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The symmetry breaking states and bifurcation of Bose–Einstein condensates in a double well

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Abstract

An analytical approximation method to clarify the symmetry-breaking stationary solutions to the Gross–Pitaevskii equation with symmetric double-well external potential is presented. By this method, we can understand that each symmetry-breaking solution bifurcates from a symmetry-preserving solution as one varies the coupling constant of the nonlinear interaction, and predict the bifurcation point. Also, the method gives a good approximation to the energy eigenvalues of the lower states, symmetry-breaking as well as symmetry-preserving, as long as the nonlinear interaction is not too strong.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The nonlinear self-trapping effect is attracting more attention both experimentally and theoretically [1–4]. In particular, the stable double-well trap [3] and the nonlinear self-trapping of Bose–Einstein condensates (BECs) in a double-well trap have been reported in a recent experiment [4]. All of these strongly motivate the study on the properties of the stationary solutions and the dynamics of the Gross–Pitaevskii equation (GPE) with double-well external potential, which turns out to give quite accurate descriptions of this system [5–7].

Recently, sets of stationary solutions have been constructed analytically and numerically, for the one-dimensional GPEs with a symmetric double-square well and a multi-well external potential [8–10]. It is interesting to note that GPE with a symmetric double well has solutions which break the symmetry of the external potential along with the solutions which share the symmetry. The former is called the symmetry-breaking solution and the latter symmetry preserving [9, 10]. It has been observed that each symmetry-breaking solution bifurcates from

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a symmetry-preserving one at a critical value (bifurcation point) of the coupling constant of the nonlinear interaction. Recently, M Trippenbach and his collaborators have reported one analytical method to predict the critical points (also in the case of weak nonlinear interaction) with help of the variational analysis [11].

This paper presents an analytical approximation method to understand the symmetry-breaking solutions and to predict the bifurcation for GPE with a symmetric double-well external potential in the case of weak (not too strong) nonlinear interaction. Also, the method gives a good approximation to the energy eigenvalues of the lower states, symmetry-breaking as well as symmetry-preserving states.

This paper is constructed as follows. In section 2, we will introduce our model and the approximation method, which consists in approximating the solution to the GPE by a finite superposition of the eigenfunctions of the linear Schrödinger equation, or the GPE with the nonlinear interaction removed, and determining the coefficients of the superposition such that the GPE is satisfied as well as possible. The condition for our approximation to be valid is given by equation (5) in terms of the energy eigenvalues of the linear Schrödinger equation (4). To illustrate our method, we shall use a double-square well as a simple example. In section 3, the formulae for the solutions are given and the bifurcations are shown to take place. The results from our approximation method will be shown in section 4 to be very well in agreement with those from the exact numerical solutions of the nonlinear GPE [10]. The conclusion and discussions are presented in the final section.

2. The model and approximation method

The one-dimensional GPE for the stationary states is given by

$$\{H_0 + \eta\Phi_n(x)^2\}\Phi_n(x) = E_n\Phi_n(x) \tag{1}$$

where, measuring lengths in unit of L and energies in unit of $\hbar^2/(2mL^2)$,

$$H_0 = -\frac{\partial^2}{\partial x^2} + V_{\text{ext}}(x), \tag{2}$$

with the nonlinear coupling constant $\eta = (2mL^2/\hbar^2)N_0 g_0$, where N_0 is the total number of the atoms trapped in V_{ext} and L is the 'effective size' of the external potential. g_0 is defined by $4\pi\hbar^2 a_s/m$ and a_s, called the reduced 1D s-wave scattering length, which depends on the properties of strongly radial frequency, along the y–z plane, of the highly elongated external potential and usual s-wave scattering length of the trapped atom (see [12] for details). The weak confinement is realized by the 1D (or quasi-1D) potential $V_{\text{ext}}(x)$ along the x-direction which is assumed to be a double well, symmetric under space reflection. We shall illustrate our method by using a symmetric double-square well,

$$V_{\text{ext}}(x) = \begin{cases} \infty & |x| \geqslant a \\ 0 & b < |x| < a, \qquad (a = 1/2,\ V_0 > 0) \\ V_0 & |x| \leqslant b, \end{cases} \tag{3}$$

as a simple example. The normalized eigenfunctions u_n to the linear Schrödinger equation,

$$H_0 u_n(x) = \varepsilon_n u_n(x), \tag{4}$$

form a complete set of orthonormal functions, which we order in the increasing order of the eigenvalues, $\varepsilon_0 < \varepsilon_1 < \cdots$. In the present case of the symmetric double-well potential, the symmetric and anti-symmetric functions alternate starting from the symmetric u_0. When the central barrier of the double well is high, the energy levels ε_{2k} and ε_{2k+1} are very closely spaced, and the next couple, ε_{2k+2} and ε_{2k+3}, lie far away compared with their spacings $(k = 0, 1, 2, \ldots)$.

