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Relaxation algorithm to hyperbolic states in Gross–Pitaevskii equation

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Abstract

A new version of the relaxation algorithm is proposed in order to obtain the stationary ground-state solutions of nonlinear Schrödinger-type equations, including the hyperbolic solutions. In a first example, the method is applied to the three-dimensional Gross–Pitaevskii equation, describing a condensed atomic system with attractive two-body interaction in a non-symmetrical trap, to obtain results for the unstable branch. Next, the approach is also shown to be very reliable and easy to be implemented in a non-symmetrical case that we have bifurcation, with nonlinear cubic and quintic terms.

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The Gross–Pitaevskii (GP) equation [1] has been extensively used in the description of Bose–Einstein condensates at temperature $T = 0$ [2]. Usually this equation provides ground state solutions that can readily be achieved with several algorithms. This equation has a cubic nonlinearity. In general, for a negative cubic term (negative two-body scattering length, $a < 0$), with a fixed and reasonable (not too large) nonlinearity, a bifurcation branch in the solutions is observed. So, two stationary solutions are present; one, given by the minimum of the energy, is the ground state; and the other, which corresponds to a maximum of the energy, is referred as the hyperbolic solution. The hyperbolic solutions are relevant for precise determination of critical points, phase transitions and tunneling effects. Hyperbolic states were first determined in spherical geometries by Newton algorithm [3] and by shooting methods [5,7]. Shooting methods are inherently one-dimensional and cannot be extended to higher dimensions. When we have a cylindrical geometry, the hyperbolic states can be found by generalizing the Newton algorithm to higher dimensions [6]. A method based on a technique that combines Fourier transform and renormalization [4] can also be employed, though it still requires the Newton method and a careful treatment in the case of negative eigenvalues. Newton method requires solution of nonlinear systems at considerable computational expense for higher dimensions. Alternatively, relaxation techniques have been extensively used to obtain ground state solutions in GP equation [8–11]; and can also be generalized to higher dimensions.

A relaxation algorithm only requires iteration and needs much less computational expense than Newton method, particularly for higher dimensions. However, the usual relaxation algorithm relax to a minimum, such that the hyperbolic states are not reachable by this procedure.

In the present work we devised a *modified relaxation algorithm* to obtain not only the ground state, but also the hyperbolic states. The proposed algorithm consists of a method that provides a convenient modification in the stability of the original problem, such that the same relaxation technique can be used to obtain the hyperbolic solutions. The Letter is organized as follows. We first review several numerical methods that have been employed to solve the GP equation. Further, we describe the relaxation algorithm and how it can be appropriately modified to achieve the new algorithm. Finally, we show a few examples that provide the reliability and usefulness of the present algorithm. The examples are given for cylindrical cases, including

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the determination of critical points, extreme cases in the quasi-1D limit, and also by considering the addition of a quintic term. The last case, with negative cubic and positive quintic terms, is an example where we can observe pitchfork bifurcations.

We should also mention other useful methods to obtain numerical solutions of nonlinear differential equations. Bao and Tang [12], for example, have proposed a method to compute the ground-state solution of trapped interacting Bose–Einstein condensate (BEC) by directly minimizing the functional energy via finite element approximation. Another efficient algorithm, based on a discrete variable representation (DVR) of the Hamiltonian, was proposed in Ref. [13], as an alternative to standard iterative techniques to solve GP equations, particularly in cases where the techniques fail to obtain convergent solutions. The DVR method was used in [13] to obtain the ground-state solutions of fully anisotropic cases. However, both methods proposed in [12] and [13], besides their advantages, are not addressing to the hyperbolic solutions of nonlinear equations with attractive two-body interactions.

