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Stationary solutions of Gross-Pitaevskii equations in a double square well

WeiDong Li
Department of Physics and Institute of Theoretical Physics, Shanxi University, Taiyuan 030006, China
and INFM-BEC and Dipartimento di Fisica, Universita di Trento, 1-38050 Povo, Italy

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We present analytical stationary solutions for the Gross-Pitaevskii equation (GPE) of a Bose-Einstein condensate (BECs) trapped in a double-well potential. These solutions are compared to those described by [Mahmud *et al.*, Phys. Rev. A **66**, 063607 (2002)]. In particular, we provide further evidence that symmetry preserving stationary solutions can be reduced to the eigenstates of the corresponding linear Schrödinger equation. Moreover, we have found that the symmetry-breaking solutions can emerge not only from bifurcations, but also from isolated points in the chemical potential–nonlinear interaction diagram. We also have found that there are some moving nodes in the symmetry-breaking solutions.

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I. INTRODUCTION

The Gross-Pitaevskii equation (GPE) describes many features of Bose-Einstein condensates (BECs) of dilute atomic gases in an external potential at zero temperature [1]. The properties of the ground state of the GPE with external potential have been extensively studied; and many interesting phenomena have been reported. Of special interest is that the mean–field interaction profoundly modifies the density profiles and the stability of the ground state [1]. Recently, the properties of the non-ground-state stationary solutions of the GPE have attracted more attention both theoretically and experimentally [2–4]. For example, the dark solitons have been created in the atomic gases with a positive scattering length by phase engineering optical techniques [4–6].

Based on [3], one can classify the stationary solutions of GPE as symmetry preserving and symmetry-breaking solutions. Whereas the vortices and solitons observed in experiments [4,5,7,8] are symmetry-preserving solutions, which can be reduced to the eigenstates of the corresponding linear Schrödinger equations, the macroscopic quantum self-trapping state in the two states [9–12] and a non-Bloch state [13,14] in periodical potential are symmetry-breaking solutions, and they cannot be reduced to the eigenstates of the corresponding linear Schrödinger equations.

The system of GPE with double wells is a good system to investigate the properties of the stationary solutions of GPE and also good for studying the special nonlinear dynamics, for example, the nonlinear self-trapping effect which was predicted theoretically in 1997 [9] and realized experimentally [11,12,15] last year. It has been shown that there are stationary solutions, which are either symmetry preserving or symmetry breaking, both numerically and analytically in this system [2,3]. With the help of the double square well [2], which allows one kind of analytical solution for GPE, Reinhardt and his collaborators have confirmed the numerical calculation for GPE with double-well traps [3]. This provides one possible way to investigate the properties of the stationary solution for GPE with double wells. It is interesting to know how the stationary solutions change as the nonlinear interaction increases or decreases, how the symmetry-breaking stationary solutions emerge, and how many kinds of the stationary solutions there are for the fixed nonlinear interaction.

In this paper, we present different stationary analytical solutions for GP equations with double square wells. Compared with the solutions of [2], ours can be reduced to the eigenstates of the corresponding linear Schrödinger equations. It is this feature which enables us to understand the above-mentioned interesting problems concerning the stationary solutions for GPE. It allows us to obtain the critical nonlinear interaction value, over which the symmetry-breaking solution emerges. And from the relation of the profiles of the stationary solutions and chemical potentials with the nonlinear interaction, we can directly see the means of the symmetry and symmetry-breaking and different stationary solutions for special nonlinear interaction.

II. MODEL AND THE SOLUTIONS

Considering that the BECs of dilute atomic gases are confined by a very anisotropic harmonic potential ($\omega_\perp \gg \omega_x$, where $\omega_{\perp,x}$ are the confined frequency in the y-z space and x direction) and that the BECs are loaded in a double square well in the weak confined direction (x direction), then the dynamics of this system is governed by the one-dimensional (1D) GP equation

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) + g_0|\Psi(x,t)|^2 \right)\Psi(x,t), \tag{1}$$

where $g_0 = 4\pi\hbar^2 a/m$ is the 1D reduced nonlinear interaction constant. The potential is of the form

$$V(x) = \begin{cases} \infty & |x| \geq a \\ 0 & b < |x| < a \quad \left(a = \frac{1}{2}, V_0 > 0\right) \\ V_0 & |x| < b. \end{cases}$$

The stationary solution can be written as

$$\psi(x) = r(x)\exp(-i\mu/\hbar\, t)$$

and after rescaling the equations, we arrive at the equation for $r(x)$

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TABLE I. The modular transformation of Jacobi elliptic functions.

