Improved numerical approach for time-independent Gross-Pitaevskii nonlinear Schrödinger equation.

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In the present work, we improve a numerical method, developed to solve the Gross-Pitaevskii nonlinear Schrödinger equation. A particular scaling is used in the equation, which permits to evaluate the wave-function normalization after the numerical solution. We have a two point boundary value problem, where the second point is taken at infinity. The differential equation is solved using the shooting method and Runge-Kutta integration method, requiring that the asymptotic constants, for the function and its derivative, are equal for large distances. In order to obtain fast convergence, the secant method is used.

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Precise and fast numerical solutions to non-linear equations have become considerable important in computational physics. So, the numerical procedure are relevant also to be described, when treating such problems, considering the computational time consuming. In the present work, we pay attention specially to this problem, proposing an alternative approach to a method recently described in Ref. [1], which was used to solve the Gross-Pitaevskii nonlinear Schrödinger equation (NLSE) for trapped neutral atoms, with positive two-body scattering lengths. In Ref. [1], the NLSE treated in Ref. [1] was extended to a time-dependent one, for both positive and negative two-body scattering lengths, where the Crank-Nicolson algorithm (appropriate for time evolution) was considered. This approach, however, has the disadvantage that can only reach the stable solutions. In case one needs to add other non-linear terms (of higher order) in the original equation [1], it is not feasible to reach another region of stable solutions if in between there is an unstable region. This implies that it should be appropriate to combine a static method (as the one used in Ref. [1]) with the method used in Ref. [1] when we are interested in obtain all the stable and unstable solutions and also the corresponding time evolutions. So, in this perspective, any improvement of the method considered in Ref. [1] would be relevant.

In the following, we briefly describe the physics related to the NLSE considered in [1], and the numerical procedure used to solve it. Then we present an alternative approach, which can considerably reduce the time to search for the solutions and the normalizations.

The nonlinear Schrödinger equation, which describes the condensed wave-function in the mean-field approximation can be written as

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + \frac{m}{2} \omega^2 r^2 - \frac{4\pi\hbar^2}{m} |a| |\Psi(\vec{r})|^2 \right] \Psi(\vec{r}) = \mu \Psi(\vec{r}),
\]

where \(m\) is the mass of a single atom, \(\omega\) the angular frequency of the trap, \(\mu\) the chemical potential and \(a\) the scattering length. In the present approach, as we are more concerned with numerical aspects, for convenience we treat only cases with negative scattering lengths \((a < 0)\). Later we also consider the inclusion of a three body interaction term.

The chemical potential \(\mu\) is fixed by the number \(N\) of atoms in the condensed state, which is given by the normalization condition:

\[
\int d^3r |\Psi(\vec{r})|^2 = N. \tag{2}
\]

In Refs. [1] and [3] the NLSE for Bose-Einstein condensates, as given in Eq. (1), was solved numerically. In Ref. [1], the shooting and the Runge-Kutta methods were combined. For a given normalization parameter \(N\) was solved the corresponding dimensionless equation. The asymptotic form of the wave-function was renormalized to be equal to the numerical wave-function for a sufficiently large distance. The wave-function normalization parameter was increased until the Wronskian of the asymptotic behavior of the numerical and the analytic function changes sign.

Next, we present in detail the numerical approach we have used, in order to show up the similarities and subtle differences between this approach and the one of Ref. [1].

As we suggest from our experience, such subtle differences in the numerical procedures will reduce considerably the time to search for the solutions. We first rewrite

\[
*\text{For the numerical considerations, there is no restrictions about the sign of the scattering length, as the solutions with } a > 0 \text{ are equally accessible using the same procedure and changing the sign of the non-linear term in Eq. (1).}
\]
Eq. (1) in dimensionless units, in order to become apparent the scales contained in Eq. (1). By rescaling Eq. (1) for the s-wave solution, we obtain

$$\left[ -\frac{d^2}{dx^2} + \frac{1}{4} x^2 - \frac{\left| \Phi(x) \right|^2}{x^2} \right] \Phi(x) = \beta \Phi(x), \quad (3)$$

where \( x \equiv \sqrt{2m\omega / \hbar} \), \( \Phi(x) \equiv \sqrt{8\pi|a|N} r \Phi(r) \), and \( \beta \equiv \mu / \hbar \omega \leq 3/2 \). The normalization for \( \Phi(x) \), obtained from Eq. (2) defines a real number \( n \) (given as \( |C_n| \) in Ref. [1]) related to the number of atoms \( N \):

$$\int_0^\infty dx |\Phi(x)|^2 = n, \quad n \equiv N(8\pi|a|) \frac{2m\omega}{\hbar}.$$

We would like to emphasize that, by using this scaling procedure, the numerical solutions for the equation are free of any normalization constraint, or other parameter dependence. The parameter \( N \), related to the number of particles, was removed from the differential equation and its not necessary to check Eq. (3) or (1) at all steps of the calculation. The normalization is found a posteriori, using Eq. (1).

