity and the attractive nonlinearity cases are worked out in section 3. We also study the similar cases in [4], and present the bound

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state wave functions normalized to unity of the condensate. In section 4, we study the time-dependent GP equation by Euler-centered scheme, and give out the eigenvalues as well as the wavefunctions, and compare the results with those obtained by the time-independent approach. Conclusions are given in section 5.

2. Time-independent GP equation and the numerical method

The time-independent GP equation for neutral atoms in 3D spherically harmonic potential trap can be written as,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) + NU_0\,|\psi(\vec{r})|^2\right]\psi(\vec{r}) = \mu\psi(\vec{r}), \tag{1}$$

where, $V(r) = m\omega_t^2 r^2/2$ is the spherical harmonic trap, m the mass of a single atom, ω_t the angular frequency of the trap, and N is the number of atoms in the condensate. $\psi(\vec{r})$ is the 'wavefunction' of the condensate, and μ is the chemical potential. $U_0 = 4\pi\hbar^2 a_s/m$ represents the interaction between atoms, and a_s is the scattering length. Since this approximation is valid at sufficiently low energies, it is enough to consider only the s-wave scattering between atoms [2]. When $a_s > 0$, the interaction between atoms is repulsive, it is positive to obtain stable condensates. When $a_s < 0$, the interaction between atoms is attractive, it is negative to obtain stable condensates. When the absolute value of the negative scattering length reaches a critical value, it can not support a stable solution. In dilute Bose gases, the condition that $|a_s|/d \ll 1$ can be satisfied very well, where d is the average distance between atoms. Just under this condition, the poseudopotential U_0 which is proportional to the scattering length can be used safely to describe the interaction between atoms.

If the following harmonic oscillator units are used,

$$r = [\hbar/2m\omega_t]^{1/2}\,x, \quad \beta = \mu/\hbar\omega_t$$

and take

$$\psi(r) = \frac{1}{\sqrt{4\pi}\,[\hbar/2m\omega_t]^{3/4}}\frac{\Phi(x)}{x}$$

the dimensionless form of equation (1) reads

$$\left[-\frac{d^2}{dx^2} + \frac{x^2}{4} + \alpha\frac{\Phi^2(x)}{x^2} - \beta\right]\Phi(x) = 0 \tag{2}$$

and the normalization condition is

$$4\pi\int_0^\infty \psi^2(r)\,r^2\mathrm{d}r = \int_0^\infty \Phi^2(x)\,\mathrm{d}x = 1. \tag{3}$$

In equation (2), $\alpha = 2Na_s/[\hbar/2m\omega_t]^{1/2}$ is the nonlinear coefficient. We rewrite equation (2) into a system of ODEs,

$$\frac{d\Psi(x)}{dx} = -\left[\beta - \frac{x^2}{4} - \alpha\frac{\Phi^2(x)}{x^2}\right]\Phi(x) = f(\Phi, x), \tag{4}$$

$$\frac{d\Phi(x)}{dx} = \Psi(x) = g(\Psi). \tag{5}$$

If we take x as the 'time' variable, $\Phi(x)$ the general position, and $\Psi(x)$ the general velocity, it is easy to see that the system equation (4), (5) is of the form of Hamiltonian equation which is a separable Hamiltonian system. The Hamiltonian function can be written as follows,

$$H = \frac{\Psi^2(x)}{2} + \frac{1}{2}\left[-\frac{x^2}{4} + \beta\right]\Phi^2(x) - \frac{1}{4}\alpha\frac{\Phi^4(x)}{x^2}. \tag{6}$$