	$m<0$	$0<m<1$	$m>1$	$m=0$	$m=1$
$\mathrm{sn}(u\|m)$	$\sqrt{m_1}\mathrm{sd}(u\sqrt{1-m}\|m_1)$	$\mathrm{sn}(u\|m)$	$\sqrt{m_2}\mathrm{sn}(u/m_2\|m_2)$	$\sin(u)$	$\tanh(u)$
$\mathrm{sc}(u\|m)$	$\sqrt{m_1}\mathrm{sc}(u\sqrt{1-m}\|m_1)$	$\mathrm{sc}(u\|m)$	$\sqrt{m_2}\mathrm{sd}(u/m_2\|m_2)$	$\tan(u)$	$\sinh(u)$
$\mathrm{cn}(u\|m)$	$\mathrm{cd}(u\sqrt{1-m}\|m_1)$	$\mathrm{cn}(u\|m)$	$\mathrm{dn}(u/m_2\|m_2)$	$\cos(u)$	$\sec h(u)$
$\mathrm{dn}(u\|m)$	$\mathrm{nd}(u\sqrt{1-m}\|m_1)$	$\mathrm{dn}(u\|m)$	$\mathrm{cn}(u/m_2\|m_2)$	1	$\sec h(u)$

$$\mu r(x) = -\frac{\partial^2}{\partial x^2} r(x) + V(x) r(x) + \eta r(x)^3, \tag{2}$$

where $\eta = N_0 g_0 2mL^2/\hbar^2$ and N_0 is the total number of the atom. The energy and the potential are measured in units of $\hbar^2/2mL^2$, and L is the length of the total space (here $L=2a$). Due to the double-well case, the stationary solution is just the real function, so we have assumed that our solution $r(x)$ is a real function. As in Ref. [2], the solution of (2) can be written in terms of the Jacobi elliptical function.

Generally, we have two different solutions depending on the relation of the chemical potential and the barrier height. First for $\mu > V_0$

$$r_1(x) = A\mathrm{sn}(Kx + \delta, n_1), \tag{3}$$

where

$$n_1 = \frac{A^2}{2K^2}\eta, \quad \mu = K^2 + V_0 + \frac{A^2}{2}\eta. \tag{4}$$

This solution is also valid for $V_0=0$, which corresponds to the region of $b<|x|<a$. It is easy to check that when $\eta=0$, our solution is reduced to $r_1(x)=A\sin(Kx+\delta)$, where $n_1=0$, $\mu=K^2+V_0$. This is nothing but the eigenstates of linear Schrödinger equations for $\mu>V_0$. We have two different Jacobi functions for $\mu<V_0$, corresponding to the region of $|x|<b$. To the case with one node in the barrier region, the solution is

$$r_2(x) = B\mathrm{sc}(Qx + \gamma, n_2), \tag{5}$$

$$n_2 = 1 - \frac{B^2}{2Q^2}\eta, \quad \mu = V_0 - Q^2 - \frac{B^2}{2}\eta \tag{6}$$

but to the case without node,

$$r_2(x) = B\mathrm{nc}(Qx + \gamma, n_2), \tag{7}$$

$$n_2 = 1 - \frac{B^2}{2Q^2}\eta, \quad \mu = V_0 - Q^2 + B^2\eta. \tag{8}$$

Same as the solution (3) in $\eta=0$, our solutions are reduced to $r_2(x)=B\sinh(Qx+\gamma)$ for (5) and $r_2(x)=B\cosh(Qx+\gamma)$ for (7), where $n_2=1$, $\mu=V_0-Q^2$. It is interesting to note that those two solutions are precisely identical with the eigenstates of linear Schrödinger equations for one node or no node within the barrier.

Please note here that we do not restrict the value of n_1 from 0 to 1 as is usually used in the Jacobi elliptic function. But this problem could be solved by the modular transformation table (see Table I, where $m_1=m/1+m$, $m_2=1/m$) [16]. The Jacobi elliptical functions sc and nc are constructed from the Jacobi elliptical sn, cn, and dn (see Table II) or [16]).