Our approximation method consists in trying a finite superposition of u_n's for the solution $\Phi_m(x)$ to the GPE (1), determining the coefficients such that the superposition satisfies the GPE as well as possible. The symmetry-preserving solutions are superpositions of u_n's of either even or odd n's, and the symmetry-breaking solutions are superpositions of both even and odd n's leading to non-symmetric effective potential $\eta\Phi_m^2$ in equation (1). We shall see in the next section that the symmetry-breaking solution $\Phi_m(x)$ can exist only when η, starting from $\eta = 0$, exceeds a certain critical value η_m^{c}, while symmetry-preserving solution exists for all η. In other words, symmetry-breaking solution bifurcates from a symmetry-preserving one at $\eta = \eta_m^{\mathrm{c}}$.

The condition for our approximation method to be valid for Φ_m is given by

$$\varepsilon_{2k+1} - \varepsilon_{2k} \ll \begin{cases} \varepsilon_{2k+2} - \varepsilon_{2k+1}, \\ \varepsilon_{2k} - \varepsilon_{2k-1} \end{cases} \qquad (n = 2k, \text{ or } 2k+1). \tag{5}$$

This is a common feature of the double-well potentials whose central barrier is very high.

3. Symmetry-breaking solution and bifurcation

In this section, we shall show that, at certain value of η_m^{c} of the coupling constant, symmetry-breaking solution to equation (1) bifurcates from the symmetry-preserving solution under the assumption of equation (5). For this purpose, let us write 'even' states $(m = 2k)$ approximately as

$$\Phi_{2k}(x) = \mathcal{N}_{2k}(u_{2k} + \alpha u_{2k+1} + \beta u_{2k+2} + \gamma u_{2k-2}) \qquad (|\alpha| < 1) \tag{6}$$

where α, β and γ ($\gamma = 0$ when $k = 0$) are real parameters to be determined such that Φ_{2k} satisfies the GPE as well as possible, and $\mathcal{N}_{2k} = (1 + \alpha^2 + \beta^2 + \gamma^2)^{-1/2}$ is the normalization factor. For better approximation, we should include more terms in equation (6). A remark is in order about the reasons for not including the terms, u_{2k+3} and u_{2k-1} in equation (6). The reasons are (i) that both these two states are far away from u_{2k} due to our condition (5), and (ii) that these states have parity different from that of u_{2k}. If α is small, the asymmetry of the effective potential Φ_{2k}^2 in equation (1) is small, so that, in view of the condition (5), the coefficients of these terms are very small, justifying the omissions from equation (6). Actually, however, α need not be small (see figure 1 below). Yet, the condition (5) would keep the coefficients of these terms small as can be inferred from the smallness of β and γ (see figure 1).

We shall show (i) that until η, starting from $\eta = 0$, reaches a critical point, $\alpha = 0$ is the only solution making the even state $\Phi_{2k}(x)$ symmetric under space reflection and (ii) beyond this point, the solution with $\alpha \neq 0$ arises realizing the symmetry-breaking solution, and coexisting with the symmetry preserving solution $(\alpha = 0)$. Namely, a bifurcation takes place at the critical point, $\eta = \eta_{2k}^{\mathrm{c}}$.

We shall also consider 'odd' states,

$$\Phi_{2k+1}(x) = \mathcal{N}_{2k+1}(u_{2k+1} + \alpha u_{2k} + \beta u_{2k+3} + \gamma u_{2k-1}) \tag{7}$$

in the similar notations as for the 'even' state. We shall see also that there occurs at $\eta = \eta_{2k+1}^{\mathrm{c}}$ a bifurcation from symmetry-preserving, antisymmetric state $(\alpha = 0)$ to coexisting symmetry-breaking $(\alpha \neq 0)$ states.

First, let us consider the 'even' states. Substituting equation (6) into equation (1), we have

$$H_0(u_{2k} + \alpha u_{2k+1} + \beta u_{2k+2} + \gamma u_{2k-2}) + \mathcal{N}_{2k}^{-1} V_{\mathrm{eff}} \Phi_{2k} = E_{2k}(u_{2k} + \alpha u_{2k+1} + \beta u_{2k+2} + \gamma u_{2k-2}) \tag{8}$$