So, the reliable method for this kind of problem is the structure-preserving method. Many symplectic schemes have been applied in solving time-independent Schrödinger equation [6–9]. In this paper, we adopt the fourth-order explicit symplectic scheme to solve equations (4) and (5). The 4-stage fourth-order explicit symlectic scheme reads [9]:

$$\begin{aligned}
&p_1 = \Psi^n + c_1 h f(\Phi^n, x^n), \qquad q_1 = \Phi^n + d_1 h g(p_1),\\
&x_1 = x^n + d_1 h,\\
&p_2 = p_1 + c_2 h f(q_1, x_1), \qquad q_2 = q_1 + d_2 h g(p_2),\\
&x_2 = x_1 + d_2 h,\\
&p_3 = p_2 + c_3 h f(q_2, x_2), \qquad q_3 = q_2 + d_3 h g(p_3),\\
&x_3 = x_2 + d_3 h,\\
&\Psi^{n+1} = p_3 + c_4 h f(q_3, x_3), \qquad \Phi^{n+1} = q_3 + d_4 h g(\Psi^{n+1}),\\
&x^{n+1} = x_3 + d_4 h = x^n + h,
\end{aligned} \tag{7}$$

where $c_1 = c_4 = \alpha/2$, $c_2 = c_3 = (\alpha+\beta)/2$, $d_1 = d_3 = \alpha$, $d_2 = \beta$, $d_4 = 0$ and $\alpha = \left(2 - 2^{1/3}\right)^{-1}$, $\beta = 1 - 2\alpha$.

Shooting method is a popular method to solve boundary value problems, and it aims at converting the boundary value problem into an initial value problem. We use the SSM that combines the structure-preserving method and the shooting method to this problem. We adopt the well-known boundary conditions [4]. When $x \sim 0$, $\Phi(x)/x$ tends to a limit, then $\Phi(0) = 0$. When $x \sim \infty$, the nonlinear term in equation (2) vanishes, and then equation (2) reduced to the form of the plain harmonic oscillator equation which has two analytical

solutions. Select the one that vanishes at sufficiently large distance, and work out its derivative, the well-known boundary conditions are,

$$x \sim 0, \quad \Phi(\varepsilon) = \varepsilon \Phi'(0), \quad \left(\varepsilon = 10^{-6}\right), \tag{8}$$

$\Phi'(0)$ unknow,

$$x \sim \infty, \quad \Phi(x)_{\text{asym}} = C \exp\left(-\frac{x^2}{4} + \left(\beta - \frac{1}{2}\right) \ln(x)\right), \tag{9}$$

$$\Phi'(x)_{\text{asym}} = C \left(-\frac{x}{2} + \left(\beta - \frac{1}{2}\right) \frac{1}{x}\right) \exp\left(-\frac{x^2}{4} + \left(\beta - \frac{1}{2}\right) \ln(x)\right). \tag{10}$$

We take the right boundary at sufficiently large distance as $x_{\max}$, and at $x_{\max}$, the numerical solution of equations (4) and (5), $\Phi(x)_{\text{num}}$ and $\Phi'(x)_{\text{num}}$, should satisfy the following condition,

$$\frac{\Phi(x)_{\text{num}}}{\Phi'(x)_{\text{num}}} = \frac{\Phi(x)_{\text{asym}}}{\Phi'(x)_{\text{asym}}} = \left[-\frac{x}{2} + \left[\beta - \frac{1}{2}\right] \frac{1}{x}\right]^{-1}. \tag{11}$$

Taking into consideration the normalization of the NSE, the criterion for our SSM at $x_{\max}$ is taken to be,

$$\left|\Phi(x)_{\text{num}} - \Phi'(x)_{\text{num}} \left[-\frac{x}{2} + \left[\beta - \frac{1}{2}\right] \frac{1}{x}\right]^{-1}\right| < \varepsilon_1 \quad \left(\varepsilon_1 = 10^{-10}\right), \tag{12}$$

$$\left|\int_0^{\infty} \Phi^2(x)_{\text{num}} \, \mathrm{d}x - 1\right| < \varepsilon_2 \quad \left(\varepsilon_2 = 10^{-5}\right), \tag{13}$$

where ε_1 and ε_2 are the accuracy in our numerical computation.