III. SYMMETRY-PRESERVING AND SYMMETRY BREAKING SOLUTIONS

As mentioned in the Introduction, we have two different kinds of stationary solutions depending on whether the stationary solution has its linear counterpart [3]. The symmetry-preserving solution has the linear counterpart, as it could be reduced to the eigenstates of the corresponding linear Schrödinger equations. But the symmetry-breaking solution could not be reduced, therefore it does not have the linear counterpart. Such being the case, we are required to find the stationary solutions of Eq. (1). It is worthwhile to note that our method is just the usual one in the linear case.

With the help of (3), (5), and (7), solutions in the three regions can be written in the form

$$f_1(x) = A_1\mathrm{sn}(K_1(x+a), n_1), \quad -a<x<-b$$

$$f_2(x) = B\mathrm{nc}(Q(x+\gamma), m), \quad |x|<b$$

$$f_3(x) = A_2\mathrm{sn}(K_2(x-a), n_2), \quad b<x<a \tag{9}$$

for the case without node inside the barrier. For the case with one node inside the barrier, we have

$$f_1(x) = A_1\mathrm{sn}(K_1(x+a), n_1), \quad -a<x<-b$$

$$f_2(x) = B\mathrm{sc}(Q(x+\gamma), m), \quad |x|<b$$

$$f_3(x) = -A_2\mathrm{sn}(K_2(x-a), n_2) \quad b<x<a. \tag{10}$$

We have considered the fact that the solutions vanish on and outside the potential $|x|\geq a$. To fix the parameters A_1,

TABLE II. Other Jacobi elliptic functions.

$\mathrm{ns}(u\|m) \equiv 1/\mathrm{sn}(u\|m)$	$\mathrm{sc}(u\|m) \equiv \mathrm{sn}(u\|m)/\mathrm{cn}(u\|m)$	$\mathrm{sd}(u\|m) \equiv \mathrm{sn}(u\|m)/\mathrm{dn}(u\|m)$
$\mathrm{nc}(u\|m) \equiv 1/\mathrm{cn}(u\|m)$	$\mathrm{cs}(u\|m) \equiv \mathrm{cn}(u\|m)/\mathrm{sn}(u\|m)$	$\mathrm{cd}(u\|m) \equiv \mathrm{cn}(u\|m)/\mathrm{dn}(u\|m)$
$\mathrm{nd}(u\|m) \equiv 1/\mathrm{dn}(u\|m)$	$\mathrm{ds}(u\|m) \equiv \mathrm{dn}(u\|m)/\mathrm{sn}(u\|m)$	$\mathrm{dc}(u\|m) \equiv \mathrm{dn}(u\|m)/\mathrm{cn}(u\|m)$

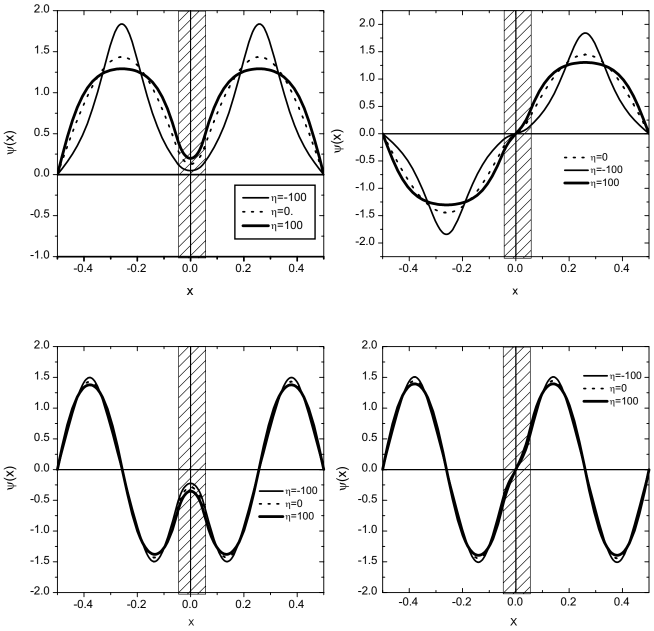

FIG. 1. The symmetry-preserving solutions of GP equations.