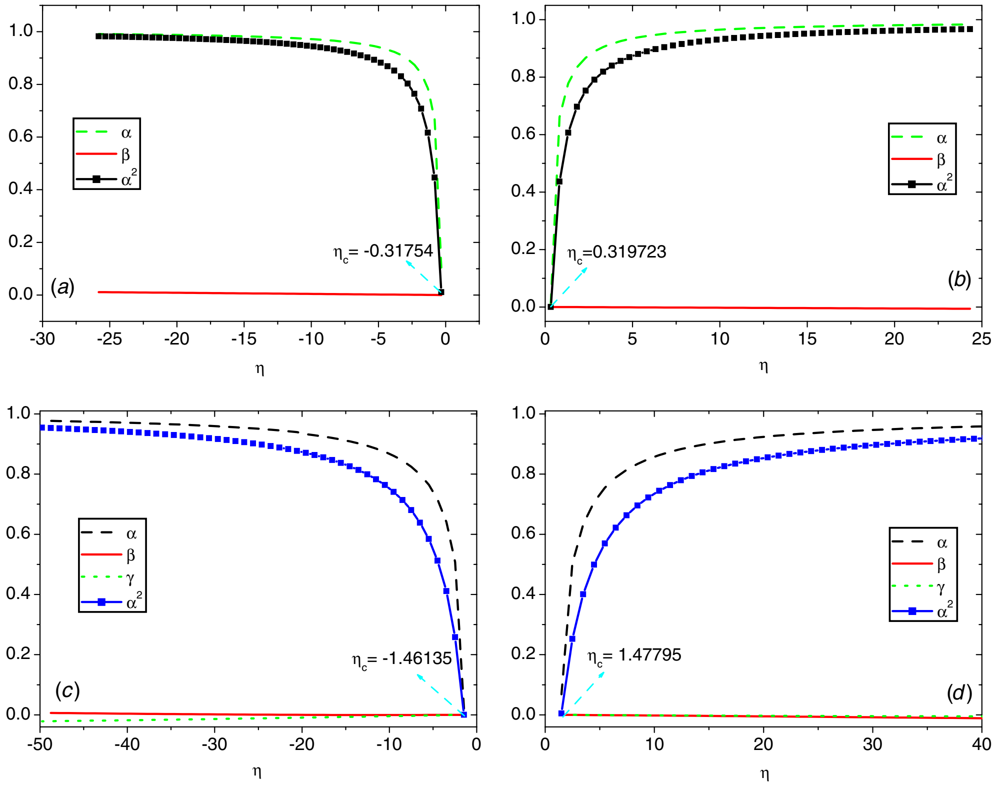

Figure 1. The expansion coefficients of symmetry-breaking states (6): (*a*) $m = 0$, (*b*) $m = 1$, (*c*) $m = 2$, (*d*) $m = 3$.

where

$$\mathcal{N}_{2k}^{-1} V_{\text{eff}} \Phi_{2k} = \eta' \big(u_{2k}^3 + 3\alpha u_{2k}^2 u_{2k+1} + 3\alpha^2 u_{2k} u_{2k+1}^2 + \alpha^3 u_{2k+1}^3 + 3\beta u_{2k}^2 u_{2k+2} + 6\alpha\beta u_{2k} u_{2k+1} u_{2k+2} + 3\alpha^2 \beta u_{2k+1}^2 u_{2k+2} + 3\gamma u_{2k}^2 u_{2k-2} + 6\alpha\gamma u_{2k} u_{2k+1} u_{2k-2} + 3\alpha^2 \gamma u_{2k+1}^2 u_{2k-2} \big) + O(\beta^2, \gamma^2) \tag{9}$$

with $\eta' = \mathcal{N}_{2k}^2 \eta$. In the following, we shall suppress $O(\beta^2, \gamma^2)$, restricting our calculations always to the first order both in β and γ, which we shall verify to be small indeed later. The α's are taken to all orders.

Taking the scalar products of equation (8) and each one of $u_{2k}, u_{2k+1}, \ldots$, we get

$$\varepsilon_{2k} + \eta' \big[\langle u_{2k}^4 \rangle + 3\alpha^2 \langle u_{2k}^2 u_{2k+1}^2 \rangle + 3\beta \langle u_{2k}^3 u_{2k+2} \rangle + 3\alpha^2 \beta \langle u_{2k} u_{2k+1}^2 u_{2k+2} \rangle + 3\gamma \langle u_{2k}^3 u_{2k-2} \rangle + 3\alpha^2 \gamma \langle u_{2k} u_{2k+1}^2 u_{2k-2} \rangle \big] = E_{2k}, \tag{10}$$

$$\alpha \varepsilon_{2k+1} + \alpha \eta' \big[3 \langle u_{2k}^2 u_{2k+1}^2 \rangle + \alpha^2 \langle u_{2k+1}^4 \rangle + 6\beta \langle u_{2k} u_{2k+1}^2 u_{2k+2} \rangle + 6\gamma \langle u_{2k} u_{2k+1}^2 u_{2k-2} \rangle \big] = \alpha E_{2k}, \tag{11}$$