We solve the time-independent NSE with existence of an external potential by the general method presented in [3]. Given a nonlinear coefficient α, we take $\Phi'(0)$ and β as variables, and then apply the SSM.

For certain $\Phi'(0)$, we let β run in a large range (choosing the appropriate searching range of β is guided by the cases of harmonic oscillator equation), and propagate the solution of equation (2) out to $x_{\max}$ by the explicit symplectic method stated above, and the numerical solutions at $x_{\max}$ are examined by the criterion of equations (12) and (13). Then we let $\Phi'(0)$ go one-step forward, $\Delta\Phi'(0)$, again let β run in the large range to test whether they are the desired $\Phi'(0)$ and β, and so on. That means we are doing SSM in the plane of $\Phi'(0)$ and β. Only when the proper values of $\Phi'(0)$ and β are reached, the corresponding numerical

solutions at $x_{\max}$ can satisfy both equations (12) and (13). Meanwhile, the eigenvalues and the corresponding wavefunctions normalized to unity are obtained. All this means that the general method is practiced in the plane of $\Phi'(0)$ and β, so the computation cost is considerably high. From our experience in computation we find that ε_1 in equations (12) behaved linearly, and that ε_2 in equation (13) largely behaved linearly too. It is promising! These two phenomenons motivate us to apply half-interval method to both variable $\Phi'(0)$ and variable β. As consequences of the utilization of half-interval method, we can choose relatively larger steps $\Delta\beta$ and $\Delta\Phi'(0)$. Undoubtedly that will save much computation cost, and make our computation stable, and furthermore, it gives advantages to attain higher accuracy. We hasten to add that we are not searching in large ranges blindfold, and we are guided by the cases of the harmonic oscillator equation.

3. Numerical results

We practice the method to the problem stated above and obtain the eigenvalues and the corresponding wavefunctions for the condensate at zero temperature as below.

3.1. The repulsive nonlinearity

In the repulsive nonlinearity cases ($\alpha > 0$), the solutions of the condensate are stable. Let α range in 0–50, we work out the ground state eigenvalues and the first excited state eigenvalues as well as the corresponding wavefunctions, which are displayed, respectively, in figures 1–3. For convenience we choose the scaling as follows: horizontal axis to be x, and vertical axis to be $\Phi(x)/x$. As can be seen from figures 1 and 2, the condensate expands with the increasing of α. There is a node in the wavefunction of the first excited state. It can be seen clearly in figure 3 that the problem reduced to the harmonic oscillator cases when $\alpha = 0$, and the plain eigenvalues 1.5 and 3.5 are obtained (Since $x \sim 0$, $\Phi(0) = 0$, the principle quantum number n can only chose odd number). Generally, we set $h = 10^{-2}$, $\Delta\beta = 10^{-4}$, and $\Delta\Phi'(0) = 10^{-2}$ in our computation. We set $\Delta\beta = 10^{-5}$ when the nonlinear coefficient is larger (i.e. $\alpha = 50$). For ground state wavefunctions we set $x_{\max} = 8$, and $x_{\max} = 8 - 9$ for the first excited state wavefunctions. Our computation results are consistent with those of [3].

3.2. The attractive nonlinearity

In the attractive nonlinearity cases ($\alpha < 0$), the solutions of the condensate are not always stable. Since interactions between atoms are attractive now, the absolute value of the nonlinear coefficient cannot increase without a limitation. The ground state wavefunctions as α ranged in 0 to -1.6 are displayed in fig-