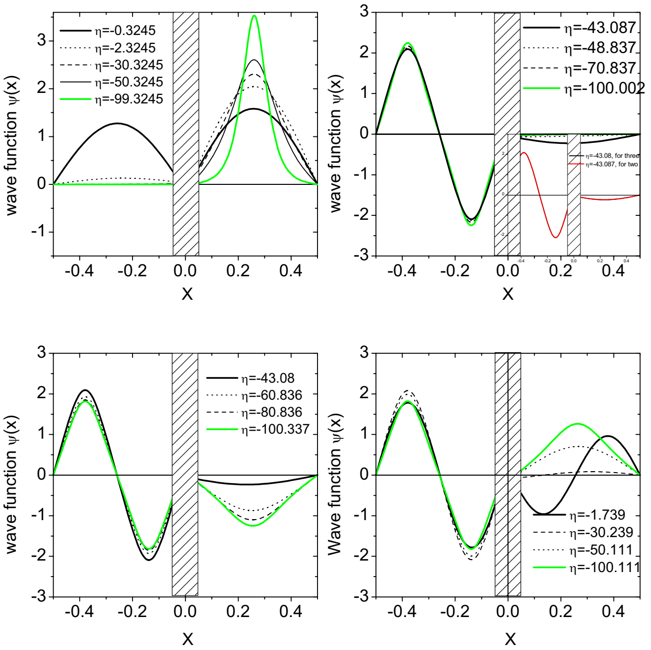

FIG. 2. (Color online) The symmetry-breaking solutions of GP equations for positive nonlinear interaction.

A_2, K_1, K_2, Q, B, and γ, we need the continuity

$$
\begin{aligned}
f_1(-b) &= f_2(-b),\\
f_1'(-b) &= f_2'(-b),\\
f_2(b) &= f_3(b),\\
f_2'(b) &= f_3'(b),
\end{aligned}
\tag{11}
$$

and normalization conditions

$$
\int_{-a}^{-b} |f_1^2(x)|dx + \int_{-b}^{b} |f_2^2(x)|dx + \int_{b}^{a} |f_3^2(x)|dx = 1, \tag{12}
$$

and we need that the chemical potential is the same in different regions ($\mu_1 = \mu_2 = \mu_3$). The definition of the chemical potential μ can be found in Eqs. (4), (6), and (8).

In Fig. 1 we present the first four symmetric and antisymmetric solutions for $-100 < \eta < 100$. It is clear that all of these solutions can be reduced to eigenstates of the corresponding linear Schrödinger equations ($\eta = 0$). All of these solutions are symmetry-preserving solutions. A barrier height of $V_0 = 1000$, barrier width $2b = 0.1$, and well width $2a = 1$ are used all through this paper. The shaded part represents the barrier region in all the figures. It is hence easy to see that the effect of the nonlinear interaction on the profile of the wave function of the high energy state is smaller than that in the case of the low energy state. This situation is the same as in the lattice case [14]. In Fig. 4, the chemical potential has been plotted as the function of the nonlinear interaction. From Fig. 4, one can read that the chemical potential difference between the ground state and the first excited state increases with the increase of the strength of the nonlinear interaction. This seems to suggest that the positive nonlinear interaction enhances tunneling effects but the negative nonlinear interaction eliminates it. When the nonlinear interaction is very large and negative ($\eta_c \sim -54.5$), the symmetrical properties of the "ground" state change from the symmetry to the antisymmetry [2,3]. In fact, when the nonlinear interaction is negative and large, the symmetry-preserving solution is not the ground state. But this will be discussed in the later part of the paper.

In Fig. 2 we present the first four symmetry-breaking solutions for positive nonlinear interactions up to 100. When $\eta = 100$, these four solutions are exactly the one presented in [2]. In [2], they also show the profile of the first kind of solution in Fig. 2 for $\eta = 15$, 30, 50, and 100. But here our results show that this solution emerges from the bifurcations of the chemical potential of the first excited state at $\eta_c \sim 0.32$ (see Fig. 4). Some more detailed behavior can be read from Fig. 2. This solution has been predicted in [10]. Its chemical potential is larger than that of the first excited state. It is easy to see that the node in this solution is moving as the nonlinear interaction increases. From 0.32 to 5.563, the node is displacing from within the barrier to the right well. The fourth solution emerges from another bifurcation ($\eta_c \sim 1.48$), at which the chemical potential is the same as the fourth symmetry-preserving solution (the third excited state). For this solution, there is one fixed node and two moving nodes. Due to the increase of the nonlinear interaction, one of the moving nodes moves from the barrier region into the well. Finally, there are two moving nodes in the right well and one fixed node in the left well. The second and third solutions in Fig. 2 belong to a new kind of symmetry-breaking solution. They occur from the same isolated point ($\eta_c \sim 51.284$) in the diagram of the chemical potential and the nonlinear interaction. Here an isolated point is one point whose chemical potential (or eigenvalue) is not the same as the neighboring points in the diagram of the chemical poten-

TABLE III. Different numbers for the first symmetric-breaking solutions

η	Λ_c	Λ
5.0627	0.4945	0.9955
10.0627	0.4940	0.9960
20.0627	0.4932	0.9985

tial and nonlinear interaction, whether it is the symmetry preserving or symmetry-breaking solution. Therefore their profiles are modified completely differently with the increase of the nonlinear interaction. The second one has one fixed node and one moving node while the third one has two moving nodes.