$$\beta \varepsilon_{2k+2} + \eta' \big[\langle u_{2k}^3 u_{2k+2} \rangle + 3\alpha^2 \langle u_{2k} u_{2k+1}^2 u_{2k+2} \rangle + 3\beta \langle u_{2k}^2 u_{2k+2}^2 \rangle + 3\alpha^2 \beta \langle u_{2k+1}^2 u_{2k+2}^2 \rangle, + 3\gamma \langle u_{2k}^2 u_{2k-2} u_{2k+2} \rangle + 3\alpha^2 \gamma \langle u_{2k+1}^2 u_{2k-2} u_{2k+2} \rangle \big] = \beta E_{2k}, \tag{12}$$

and

$$\gamma \varepsilon_{2k-2} + \eta' \big[\langle u_{2k}^3 u_{2k-2} \rangle + 3\alpha^2 \langle u_{2k} u_{2k+1}^2 u_{2k-2} \rangle + 3\gamma \langle u_{2k}^2 u_{2k-2}^2 \rangle + 3\alpha^2 \gamma \langle u_{2k+1}^2 u_{2k-2}^2 \rangle + 3\beta \langle u_{2k}^2 u_{2k+2} u_{2k-2} \rangle + 3\alpha^2 \beta \langle u_{2k+1}^2 u_{2k+2} u_{2k-2} \rangle \big] = \gamma E_{2k}, \tag{13}$$

where the angular bracket means integration $\langle f \rangle = \int_{-a}^{a} f(x)\,\mathrm{d}x$. Note that equation (11) is trivial with $\alpha = 0$, in which case equations (10), (12) and (13) determine the value of β, γ and E_{2k} for a given value of η and yields a symmetry-preserving solution to equation (8).

To exhibit the bifurcation, we shall show that these equations have a solution with non-vanishing α, corresponding to $\eta \leqslant \eta_{2k}^{\mathrm{c}} < 0$. For this purpose, we assume $\alpha \neq 0$ to divide out α from both sides of equation (11).

Eliminating E_{2k} from equations (10) and (11), from equations (11) and (12), and from equations (11) and (13), we get

$$\begin{aligned} &A_0 + A_1\beta + A_2\gamma = 0 \\ &B_0 + B_1\beta + B_2\gamma = 0 \\ &C_0 + C_1\beta + C_2\gamma = 0 \end{aligned} \tag{14}$$

where

$$A_i = a_{i0} + (a_{i1} + a_{i2}\,\alpha^2)\eta' \qquad (i = 0, 1, 2) \tag{15}$$

with

$$\begin{aligned} &a_{00} = \varepsilon_{2k+1} - \varepsilon_{2k}, && a_{01} = 3\langle u_{2k}^2 u_{2k+1}^2\rangle - \langle u_{2k}^4\rangle, && a_{02} = \langle u_{2k+1}^4\rangle - 3\langle u_{2k}^2 u_{2k+1}^2\rangle, \\ &a_{10} = 0, && a_{11} = 6\langle u_{2k} u_{2k+1}^2 u_{2k+2}\rangle - 3\langle u_{2k}^3 u_{2k+2}\rangle, && a_{12} = -3\langle u_{2k} u_{2k+1}^2 u_{2k+2}\rangle, \\ &a_{20} = 0, && a_{21} = 6\langle u_{2k} u_{2k+1}^2 u_{2k-2}\rangle - 3\langle u_{2k}^3 u_{2k-2}\rangle && a_{22} = -3\langle u_{2k-2} u_{2k} u_{2k+1}^2\rangle, \end{aligned} \tag{16}$$

and similarly for B_i and C_i with

$$\begin{aligned} &b_{00} = 0, && b_{01} = \langle u_{2k}^3 u_{2k+2}\rangle, && b_{02} = 3\langle u_{2k} u_{2k+1}^2 u_{2k+2}\rangle, \\ &b_{10} = \varepsilon_{2k+2} - \varepsilon_{2k+1}, && b_{11} = 3\langle u_{2k}^2 u_{2k+2}^2\rangle - 3\langle u_{2k}^2 u_{2k+1}^2\rangle, && b_{12} = 3\langle u_{2k+1}^2 u_{2k+2}^2\rangle - \langle u_{2k+1}^4\rangle, \\ &b_{20} = 0, && b_{21} = 3\langle u_{2k}^2 u_{2k-2} u_{2k+2}\rangle, && b_{22} = 3\langle u_{2k-2} u_{2k+1}^2 u_{2k+2}\rangle, \end{aligned} \tag{17}$$

and

$$\begin{aligned} &c_{00} = 0, && c_{01} = \langle u_{2k}^3 u_{2k-2}\rangle, && c_{02} = 3\langle u_{2k} u_{2k+1}^2 u_{2k-2}\rangle, \\ &c_{10} = 0, && c_{11} = 3\langle u_{2k}^2 u_{2k+2} u_{2k-2}\rangle, && c_{12} = 3\langle u_{2k+1}^2 u_{2k+2} u_{2k-2}\rangle, \\ &c_{20} = \varepsilon_{2k-2} - \varepsilon_{2k+1}, && c_{21} = 3\langle u_{2k}^2 u_{2k-2}^2\rangle - 3\langle u_{2k}^2 u_{2k+1}^2\rangle, && c_{22} = 3\langle u_{2k+1}^2 u_{2k-2}^2\rangle - \langle u_{2k+1}^4\rangle. \end{aligned} \tag{18}$$