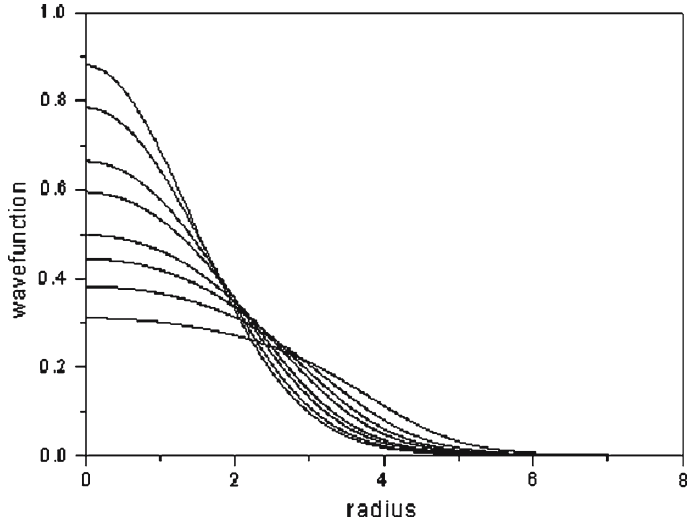

Figure 1. The ground state wavefunctions of the condensate. The nonlinear coefficient is taken to be 0.1, 1, 3, 5, 10, 15, 25, and 50 down the vertical axis. Horizontal axis is x, and vertical axis is $\Phi(x)/x$.

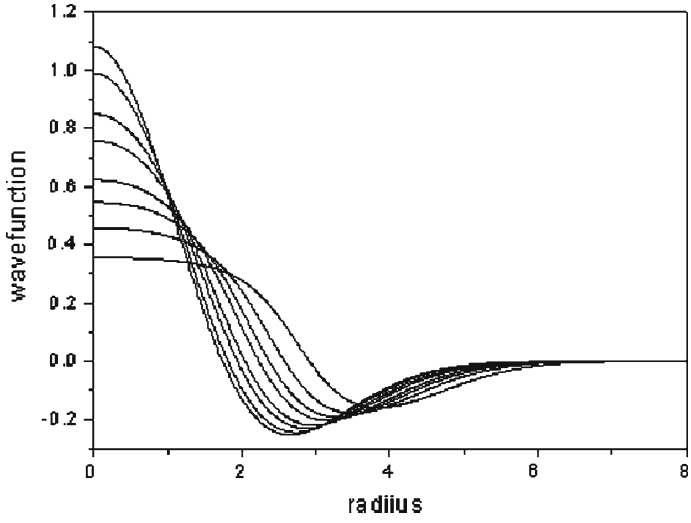

Figure 2. The first excited state wavefunctions of the condensate. The nonlinear coefficient is taken to be 0.1, 1, 3, 5, 10, 15, 25, and 50 down the vertical axis. Horizontal axis is x, and vertical axis is $\Phi(x)/x$.

ure 4. It can be seen from figure 4 that the condensate peaks with the increasing of the absolute value of the nonlinear coefficient. Here, we set $x_{\max} = 7$. We also give out the picture of the boundary value $\Phi'(0)$ via α, the latter ranges in -1.6–50, as displayed in figure 5. The picture corresponding to the positive part of α largely coincides with that of [3].

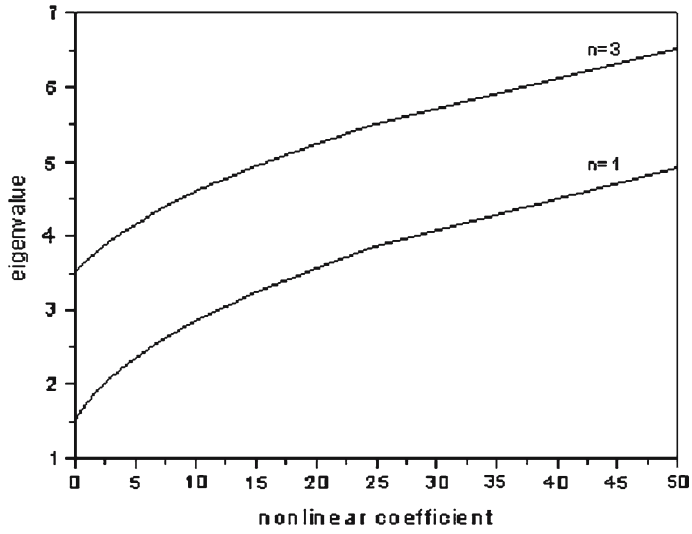

Figure 3. The evolution of the eigenvalues of the ground state ($n = 1$) and the first excited state ($n = 3$) with the nonlinear coefficient. Horizontal axis is α, and vertical axis is β. n is the principle quantum number.