The boundary conditions for Eq. (3) are given as [1]:

$$\Phi(0) = 0 \quad \text{and} \quad \Phi(x)|_{x \rightarrow \infty} \rightarrow \Phi_{\text{asym}}(x)$$

$$\Phi_{\text{asym}}(x) \equiv C \exp \left[ -\frac{x^2}{4} + \left( \beta - \frac{1}{2} \right) \ln(x) \right], \quad (5)$$

where \( C \) is a constant to be determined. By using Runge-Kutta method and starting with the given \( \Phi(0) \), the problem is reduced to determine the value of the corresponding derivative, \( \Phi'(0) \), which satisfies the asymptotic condition at infinity. So, we are tempted to shoot [3,4] many values for \( \Phi'(0) \) until we obtain numerically a constant for large distances. At a certain \( x_{\text{max}} \) we expect a constant, given by

$$C_{\Phi} \equiv \Phi_{\text{num}}(x) \exp \left[ -\frac{x^2}{4} - \left( \beta - \frac{1}{2} \right) \ln(x) \right] \quad (6)$$

This process is very laborious and difficult to reach precise solutions due to the problem of verifying, for some large \( x \), when \( C_{\Phi} \) is constant, within the required numerical precision. The way to overcome these difficulties is to consider the asymptotic derivative of \( \Phi(x) \), that is

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

and also determine (numerically) the expression

$$C_{\Phi'} \equiv \Phi'_{\text{num}}(x) \times$$

$$\times \left[ -\frac{x}{2} + \left( \beta - \frac{1}{2} \right) \frac{1}{x} \right]^{-1} \exp \left[ -\frac{x^2}{4} - \left( \beta - \frac{1}{2} \right) \ln(x) \right], \quad (7)$$

with \( x_{\text{max}} \) such that both (3) and (2) are constants. When we are using the correct value of \( \Phi'(0) \) we also should obtain \( C_{\Phi} = C_{\Phi'} = C \) for a large enough \( x = x_{\text{max}} \).

An useful remark we can make is that when we overestimate the value of \( \Phi'(0) \), \( C_{\Phi} \) increases and \( C_{\Phi'} \) decreases. The inverse happens when we underestimate \( \Phi'(0) \). So, this condition is valuable to tune \( \Phi'(0) \). It corresponds to solve the equation

$$C_{\Phi} - C_{\Phi'} = 0,$$

having \( \Phi'(0) \) as the unknown variable. Substituting (5) and (6) in (3) we recover the expression for the Wronskian \( W(\Phi_{\text{num}}(x_{\text{max}}), \Phi_{\text{asym}}(x_{\text{max}})) = 0 \) stated in [1]. Eq. (3) can be solved by secant method [3]. So, we begin with an approximate solution for \( \Phi'(0) \), as an input to the secant method, where \( C_{\Phi} \) and \( C_{\Phi'} \) are evaluated by the Runge-Kutta method. We should emphasize that, to succeed with such method the original guess for \( \Phi'(0) \) should be not far from the correct value, otherwise the method can conduct to the trivial solution \( \Phi(x) = 0 \) or to overflows. In our procedure, for a fixed \( \beta, x_{\text{max}} \) was first estimated to be equal to 4.2 and \( \Phi'(0) \) was used as an initial trial to extend \( x_{\text{max}} \) to 5.6 and subsequently to 7.0. Once we find a solution for \( \Phi'(0) \), for a given \( \beta \), we decrease \( \beta \) slightly by \( \Delta \beta \) using the previous \( \Phi'(0) \) to find the new \( \Phi'(0) \). This process allows us to “walk” along \( \beta \) values, obtaining the corresponding solutions and results for \( n \).

Although the secant method can become unstable under certain conditions, in this case it will not occur, as we explain in the following. We found that the secant method is appropriate, as we can be as near as desired to the solution, starting with a given analytical solution of the corresponding linear Schrödinger equation. So, we just need to implement an automatic algorithm routine to make slow variations of \( \beta \) and the corresponding slow shift (from the initially zero) of \( \Phi'(0) \), in order to satisfy the corresponding non-linear equation. In this way, we are always near the solution, such that the secant method can be applied. We think the same procedure can be generally applied for solitary equations. The algorithm of slow variation of \( \beta \) (deformation algorithm) does not need the estimation for the derivative of the wave-function at \( x = 0 \), as given in Eq.(3.7) of Ref. [1], for every solution, except for the first one were we take it near the harmonic oscillator solution. We understand that the analytical approximation given in Ref. [1] to estimate the derivative at \( x = 0 \) is not the most convenient in the present case. Considering that in general such equations are highly non-linear, the initial guess for the derivative of \( \Phi \) at \( x = 0 \) can easily cause overflow when determining the asymptotic constants (Wronskian) at large distances. Our initial guess can be very close to the harmonic oscillator solution, which corresponds to \( \Phi'(0) = 0 \), avoiding possible overflows for sufficient large distances. In our numerical approach, considering that \( \beta = 1.5 \) is a trivial
solution of the linear harmonic oscillator, we started with $\beta = 1.4$, trial $\Phi'(0) = 0.6$ and $\Delta \beta = 0.02$. For each $\beta$ it was necessary 4 ~ 6 iterations in the secant method [3], for each $x_{\text{max}}$.