In order that the linear simultaneous equations (14) for β and γ have solutions, we must have

$$\begin{vmatrix} A_0 & A_1 & A_2 \\ B_0 & B_1 & B_2 \\ C_0 & C_1 & C_2 \end{vmatrix} = 0, \qquad (k \neq 0) \tag{19}$$

which gives an algebraic equation for η' of the third order for a given value of α. Thus, we can equivalently regard η' as a function of α in place of reading α as a function of η'.

To estimate the critical value ${\eta'_{2k}}^{\mathrm{c}}$, we have to know the values of the integrals $\langle\cdots\rangle$ appearing in equations (16)–(18).

If the central barrier of equation (3) is very high, then the eigenfunctions of equation (4) can be approximated by

$$u_{2k}(x) = \begin{cases} f_k(x) & b \leqslant x \leqslant a, \\ 0 & |x| < b, \\ f_k(-x) & -a \leqslant x \leqslant -b, \end{cases} \tag{20}$$

and

$$u_{2k+1}(x) = \begin{cases} f_k(x) & b \leqslant x \leqslant a \\ 0 & |x| < b, \\ -f_k(-x) & -a \leqslant x \leqslant -b, \end{cases} \quad (21)$$

with

$$f_k(x) = \sqrt{\frac{2}{1-2b}} \sin \frac{2(k+1)\pi(x-b)}{1-2b},$$

where $2b$ is the size of the central barrier and $a = 1/2$, when the central barrier is very high, the integrals of the eigenfunctions within the barrier can be neglected. Then,

$$\begin{aligned} \langle u_{2k}^2 u_{2k+1}^2 \rangle &= \langle u_{2k}^4 \rangle = \langle u_{2k+1}^4 \rangle \\ &= \left(\frac{2}{1-2b}\right)^2 \int_b^{1/2} \sin^4 \frac{2(k+1)\pi(x-b)}{1-2b} \, \mathrm{d}x = \frac{3}{2(1-2b)} \end{aligned} \quad (22)$$

$$\begin{aligned} \langle u_{2k}^2 u_{2k+2}^2 \rangle &= \langle u_{2k}^2 u_{2k+3}^2 \rangle = \langle u_{2k+1}^2 u_{2k+2}^2 \rangle = \langle u_{2k+1}^2 u_{2k+3}^2 \rangle \\ &= 2 \left(\frac{2}{1-2b}\right)^2 \int_b^{1/2} \sin^2 \frac{2(k+1)\pi(x-b)}{1-2b} \sin^2 \frac{2(k+2)\pi(x-b)}{1-2b} \mathrm{d}x \\ &= \frac{1}{1-2b} \end{aligned} \quad (23)$$

$$\begin{aligned} \langle u_{2k-2} u_{2k}^2 u_{2k+2} \rangle &= \langle u_{2k-2} u_{2k+1}^2 u_{2k+2} \rangle = \langle u_{2k-1} u_{2k}^2 u_{2k+3} \rangle = \langle u_{2k-1} u_{2k+1}^2 u_{2k+3} \rangle \\ &= 2 \left(\frac{2}{1-2b}\right)^2 \int_b^{1/2} \sin \frac{2(k)\pi(x-b)}{1-2b} \sin^2 \frac{2(k+1)\pi(x-b)}{1-2b} \\ &\quad \times \sin \frac{2(k+2)\pi(x-b)}{1-2b} \mathrm{d}x \\ &= \frac{1}{2(1-2b)}. \end{aligned} \quad (24)$$

For $b = 0.05$ of the illustrative example to be treated in section 4,

$$\begin{aligned} \langle u_{2k}^2 u_{2k+1}^2 \rangle &= \frac{3}{2 \times 0.9} = 1.67 \\ \langle u_{2k}^2 u_{2k+2}^2 \rangle &= \frac{1}{0.9} = 1.11 \\ \langle u_{2k-2} u_{2k}^2 u_{2k+2} \rangle &= \frac{1}{2 \times 0.9} = 0.556 \end{aligned}$$

a little too large compared with the value, $\langle u_0^2 u_1^2 \rangle = 1.55275$, $\langle u_0^2 u_2^2 \rangle = 1.019997$, $\langle u_0 u_2^2 u_4 \rangle = 0.49728$ for our illustrative example in section 4 (see table 2). We note that the estimates similar to the above give