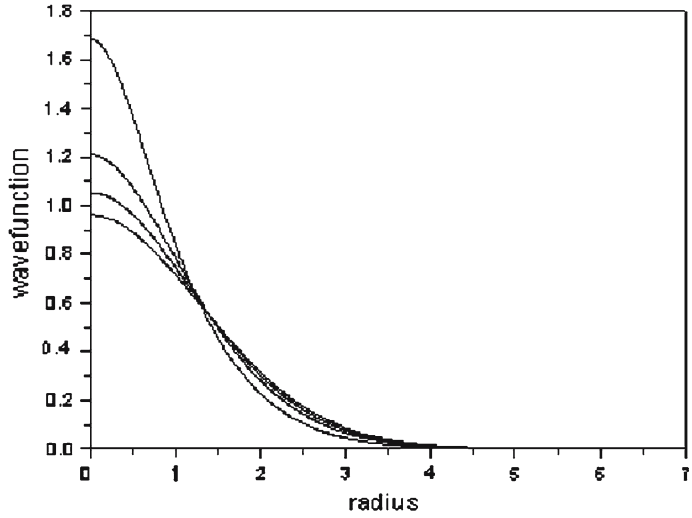

Figure 4. The ground state wavefunctions of the condensate. The nonlinear coefficient is taken to be $-1.6, -1.2, -0.8$, and -0.4 down the vertical axis. Horizontal axis is x, and vertical axis is $\Phi(x)/x$.

In order to test our SSM further, we study the similar case in [4] that deals with the very stationary NSE but concentrates on the cases of attractive nonlinearity. This literature presents another way of normalization that saves much

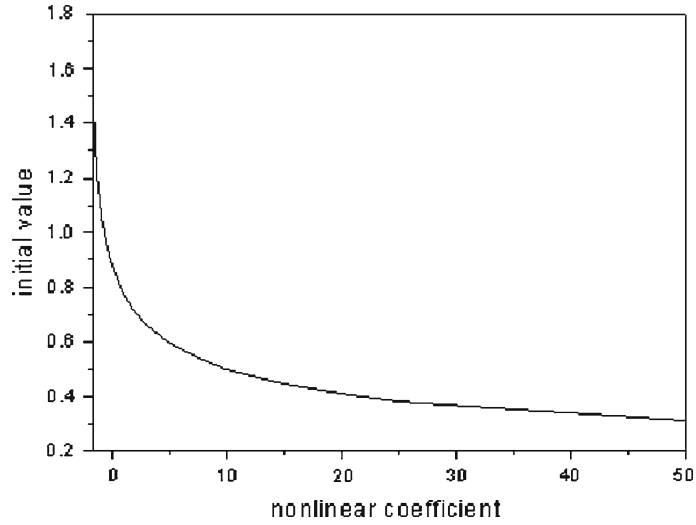

Figure 5. Boundary value $\Phi'(0)$ via α. α is taken to be in -1.6–50.