The Gross–Pitaevskii equation is given by

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \left[H_{\mathrm{ho}} + \frac{4\pi N\hbar^2 a}{m}|\Psi|^2\right]\Psi, \tag{1}$$

where $\Psi \equiv \Psi(\vec{r},t)$ is the system wave-function normalized to unity. H_{ho} is the Hamiltonian harmonic oscillator operator for a particle with mass m:

$$H_{\mathrm{ho}} \equiv -\frac{\hbar^2}{2m}\nabla^2 + \frac{m}{2}\sum_{i=1}^{3}\omega_i^2 x_i^2. \tag{2}$$

Next, we write the above equations in dimensionless units. We consider a unit of frequency ω, to be defined appropriately according to the geometry of the problem. In this case, the physical frequencies ω_i $(i = 1, 2, 3)$ are redefined to dimensionless quantities as $\omega_x \equiv \omega_1/\omega$, $\omega_y \equiv \omega_2/\omega$ and $\omega_z \equiv \omega_3/\omega$ and the unit of energy is $\hbar\omega$. The unit of length is defined as $l_\omega \equiv \sqrt{\hbar/(m\omega)}$. Usually, in the three-dimensional geometries, ω is taken as the mean geometric value, such that $\omega^3 \equiv \omega_1\omega_2\omega_3$. In this case, we define the unit of length as $l_0 \equiv l_\omega$, In the cylindrically symmetric case, when $\omega_1 = \omega_2 \neq 0$, in some cases it is also convenient to define ω as ω_1 and the unit of length as $l_\rho \equiv \sqrt{\hbar/(m\omega_1)}$. For future numerical purposes, we also consider an imaginary time variable, which in dimensionless units is defined as $\tau \equiv \mathrm{i}\omega t/2$. So, with the wave function of Eq. (1) being redefined such that $|\Psi(\vec{r},t)|^2 \equiv |\psi(\vec{x},\tau)|^2/l_\omega^3$, we have

$$\begin{aligned} -\frac{\partial\psi(\vec{x},\tau)}{\partial\tau} &= \left[H_0 + 8\pi\eta\left|\psi(\vec{x},\tau)\right|^2\right]\psi(\vec{x},\tau) \\ &= 2\mu\psi(\vec{x},\tau), \end{aligned} \tag{3}$$

where $\eta \equiv Na/l_\omega$, μ is the dimensionless chemical potential (with $\hbar\omega$ the energy dimension) and

$$H_0 \equiv -\frac{\partial^2}{\partial x^2} + \omega_x^2 x^2 - \frac{\partial^2}{\partial y^2} + \omega_y^2 y^2 - \frac{\partial^2}{\partial z^2} + \omega_z^2 z^2. \tag{4}$$

$\psi \equiv \psi(\vec{x},\tau)$ in Eq. (3) is normalized to one. Note that, in the spherically symmetric case ($\omega \equiv \omega_1 = \omega_2 = \omega_3$) we have $\omega_x = \omega_y = \omega_z = 1$; and, in a cylindrically symmetric case, with $\omega = \omega_1 = \omega_2$, we have $\omega_x = \omega_y = 1$ and $\omega_z = \omega_3/\omega$.

In the following we present several relaxation schemes that finally lead to scheme C to obtain stable and unstable solutions for $\eta < 0$.

Usual relaxation scheme

The usual relaxation scheme is considered, for example, in Ref. [11]. For a given η either positive or negative, Eq. (3) is propagated in time. For very long time it converges to the ground state solution. Because this process is dissipative, we must renormalize ψ to one at each time step. The chemical potential is obtained a posteriori using $\mu = \int \psi^*[H_0 + 8\pi\eta\psi^2]|\psi\, d\vec{x}$. The propagation is made by split-step technique, where the diffusion term is implemented by Crank–Nicolson algorithm, and the potential and nonlinear terms are just exponentiated.

In the above procedure, usually one provides η to obtain μ. Considering only ground state, when η is negative (attractive two-body interaction) we also have hyperbolic solutions (maxima for the energies), that are not reachable through this relaxation algorithm. As our aim is also to obtain the hyperbolic solutions within the same algorithm, a first trial approach is to provide μ to obtain η. With this parametrization there is no multivalued solution. Two similar relaxation schemes (A and B) are found appropriate to obtain the solutions of a nonlinear Schrödinger-type equation, when the (cubic) nonlinear interaction is positive. With a convenient modification of the scheme B, we finally reach a scheme C that works to obtain all the solutions for $\eta < 0$, including the hyperbolic ones.