$$\begin{aligned} &\langle u_{2k}^3 u_{2k+2} \rangle, \quad \langle u_{2k} u_{2k+1}^2 u_{2k\pm 2} \rangle, \quad \langle u_{2k}^3 u_{2k-2} \rangle, \quad \langle u_{2k}^2 u_{2k+1} u_{2k+3} \rangle, \\ &\langle u_{2k+1}^3 u_{2k+3} \rangle, \quad \langle u_{2k+1} u_{2k+3}^3 \rangle, \quad \langle u_{2k+1} u_{2k+2}^2 u_{2k+3} \rangle \sim 0. \end{aligned} \quad (25)$$

Then,

$$B_1 \sim b_{10} = \varepsilon_{2k+2} - \varepsilon_{2k+1}, \qquad -C_2 \sim -c_{20} = \varepsilon_{2k+1} - \varepsilon_{2k-2} \quad (26)$$

are very large compared with 1, which is the order of magnitudes of the integrals $\langle \cdots \rangle$ appearing in equation (14). Therefore, equation (19) can be approximated roughly by $A_0 \sim a_{00} + (a_{01} + a_{02}\alpha^2)\eta' = 0$, and hence

$$\eta' \sim -\frac{a_{00}}{a_{01} + a_{02}\alpha^2} \sim -\frac{\varepsilon_{2k+1} - \varepsilon_{2k}}{3(1-\alpha^2)}, \quad (27)$$

which is small and negative by our assumption, equation (5), and $a_{01} \sim 3$, $a_{02} \sim -3$. We arrive at

$$\eta_{2k} \leqslant \eta_{2k}^{c} \sim -\mathcal{N}_{2k}^{2}\big|_{\alpha=0}\frac{\varepsilon_{2k+1}-\varepsilon_{2k}}{3},$$

giving the bifurcation point η_{2k}^{c}.

From the second and third of equation (14), we obtain

$$\beta \sim -\frac{B_0C_2 - C_0B_2}{B_1C_2 - C_1B_2} \sim -\frac{B_0}{B_1} \sim -\frac{(b_{01}+b_{02}\alpha^2)\eta'}{b_{10}+(b_{11}+b_{12}\alpha^2)\eta'}, \tag{28}$$

and

$$\gamma \sim -\frac{C_0}{C_2} \sim -\frac{(c_{01}+c_{02})\eta'}{c_{20}+(c_{21}+c_{22}\alpha^2)\eta'}. \tag{29}$$

Both β and γ are small as expected, so $\mathcal{N}_{2k}|_{\alpha=0} \sim 1$ and $\eta_{2k}^{c} = -(\varepsilon_{2k+1} - \varepsilon_{2k})/3$, a negative value.

We remark that, when $k = 0$, we know $\gamma = 0$ and find $C_0 = C_1 = 0$ from equation (18). Consequently, equation (13) drops out and the determinant equation (19) reduces to

$$\begin{vmatrix} A_0 & A_1 \\ B_0 & B_1 \end{vmatrix} = 0 \qquad (k = 0), \tag{30}$$

yet giving the same η' as equation (27), and the same η_{2k}^{c}.

For the 'odd' symmetry-breaking solutions, we have similarly

$$\begin{aligned} &A_0 + A_1\beta + A_2\gamma = 0\\ &B_0 + B_1\beta + B_2\gamma = 0\\ &C_0 + C_1\beta + C_2\gamma = 0 \end{aligned} \tag{31}$$