computation. The equation in [4] is

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{1}{4}x^2-\frac{|\Phi(x)|^2}{x^2}\right]\Phi(x)=\beta\Phi(x), \tag{14}$$

$$\int_0^\infty |\Phi(x)|^2\,\mathrm{d}x = n, \tag{15}$$

$$n = 2N|a_\mathrm{s}|\sqrt{\frac{2m\omega_\mathrm{t}}{\hbar}}, \tag{16}$$

where n is a real number related to the number of atoms N. The author pointed out that n is given out as the nonlinear coefficient $\left|C_{nl}^{3D}\right|$ of [2]. In our paper for the attractive nonlinearity cases, we have $-n=\alpha$. We list part of their results [4] in the first three columns of table 1. It can be seen that for given β, they worked out the corresponding n. Recall that $-n=\alpha$, on the premise of the same conditions that are adopted in our computation, for certain α, we can work out the related β. So we do our computation on the basis of $-n$, and the results are listed in the last three columns in table 1. We set $x_{\max}=7$. On the whole the results of the two methods coincide very well except one point $n=-1.6237$. By further computation we found out that the nonlinear coefficient should be -1.6112 corresponding to $\beta=0.2$. Furthermore, we display the ground state

Table 1
The first three columns are the results of [4], and the last three columns are our computation results.

β	$\Phi'(0)$	$-n$	α	$\Phi'(0)$	β
1.5	0	0	0	0.89325	1.50000
1.4	0.5448721	−0.3310	−0.3310	0.94703	1.40000
1.2	0.9939222	−0.8597	−0.8597	1.07195	1.20000
1.0	1.3567267	−1.2282	−1.2282	1.22406	1.00009
0.8	1.7022822	−1.4607	−1.4607	1.40844	0.80003
0.6	2.0495486	−1.5839	−1.5839	1.62844	0.60006
0.4	2.4045809	−1.6254	−1.6254	1.88594	0.40009
0.2	2.5851166	−1.6237	−1.6237	2.03008	0.29906
0.0	3.1340461	−1.5632	−1.5632	2.50742	−0.00050
−1.0	4.8924036	−1.2234	−1.2234	4.42383	−1.00041
−2.0	6.3914678	−0.9843	−0.9843	6.44258	−2.00026

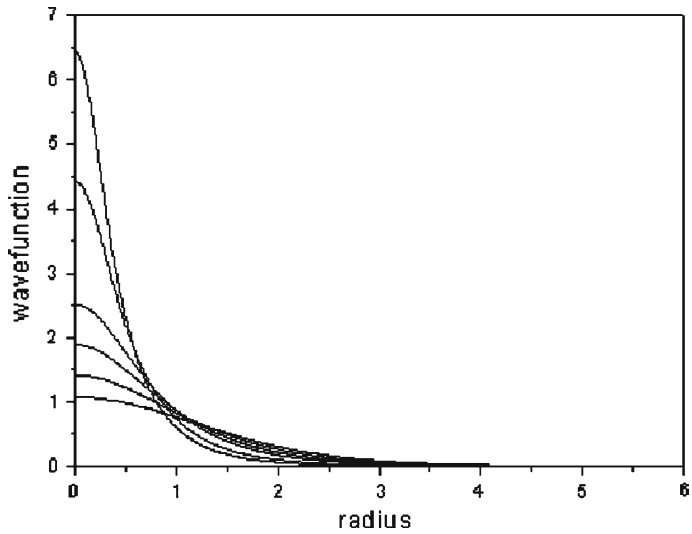

Figure 6. The ground state wavefunctions of the condensate of the attractive nonlinearity cases. β is taken to be −2.0, −1.0, 0.0, 0.4, 0.8, 1.2 down the vertical axis. Horizontal axis is x, and vertical axis is $\Phi(x)/x$.

wavefunctions normalized to unity in figure 6. In figure 6, we can see clearly the shape of the condensates corresponding to different values of β. But the stability of the wavefunctions corresponds to the negative eigenvalues is doubtful.