Scheme A

The solution of Eq. (3) for $\eta > 0$ can also be accomplished by evolving the equation [3]

$$-\frac{\partial\tilde{\psi}}{\partial\tau} = \left[H_0 + 8\pi|\tilde{\psi}|^2 - 2\mu\right]\tilde{\psi}, \tag{5}$$

where

$$|\tilde{\psi}|^2 \equiv \eta|\psi|^2, \tag{6}$$

and the stationary solutions are given by $\partial\tilde{\psi}/\partial\tau = 0$. In this process, given μ, the equation is propagated without normalization to one, with η being obtained a posteriori by

$$\eta = \int d^3r\,|\tilde{\psi}|^2. \tag{7}$$

However, this approach does not work for negative nonlinearity.

Scheme B

Another scheme to solve Eq. (3), similar to the scheme A, is to obtain the numerical solution for

$$-\frac{\partial\psi}{\partial\tau} = \left[H_0 + 8\pi\eta|\psi|^2 - 2\mu\right]\psi, \tag{8}$$

with the time discretization followed by

$$\eta_{n+1} \leftarrow \eta_n \int d^3r\, |\psi_{n+1}|^2, \tag{9}$$

where ψ is normalized to one at each time step.

Scheme C

The schemes A and B are completely equivalent. However, the scheme B has the advantage that the normalization is performed at each time step. It converges to stable solutions and the norm evoles in a controlled way. It was expected that solutions for $a < 0$ [negative nonlinear term in Eq. (8)] would also be achieved with scheme B. However, if the nonlinear term in Eq. (8) is negative, the norm η grows exponentially and the scheme B fails. We tested several alternatives, and we have observed that a particular normalization, which consists of reversing Eq. (9), presents the peculiarity to control the growing of η parameter:

$$\eta_{n+1} \leftarrow \frac{\eta_n}{\int d^3r\, |\psi_{n+1}|^2}. \tag{10}$$

This procedure defines a new scheme C to obtain numerical solution of Eq. (8), that is valid in the cases that we have negative cubic term in the nonlinear Schrödinger equation.

So, considering the nonlinear equation

$$-\frac{\partial\psi}{\partial\tau} = \big[-\nabla^2 + V + 8\pi\eta|\psi|^2 - 2\mu\big]\psi, \tag{11}$$

where V is the harmonic potential, the set of operations needed to implement this relaxation approach is given by

$$\left.\begin{aligned}
&\psi_{n+1/3} \leftarrow \psi_n + \tfrac{\Delta\tau}{2}[2\mu - V - 8\pi\eta_n|\psi_n|^2]\psi_n\\
&\psi_{n+2/3} \leftarrow \mathcal{O}_{\mathrm{CN}}\psi_{n+1/3}\\
&\psi_{n+1} \leftarrow \psi_{n+2/3} + \tfrac{\Delta\tau}{2}[2\mu - V - 8\pi\eta_n|\psi_n|^2]\psi_n\\
&\eta_{n+1} \leftarrow \eta_n[\textstyle\int d^3x\, |\psi_{n+1}|^2]^{-1}\\
&\psi_{n+1} \leftarrow \psi_{n+1}[\textstyle\int d^3x\, |\psi_{n+1}|^2]^{-1}
\end{aligned}\right\}, \tag{12}$$

where $\eta_n < 0$ and n refers to the nth time step. In the second line of (12), $\mathcal{O}_{\mathrm{CN}}$ is the evolving operator of ∇^2 by the Crank–Nicolson algorithm with a time step $\Delta\tau$. Let $K \equiv \nabla^2$ in dimensionless spherical coordinates, which is reduced to a single second-order differential equation in the dimensionless radial coordinate $\tilde{r}$, in our case that we are considering just the s-wave. With j indicating the corresponding radial space-step grid, this $\mathcal{O}_{\mathrm{CN}}$ operation on ψ results in

$$\psi_{n+2/3,j} = \psi_{n+1/3,j} + \frac{\Delta\tau}{2}[K_j\psi_{n+2/3,j} + K_j\psi_{n+1/3,j}], \tag{13}$$