The self-trapping effect as predicted in 1997 [10] was experimentally realized in [11,12,15]. This dynamical effect can be understood very well based on the two mode approximation [10]. In our case, due to the zero phase difference between the two well wave functions, the condition for the self-trapping can be written as $\Lambda=2(1+\sqrt{1-\Lambda^2})/\Lambda^2$. It is easy to check that all of the symmetry-breaking solutions satisfy this condition. We show this calculation in Table III, where Λ_c is the critical value for the self-trapping [10] and Λ is our solutions.

In Fig. 3, the symmetry-breaking solution for negative nonlinear interaction has been presented up to −100. When $\eta=-100$, they are the same as the Fig. 4 in [2] but with a different order. Same as the symmetry-breaking solutions in positive nonlinear interaction, the first and fourth solutions emerge from the symmetry-preserving solution at $\eta_c\sim-0.32$ and at $\eta_c\sim-1.46$, respectively. Please note that the first kind of symmetry-breaking solution emerges from the ground state and its chemical potential is less than that of the ground state. Therefore this state is the ground state of the system (from Fig. 4). This is what is called the quantum phase transition in this system [2,3]. This solution does not have any node and its profile shows that the particle would stay in one of the wells for negative nonlinear interaction. The fourth solution includes one fixed node and a moving one. Now the node moves from the well into the barrier region with the decrease of the nonlinear interaction. Around $\eta\sim-33.239$ the node is in the barrier region.

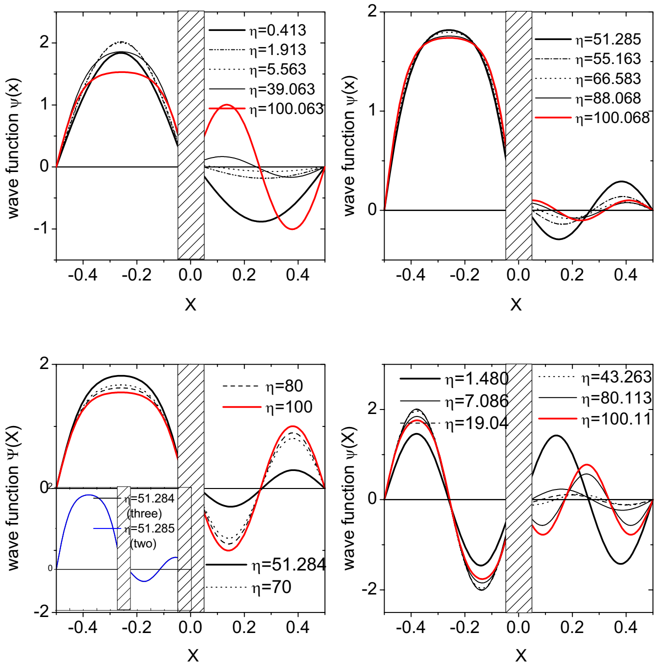

FIG. 3. (Color online) Same as Fig. 2 for negative nonlinear interaction.