4. Time-dependent GP equation and the numerical method

For neutral atoms in 3D spherically harmonic potential trap, the time-dependent GP equation reads

$$\left[-\frac{\hbar^2}{2m}\nabla^2+\frac{1}{2}m\omega_{\mathrm{t}}^2r^2+NU_0\left|\psi(\vec{r},t)\right|^2\right]\psi(\vec{r},t)=i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}, \tag{17}$$

$$\int\left|\psi\left(\vec{r},t\right)\right|^2\mathrm{d}\vec{r}=1. \tag{18}$$

The wavefunction can be written as

$$\psi(\vec{r},t)\equiv\psi(r,t)=\psi(r)\exp(-i\mu t/\hbar).$$

Equations (17) and (18) can be rescaled by $r=[\hbar/2m\omega_{\mathrm{t}}]^{1/2}x$, $t=\tau\omega_{\mathrm{t}}$ into the dimensionless form

$$\left[-\frac{\partial^2}{\partial x^2}+\frac{x^2}{4}+\alpha\frac{|\Phi(x,\tau)|^2}{x^2}\right]\Phi(x,\tau)=i\frac{\partial\Phi(x,\tau)}{\partial\tau}, \tag{19}$$

$$\int_0^\infty|\Phi(x,\tau)|^2\,\mathrm{d}x=1, \tag{20}$$

where

$$\psi(r,t)=\frac{1}{\sqrt{4\pi}\,[\hbar/2m\omega_{\mathrm{t}}]^{3/4}}\frac{\Phi(x,\tau)}{x},\ \beta=\mu/\hbar\omega_{\mathrm{t}},\ \Phi(x,\tau)=\Phi(x)\exp(-i\beta\tau).$$
$$\alpha=2Na_{\mathrm{s}}/[\hbar/2m\omega_{\mathrm{t}}]^{1/2}$$

is the nonlinear coefficient.

If we write the wavefunction in terms of its real and imagine parts separately as $\Phi(x,\tau)=a(x,\tau)+ib(x,\tau)$, equation (19) becomes

$$\dot{a}=-b_{xx}+\frac{x^2}{4}b+g\frac{(a^2+b^2)}{x^2}b, \tag{21}$$

$$\dot{b}=-\left[-a_{xx}+\frac{x^2}{4}a+g\frac{(a^2+b^2)}{x^2}a\right] \tag{22}$$

and further becomes

$$\dot{a}_j=-\frac{1}{h^2}\left[b_{j+1}-2b_j+b_{j-1}\right]+\frac{x_j^2}{4}b_j+g\frac{(a_j^2+b_j^2)}{x_j^2}b_j, \tag{23}$$

$$\dot{b}_j=-\left[-\frac{1}{h^2}\left[a_{j+1}-2a_j+a_{j-1}\right]+\frac{x_j^2}{4}a_j+g\frac{(a_j^2+b_j^2)}{x_j^2}a_j\right], \tag{24}$$

where they are discretized in space by central difference, $j = 0, \ldots, N$. We take the boundary conditions to be

$$x \to 0, \qquad \Phi(\varepsilon, \tau) = 0, \qquad \varepsilon = 10^{-6}, \quad x \to \infty, \qquad \Phi(x, \tau) = 0. \quad (25)$$

It can be verified that equations (23) and (24) are of the form of Hamiltonian equation, and the Hamiltonian function is

$$H = \frac{1}{2h^2} \sum_{j=1}^{N-1} \left[b_j (b_{j+1} - 2b_j + b_{j-1}) + a_j (a_{j+1} - 2a_j + a_{j-1}) \right] + \sum_{j=1}^{N-1} \left[\frac{x_j^2}{8} (a_j^2 + b_j^2) + \frac{g}{4x_j^2} (a_j^4 + b_j^4) + \frac{g}{2x_j^2} a_j^2 b_j^2 \right]. \quad (26)$$

Therefore, we can apply symplecic algorithm in solving this equations, such as the Euler-centered scheme or the symplectic RK scheme. We adopt the Euler-centered scheme

$$z^{k+1} = z^k + \tau J^{-1} (\nabla H)_{(z^{k+1} + z^k)/2}. \quad (27)$$

The normalization condition is naturally preserved.