where

$$K_j\psi_j = \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta\tilde{r})^2} + \frac{\sigma}{\tilde{r}}\frac{\psi_{j+1} - \psi_{j-1}}{2\Delta\tilde{r}}, \tag{14}$$

with $\sigma = 2$. In this numerical calculation, we are using the von Neumann boundary condition $d\psi/d\tilde{r} = 0$ at $\tilde{r} = 0$. When we have the 3D equation for ∇^2 in cylindrical symmetry, the $\mathcal{O}_{\mathrm{CN}}$ operation on ψ is split in axial and radial parts, with the radial part being the 2D implementation (with $\sigma = 1$) of the above expressions.

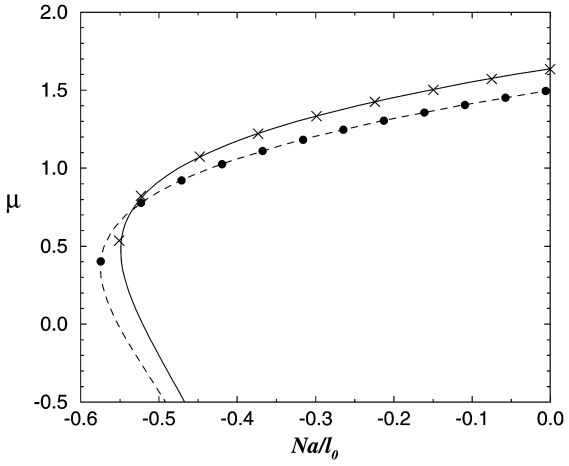

Fig. 1. Full numerical results, using the scheme C, for the chemical potential μ (in units of $\hbar\omega$) as a function of the dimensionless $\eta = Na/l_0$, when $a < 0$, for the spherical case (dashed line) and also for a cylindrical case, with $\omega_1 = \omega_2 = 2\pi \times 17.5$ Hz, $\omega_3 = 2\pi \times 6.8$ Hz (solid line). With bullet (spherical) and with $\times$ (cylindrical), we show the results obtained with the relaxation algorithm presented in Ref. [11], which does not access hyperbolic states.

About the numerical discretization, we used grid with 1000 points in the space, in the spherical case. In the cylindrical case, the grid used was 200×200. In both the cases, the time step was $\Delta\tau = 0.001$. The number of grid points was enlarged and the time step diminished in some cases to improve the precision.

We should emphasize that with this procedure the relaxation method can be applied to obtain stable solutions of cubic nonlinear Schrödinger equation with negative scattering lengths. When $\eta < 0$, all the stationary solutions (including the hyperbolic ones) can be obtained within the same code; in a method that can easily be extended to obtain dynamical solutions, considering quite different three-dimensional geometries.

So, following the scheme C, in case that $a < 0$, we were able to find both branch solutions for the stationary observables of the system, as the energy, chemical potential, mean-square radius, density, etc. Three-dimensional results for the chemical potential μ, as a function of the $\eta \equiv Na/l_0$, given by Eq. (3), are shown in Fig. 1, for $a < 0$. The results are shown for symmetric geometry, as well as for the case with the cylindrical geometry considered in Ref. [14] (the corresponding frequencies are given in the caption). All the results for the case with spherical symmetric (dotted line), including the hyperbolic solutions (the maxima for the energies), coincide with previous results obtained using shooting method [5]. Note that the relaxation method presented in Ref. [11] can only reproduce the results corresponding to minima for the energies. However, as we show in Fig. 1, with solid line, with the relaxation method we can also obtain the hyperbolic solutions for asymmetric cases. Such hyperbolic results (in the non-symmetric case) cannot be reached either by the shooting method, or by the usual relaxation method.