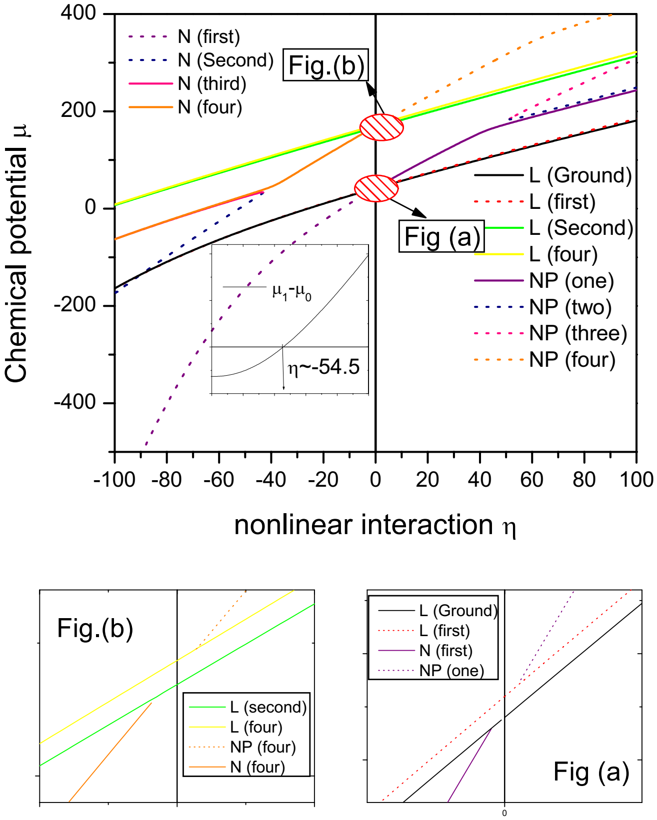

FIG. 4. (Color online) The chemical potential as the function of nonlinear interaction.

Again, the second and the third solutions occur from the isolated point at $\eta_c\sim-43.08$ in the diagram of the chemical potential with the nonlinear interaction. Now their nodes become fixed. Again the density profile has a completely different behavior with the decrease of the nonlinear interaction. The second solution will collect the particles to one well but the third one keeps them in two wells. There is still another crossover between the third and the fourth solutions near −100. That is why my order of the solution is different from [2] at $\eta=-100$.

In Fig. 4 we plot the chemical potential as the function of nonlinear interaction both for symmetry-preserving and breaking solutions. Due to the high barrier, the quantum tunneling effect between the two wells is small and the chemical potential difference between the ground state and the first excited state is small also. From Fig. 4, one can directly see that the symmetry-preserving solution can be reduced to the eigenstate of the linear Schrödinger equations ($\eta=0$), while the symmetry-breaking one cannot. To see this more clearly, we amplify the figure around $\eta=0$ [Fig. 4(a) is for the ground state and the first excited state and Fig. 4(b) is for the second excited state and the third excited state]. The embedded figure in Fig. 4 (left) shows the critical point for the quantum phase transition [2,3]. We denote the symmetry-preserving solutions as "*L*," and the symmetry-breaking solutions and positive nonlinear interaction as "NP," and the symmetry-breaking solutions and negative nonlinear interaction as "*N*." It is clearly shown that the symmetry-breaking solution can emerge from two kinds of points. One is the bifurcation and the other one is the isolated point in this diagram. We arrange our solution in Figs. 1–3 in the chemical potential order. It is easy to see that the nature of the mean-field ground state and the structure of the energy spectrum of the nonlinear system depend on the value of the nonlinear interaction.

IV. CONCLUSION

We have presented one analytical solution which could be reduced to eigenstates of the corresponding linear Schrödinger equations. And we have shown the clear and direct evidence to the relation of the symmetry-preserving stationary solution and the eigenstates of the linear Schrödinger equations. Based on the origin of the symmetry breaking state, one can find two kinds of different symmetry-breaking solutions, neither of which can be reduced to the eigenstates of the corresponding linear Schrödinger equations and have one critical nonlinear interaction, over which the symmetry-breaking solution emerges. One of the interesting things is that the first kind of symmetry-breaking solution can exist under the following conditions: (1) for positive nonlinear interaction, it emerges from the first excited state and the third excited state; (2) for negative nonlinear interaction, it emerges from the ground state and the second excited state. We understand this based on the superposition of the eigenfunctions of the linear Schrödinger equations. And high accuracy of the critical value of the nonlinear interaction has been found for the first kind of symmetry-breaking solution which emerges from the symmetry preserving one. This explains why we cannot find the symmetry-breaking solution from the ground state for the positive nonlinear interaction [17]. As this method is just valid for the small nonlinear interaction, we cannot yet understand the second kind of symmetry-breaking solution. But how the profile of the stationary solution changes with the nonlinear interaction has also been presented. Our calculation shows that the symmetry-breaking solution satisfies the self-trapping condition. This will help one to understand this effect from stationary solutions.

Considering the situations realized in the experiment, our model can be regarded as too simple. But this model can be solved analytically and is good enough to provide qualitative description. Usually, one can understand the realistic double well by the quartic function ax^4+bx^2+c. The chemical potential or the eigenvalue of GPE may show a little difference from the results of our simple model, but they are consistent quantitatively [3].

Note added. Recently, we noted two papers [18,19] which approach the same problem with similar techniques. In the present work we provide a more detailed analysis of the density profiles of stationary solutions as a function of the nonlinear interaction and we find a symmetry-breaking solution.

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