where

$$A_i = a_{i0} + (a_{i1} + a_{i2}\alpha^2)\eta' \qquad (i = 0, 1, 2) \tag{32}$$

and similarly for B_i and C_i with

$$\begin{aligned}
&a_{00} = \varepsilon_{2k} - \varepsilon_{2k+1}, && a_{01} = 3\langle u_{2k}^2 u_{2k+1}^2\rangle - \langle u_{2k+1}^4\rangle, && a_{02} = \langle u_{2k}^4\rangle - 3\langle u_{2k}^2 u_{2k+1}^2\rangle,\\
&a_{10} = 0, && a_{11} = 6\langle u_{2k}^2 u_{2k+1} u_{2k+3}\rangle - 3\langle u_{2k+1}^3 u_{2k+3}\rangle, && a_{12} = -3\langle u_{2k}^2 u_{2k+1} u_{2k+3}\rangle,\\
&a_{20} = 0, && a_{21} = 6\langle u_{2k-1} u_{2k}^2 u_{2k+1}\rangle - 3\langle u_{2k-1} u_{2k+1}^3\rangle, && a_{22} = -3\langle u_{2k-1} u_{2k}^2 u_{2k+1}\rangle,\\
&b_{00} = 0, && b_{01} = \langle u_{2k+1}^3 u_{2k+3}\rangle, && b_{02} = 3\langle u_{2k}^2 u_{2k+1} u_{2k+3}\rangle,\\
&b_{10} = \varepsilon_{2k+3} - \varepsilon_{2k}, && b_{11} = 3\langle u_{2k+1}^2 u_{2k+3}^2\rangle - 3\langle u_{2k}^2 u_{2k+1}^2\rangle, && b_{12} = 3\langle u_{2k}^2 u_{2k+3}^2\rangle - \langle u_{2k}^4\rangle,\\
&b_{20} = 0, && b_{21} = 3\langle u_{2k-1} u_{2k+1}^2 u_{2k+3}\rangle, && b_{22} = 3\langle u_{2k-1} u_{2k}^2 u_{2k+3}\rangle,\\
&c_{00} = 0, && c_{01} = \langle u_{2k-1} u_{2k+1}^3\rangle, && c_{02} = 3\langle u_{2k-1} u_{2k}^2 u_{2k+1}\rangle,\\
&c_{10} = 0, && c_{11} = 3\langle u_{2k-1} u_{2k+1}^2 u_{2k+3}\rangle, && c_{12} = 3\langle u_{2k-1} u_{2k}^2 u_{2k+3}\rangle,\\
&c_{20} = \varepsilon_{2k-1} - \varepsilon_{2k}, && c_{21} = 3\langle u_{2k-1}^2 u_{2k+1}^2\rangle - 3\langle u_{2k}^2 u_{2k+1}^2\rangle, && c_{22} = 3\langle u_{2k-1}^2 u_{2k}^2\rangle - \langle u_{2k}^4\rangle.
\end{aligned} \tag{33}$$

Using the same method, we can get the critical $\eta_{2k+1}^{c} \sim (\varepsilon_{2k+1} - \varepsilon_{2k})/3 > 0$. In this case, we have a positive critical value for the symmetry-breaking solutions. Then combining the results

Table 1. The first six eigenvlues of equation (4).

$\varepsilon_0 = 41.998$	$\varepsilon_1 = 42.987$	$\varepsilon_2 = 167.20$
$\varepsilon_3 = 171.72$	$\varepsilon_4 = 372.71$	$\varepsilon_5 = 385.45$

Table 2. The values of the integrals.

$\langle u_0^4\rangle = 1.5426$	$\langle u_1^4\rangle = 1.5639$	$\langle u_2^4\rangle = 1.5240$	$\langle u_3^4\rangle = 1.5587$
$\langle u_0^2u_1^2\rangle = 1.5528$	$\langle u_2^2u_3^2\rangle = 1.5386$	$\langle u_0^2u_2^2\rangle = 1.0200$	$\langle u_1^2u_2^2\rangle = 1.0168$
$\langle u_1^2u_3^2\rangle = 1.0402$	$\langle u_0^2u_3^2\rangle = 1.0431$	$\langle u_2^2u_4^2\rangle = 0.997\,71$	$\langle u_3^2u_4^2\rangle = 0.989\,18$
$\langle u_3^2u_5^2\rangle = 1.0347$	$\langle u_2^2u_5^2\rangle = 1.0405$	$\langle u_0^3u_2\rangle = -0.007\,6541$	$\langle u_3^3u_5\rangle = -0.004\,8963$
$\langle u_1^3u_3\rangle = -0.002\,2162$	$\langle u_2^3u_4\rangle = -0.018\,363$	$\langle u_0u_2^3\rangle = -\,0.003\,8937$	$\langle u_1u_3^3\rangle = -0.001\,1890$
$\langle u_0^2u_1u_3\rangle = 0.023\,223$	$\langle u_0u_1^2u_2\rangle = -0.033\,716$	$\langle u_2u_3^2u_4\rangle = -0.060\,834$	$\langle u_2^2u_3u_5\rangle = 0.032\,752$
$\langle u_0u_2u_3^2\rangle = 0.011\,577$	$\langle u_1u_2^2u_3\rangle = -0.018\,826$	$\langle u_0u_2^2u_4\rangle = 0.497\,28$	$\langle u_0u_3^2u_4\rangle = 0.488\,13$
$\langle u_1u_2^2u_5\rangle = 0.520\,49$	$\langle u_1u_3^2u_5\rangle = 0.516\,86$		

of η_{2k+1}^{c} and η_{2k}^{c}, we have

$$\left.\begin{array}{r}\eta_{2k}^{\mathrm{c}}\\ \eta_{2k+1}^{\mathrm{c}}\end{array}\right\} \sim \mp\frac{\varepsilon_{2k+1}-\varepsilon_{2k}}{3}. \tag{34}$$

This equation is valid for $k = 0$ also, though equation (19) reduces in the case of equation (30).