The applicability of the procedure is demonstrated by considering the same set of parameters used in Ref. [14]. The criti-

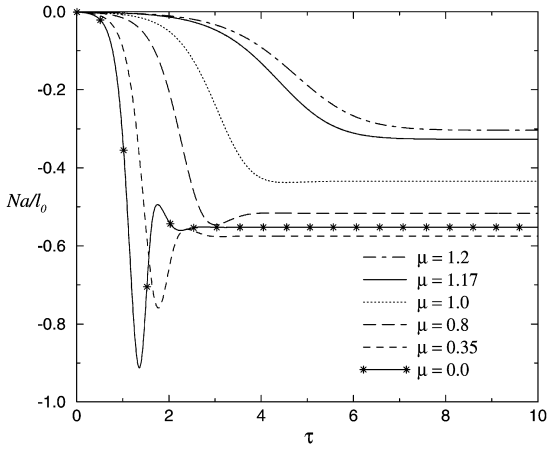

Fig. 2. Evolution of convergence of the GP solution, in the spherical case with negative scattering length. We use the modified version of the relaxation method, considering several chemical potential parameters μ (in units of $\hbar\omega$), as given inside the figure. As observed, the convergence is improved as we decrease μ. τ is given in units of $2/\omega$.

cal point for the number of particles is obtained when the stable and unstable branches are meeting. Using this technique we found the critical constant $N|a|/l_0 = 0.549$, in good agreement with previous results obtained in Ref. [11]. The critical point is achieved either by increasing the number of atoms or equivalently the magnitude of the negative scattering length. At this point, the system collapses. In fact, the collapse was first experimentally observed by Bradley et al. and reported in Ref. [15].

The results shown in Fig. 2 are very illustrative on the effectiveness of the approach, as well as, about the way the scheme C is working. In Fig. 2, we present, as a function of the imaginary time τ, results for the parameter Na/l_0 related to the number of particles N, given by the GP Eq. (3). We consider in this figure the spherical case with negative scattering length, using the present modified version of the relaxation method. We show results for several chemical potential parameters μ, from 0 till 1.2 units of $\hbar\omega$. With the help of Fig. 1, we can identify the values of μ corresponding to the hyperbolic states, as well as the ones corresponding to minima for the energies. We should emphasize that with the schemes A and B we can only obtain results for $Na/l_0 > 0$.

The scheme C is a strategy to avoid the numerical instabilities that we observe in the stationary point of the analog model of scheme A and B, when we consider μ as our input. The inversion of the procedure represented by Eq. (9), given by Eq. (10), leads us to an algorithm that can reach all the stationary solutions when the nonlinear interaction is negative. The most relevant outcome of this procedure occurs for the unstable branch, where we have the hyperbolic solutions. A curious aspect of the results given by the scheme C, when the nonlinear term is negative, is the fact that the observed convergence (related to the number of imaginary time steps n) to the correct solution is improved as we decrease the value of μ. As we approach the linear oscillator (the case where $Na/l_0 = 0$) the convergence *slows down*. This implies that the convergence is more sensitive to the changes of the chemical potential than to the numerical variation of the wave-function, at each time step n. As the negative

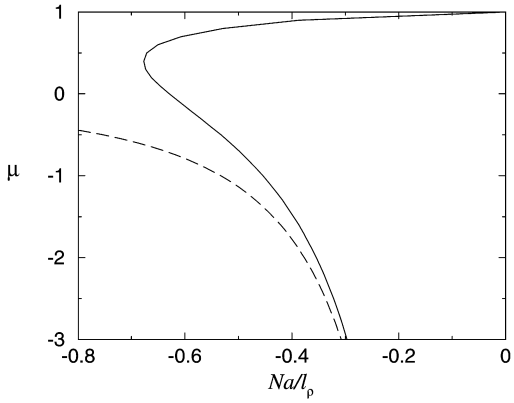

Fig. 3. Chemical potential (in units of $\hbar\omega_1$) as a function of Na/l_ρ, where $l_\rho \equiv \sqrt{\hbar/(m\omega_1)}$, for the cylindrically symmetrical case ($\omega_1 = \omega_2$). The results, considering the modified version of the relaxation method, are shown by solid line. With dashed line, we have the limiting analytical solution.