For ground state solution of the condensate, we start with the following normalized analytically known ground state solution of equation (19) with $\alpha = 0$

$$\Phi(x, 0) = 2^{-0.5} (2\pi)^{-0.25} 2x \exp\left(-\frac{x^2}{4} \right) \quad (28)$$

as the initial input.

We begin the iteration by the equation with $\alpha = 0$, and then at each time step $\Delta\tau = 10^{-3}$, α is slowly increased by $\Delta\alpha = 10^{-5}$, the same boundary condition is implemented and convergence is required. When the desired α is reached, the wavefunction is propagated in time, and the stability of the wavefunction is tested, and the corresponding eigenvalue is calculated [1]. Space step is $h = 0.1$. The wavefunctions obtained are presented in figure 7, and the eigenvalues calculated with $h = 0.1$ and $h = 0.01$ for different nonlinear coefficient are displayed in table 2. It can be seen clearly that the energies calculated agree well with those obtained by the time-independent approach in section 3.

5. Conclusions

In this paper, we study the time-independent GP equation, which describes the stationary states for neutral atoms in a spherical harmonic trap. Since it is

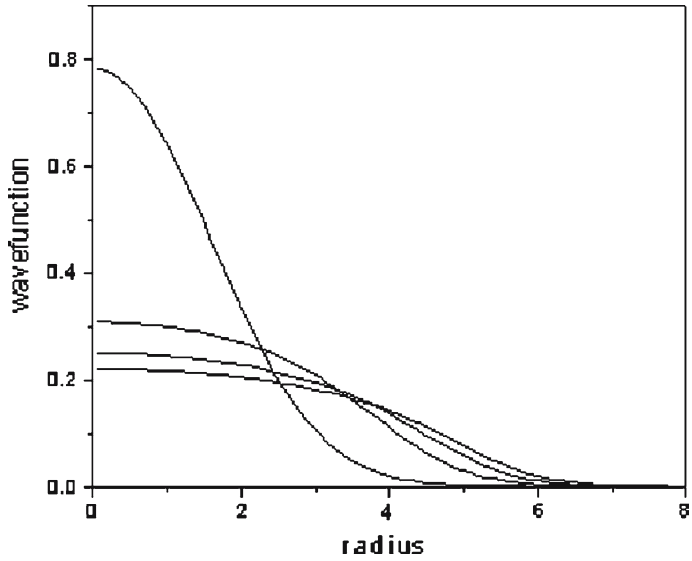

Figure 7. The ground state wavefunctions obtained by the time-dependent approach. α is taken to be 1, 50, 100, and 150 down the vertical axis. Horizontal axis is x, and vertical axis is $\Phi(x)/x$.

Table 2
Comparison of the eigenvalues calculated by the time-independent approach and the time-dependent approach.

α	1	3	10	15	25	50
$\beta^{h=0.01}_{\text{time-independent}}$	1.74147	2.09148	2.86105	3.24668	3.84852	4.91831
$\beta^{h=0.01}_{\text{time-dependent}}$	1.74146	2.09141	2.86103	3.24655	3.84873	4.91846
$\beta^{h=0.1}_{\text{time-dependent}}$	1.74107	2.09136	2.86104	3.24678	3.84865	4.91797

a Hamiltonian system, and has symplectic structure, so the structure-preserving method is an efficient method to solve this kind of problem. By the general method presented in literature and the well-known boundary conditions, we apply SSM accompanied by the half-interval method to this Hamiltonian system. Both the repulsive nonlinearity and the attractive nonlinearity cases are considered, and the eigenvalues and the corresponding wavefunctions of the condensate are given. We also study the time-dependent GP equation, and give out the results by the Euler-centered scheme, which is a symplectic algorithm too. It is assured that our method is reliable and efficient from the computation results.

Acknowledgments

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