Our results, for several values of $\beta$, are partially listed in Table I. The solutions with $\beta \leq 0.4$ are unstable and not shown in Ref. [3]. However, the solutions with $\beta \geq 0.4$ well agree with their results. As one can observe in Table I, the method also can reach solutions with negative chemical potentials ($\beta < 0$). A numerical stability check, which can be done by evolving the static solutions, can easily be followed by using a time dependent method, as the Crank-Nicolson method [3,6].

In Fig. 1 we also show three plots for the chemical potential, $\beta$, as a function of $n$, in case of zero angular momentum. The three plots shown correspond to the lower radial states ($n_r = 0, 2, 4$) of Eq. (3). The plot labeled with $n_r = 0$ corresponds to Table I. In the limit of the harmonic oscillator solution, where $n = 0$ and the equation is linear, we obtain the usual known solutions.

In Fig.2 we have another example of the application of the method described here. In this case, we consider the addition of another non-linear term inside the square brackets of Eq. (3), given by

$$g_3 \frac{|\Phi(x)|^4}{x^4},$$

which can be directly related to the three-body effects, where $g_3$ is the non-dimensional strength of the corresponding three-body interaction. The physical consequences of the addition of such a term in the NLSE is discussed in both references given in [3].

**TABLE I.** Numerical solutions for the NLSE including two-body interaction, when the two-body scattering $a$ is negative. We consider that at $x_{\text{max}} = 7.0$ we have achieved the asymptotic limit.

| $\beta$ | $\phi'(0)$ | $C$ | $n$ |
|--------|------------|-----|-----|
| 1.5    | 0.5448721  | 0.535 | 0.3310 |
| 1.4    | 0.9939222  | 0.929 | 0.7854 |
| 1.2    | 1.3567267  | 1.187 | 1.2282 |
| 1.0    | 1.7022822  | 1.374 | 1.4607 |
| 0.8    | 2.0495486  | 1.510 | 1.5839 |
| 0.6    | 2.4054809  | 1.608 | 1.6254 |
| 0.4    | 2.5851166  | 1.648 | 1.6237 |
| 0.2    | 3.1340461  | 1.741 | 1.5632 |
| -1.0   | 4.8924036  | 2.110 | 1.2234 |
| -2.0   | 6.3914678  | 2.995 | 0.9843 |

**FIG. 1.** We show the chemical potential, $\beta$, as a function of $n$, which is related to the number of particles by the Eq.(4). The three plots shown correspond to the lower radial states ($n_r$) of Eq. (3) (with zero angular momentum), such that in the limit of the harmonic oscillator solution, where $n = 0$, we have the usual known solutions. The plot labeled with $n_r = 0$ corresponds to Table I.

**FIG. 2.** We show the chemical potential, $\beta$, as a function of $n$, in case we consider three-body effects. The three plots shown correspond to the radial state solutions for $g_3 = 0$ (no quintic term), $g_3 = 0.016$ and $g_3 = 0.03$. The plot labeled with $g_3 = 0$ corresponds to Table I.

To finalize, we have presented in detail an improvement to a numerical procedure used to solve a non-linear differential equation, which is commonly applied for Bose-condensed states. In our example, we solve the Gross-Pitaevskii equation with an attractive two-body and a repulsive three-body interaction. We should note that, by using a simplified scaling procedure [given in Eqs.(3) and (4)], the numerical solutions for the equation are free of any normalization constraint, or other parameter dependence. The parameter $N$, related to the number of
particles, was removed from the differential equation and it is not necessary to obtain the normalization at each step of the calculation. Eq. (4) gives the normalization \textit{a posteriori}. So, by using the above scaling procedure, it emerges the main difference between the present method and the one given in Ref. [1], when looking for the solutions of the NLSE:

- in our approach, we searched for the derivative of the wave-function at \( x = 0 \) till the asymptotic constants match (when the Wronskian vanishes), and the normalization is given at the end;

- in [1] the normalization parameter \( A \) is incremented till the sign of the Wronskian is reached. For the final renormalization they also use other intermediate parameters, as \( A_0, N_0, A_1, N_1 \).

As we are not restricted by the normalization, our approach is a clear improvement to the method given in Ref. [1], particularly when considering the simplification and the transparency in the normalization procedure. Such advantage can be further explored when more involved calculation are presented, as in Ref. [7] where collective excitations are evaluated. A different scaling removes the normalization constraint and allows one to obtain it \textit{a posteriori}, after the numerical solutions are achieved for the eigenvalues.

In our numerical procedure, we employ the shooting method on Runge-Kutta integration, matching the asymptotic constants for the wave-function and for the corresponding derivative. This procedure is shown to be equivalent to make the Wronskian vanish at such large distances. In order to obtain a faster convergence to the solution, we also included the secant method. The numerical optimization to the method employed in Ref. [1], described here, is not restricted to the NLSE we have used. It can be used quite generically for second order solitonic differential equations whose solutions asymptotically vanish at large distances. We consider particularly relevant an optimization of the method of Ref. [1] in the perspective of looking for solutions of differential equations with higher order non-linear terms; and also in the perspective of combining such method (appropriate for static solutions) with a time-dependent one.

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