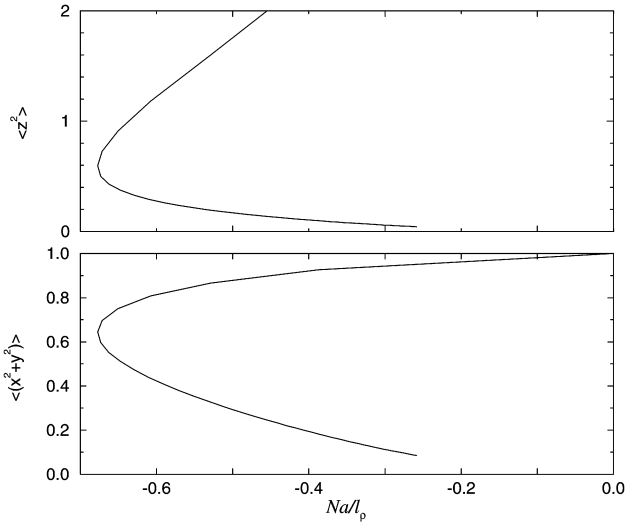

Fig. 4. Mean-square radii $\langle z^2\rangle$ (upper frame) and $\langle x^2 + y^2\rangle$ (lower frame), in units of $l_\rho^2 \equiv \hbar/(m\omega_1)$, are shown as functions of Na/l_ρ, for the cylindrically symmetric case ($\omega_1 = \omega_2$). The numerical results are obtained with the scheme C.

nonlinear term becomes larger, the convergence is improved; but we also observe a fast dumped oscillation with increasing amplitude. This numerical behavior of the convergence of the solutions for η, as a function of the imaginary time, needs a more detailed analysis, which is out of the scope of the present work.

For cylindrically symmetric case with $\omega_3 = 0$, and $\omega_1 = \omega_2$, we show in Figs. 3 and 4, respectively, results for the chemical potential and the mean-square-radius, obtained by considering the scheme C. In Fig. 3, our results for μ are shown by solid line. The branch of the hyperbolic solutions (lower branch) of this curve converges asymptotically to the corresponding analytical solution, shown by dashed line, which is given by $\eta = Na/l_\rho = -18.94/[8\pi\sqrt{-2\mu}\,]$ [18]. The results of Ref. [17] use a NPSE (non-polinomial Schrödinger equation) and is an approximate solution that gives pretty good results for the stable solutions and also for the hyperbolic ones near the bending of the bifurcation. However, the hyperbolic solutions

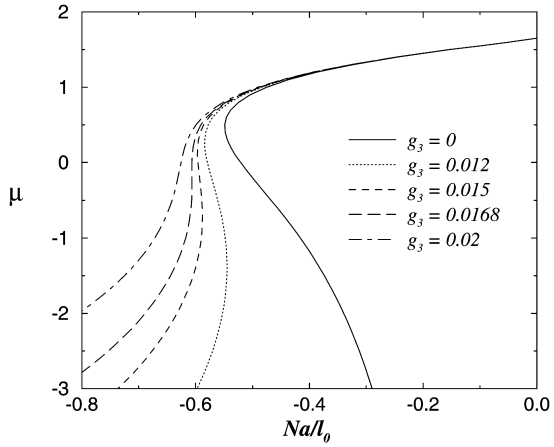

Fig. 5. Chemical potential (in units of $\hbar\omega$), as a function of Na/l_0, for a cylindrically symmetric GP equation with negative two body scattering length and with quintic nonlinear term, obtained using the relaxation method with the scheme C. The frequency relations are given by $\omega_1 = \omega_2 = 2\pi \times 17.5$ Hz and $\omega_3 = 2\pi \times 6.8$ Hz. The strengths g_3 of the quintic term, corresponding to the curves, are given inside the figure.

of [17], with weak nonlinearity, are not correct even topologically: the eigenvalues go to a constant when they should go to $-\infty$.

In Fig. 4, we have two frames considering the mean-square radius in the axial direction as well as in the perpendicular direction. The stable branches, in both frames, are the upper part of the plots. Note that such stable branch of $\langle x^2 + y^2\rangle$ goes to one, in units of $\hbar\omega_1$, when $Na \to 0$. As the system is not trapped in the z-direction, $\langle z^2\rangle$ diverges as $Na \to 0$. In both the cases, the mean-square radius for the unstable branches collapse to zero as $Na \to 0$.

To demonstrate the applicability of the approach given by the scheme C in a case that we have bifurcation, we also consider a positive quintic term in Eq. (8), with $\eta < 0$. This possibility, of an extended GP formalism with a quintic nonlinear term, can occur for some hypothetical atomic system, with attractive two-body and repulsive three-body interactions, as discussed in Refs. [16,19]. The corresponding equation is given by

$$-\frac{\partial\psi}{\partial\tau} = \big[H_0 + 8\pi\eta|\psi|^2 + 2(4\pi\eta)^2 g_3|\psi|^4 - 2\mu\big]\psi, \qquad (15)$$

where g_3 is related to the strength of the quintic term. By using the scheme C, we have first verified a perfect agreement of the actual results with the ones obtained in Ref. [19], in a spherically symmetric case. Next, we consider the *cigar-type* cylindrical symmetry considered in the experiments described in Ref. [14], as given in the caption of Fig. 1. The final numerical results are shown in Fig. 5, for several values of g_3 (given inside the figure). As observed, we have a pitchfork bifurcation when $0 < g_3 < 0.0168$. Note that this upper value of g_3 is lower than the upper value (0.0183) obtained in a spherically symmetric case [19]. So, with the present relaxation method we are able to reach all the stationary solutions of an equation with negative cubic and positive quintic nonlinear terms as the Eq. (15), with precise definitions of the critical limits for the observables. By following Refs. [16,19], one can easily extend the present approach to obtain several other stationary, as well as dynamical observables, in a non-spherically symmetric case; and also consider non-conservative cases.

About the applicability of the scheme C to the case that we have included a positive quintic term, we should point out that our results shown in Fig. 5 are in a region of parameters where the nonlinearity is dominated by the negative cubic term (with $\eta = Na/l_0 < 0$). As observed from Eq. (15), the effective nonlinear potential that we have is given by

$$-8\pi|\eta||\psi|^2\big[1 - 4\pi|\eta|g_3|\psi|^2\big],$$

such that the quintic term is dominant only when $g_3|\psi|^2 > 1/[4\pi|\eta|]$. By replacing $|\psi|$ by its maximum value, $|\psi|_{\max}$, we obtain the following sufficient condition for the applicability of the scheme C:

$$g_3 < \frac{1}{4\pi|\eta||\psi|^2_{\max}}. \qquad (16)$$

But, it is easy to verify that this condition is satisfied for all the results presented in Fig. 5, as $0 \leqslant g_3 \leqslant 0.02$. For larger g_3 there is no particular interest in the solutions (see Fig. 5), within the motivations of the present work, because there is no possibility of occurrence of bifurcations (there is no maxima for the energies). And, in the case that the condition (16) is violated, as the effective nonlinear interaction becomes positive, we already know that we should apply the scheme A or B. All these results are numerically confirmed.

In conclusion, we demonstrate how the relaxation algorithm can be suitable modified in order to achieve all the stationary solutions of the Gross–Pitaevskii equation for negative scattering length (negative nonlinear cubic term), including the hyperbolic ones. Determination of unstable branches provided precise critical numbers also in the non-symmetric cases. An example of application of the method in case that we have attractive cubic term and repulsive quintic term is provided to test the approach for a case that one has higher order nonlinearity. As shown, the scheme C is appropriate to obtain all the solutions, including the hyperbolic ones, when the effective nonlinear interaction is negative. From the other side, as the scheme B can be implemented by a minimal modification in the algorithm, one can reach all the stationary solutions (including the hyperbolic ones) for both signs of the effective nonlinear interaction, with the same numerical code. Besides that, the approach can be easily extended to obtain dynamical solutions. We believe that the proposed modified relaxation algorithm can also be used to obtain solutions to many other problems that can be described by nonlinear differential equations. It is certainly a valuable alternative tool for determining precisely points of instability and bifurcations.

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