These conclusions about the bifurcation are not restricted to the example of the double-square well, equation (3). Most of the above calculations are valid in general except for the concrete estimates of the integrals $\langle\cdots\rangle$. A more careful estimate of the bifurcation points will be carried out in the next section.

4. Comparison with the exact solutions

To illustrate how good our approximation method is, we consider the double-square well example, equation (3), with the parameters

$$a = 0.5, \qquad b = 0.05, \qquad V_0 = 1000. \tag{35}$$

The high V_0 guarantees the approximation condition (5) for $k = 0, 1, 2, \ldots$. The linear Schrödinger equation (4) can be solved easily. The eigenvalues and the integrals $\langle u_{2k}^4\rangle$ etc are given in tables 1 and 2.

Solving equations (14) and (15) and equations (31) and (32) exactly for vanishing α, we can find the critical values, η_m^c, for the coupling constant of the nonlinear interaction. We hasten to remark that, when $m = 0$, we have added one more state, u_4, to equation (6) to improve the approximation. The results agree very well with the exact values from the numerical solution of the GPE [10] as shown in table 3.

By solving equation (14) for given values of η' $\left(\eta'\langle\eta_{2k}^{\mathrm{c}\prime}\text{ or }\eta'\rangle\eta_{2k+1}^{\mathrm{c}\prime}\right)$, we find the coefficients α, β and γ in equation (6) for the symmetry-breaking solutions. We remark that, though equation (31) is a higher order algebraic equation for α, β and γ, the set of real solutions with $|\alpha| < 1$ is unique. The results are shown in figure 1 as functions of η. Note that $\beta, \gamma \ll \alpha < 1$ as expected, justifying our approximation in equation (9) to neglect the second or higher order

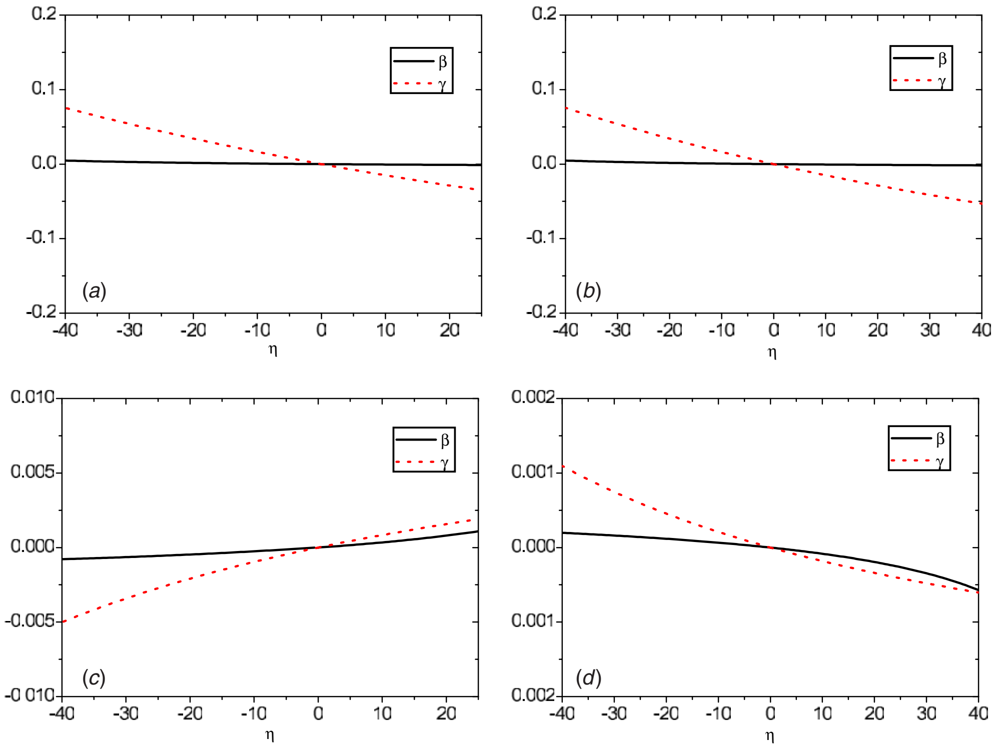

Figure 2. The expansion coefficients of symmetry-preserving states (6) with $\alpha = 0$. (*a*) $m = 0$, (*b*) $m = 1$, (*c*) $m = 2$, (*d*) $m = 3$.

Table 3. The critical coupling constants, η_m^c.

n	Our approximation	Exact (numerical calc.)
0	−0.317 54	−0.317 21
1	0.319 72	0.319 98
2	−1.461 4	−1.459 2
3	1.477 9	1.479 9

terms in β and γ. For $\alpha = 0$, the equation (11) is removed, and the remaining simultaneous equations (10), (12) and (13) have solutions β and γ and eigenvalue of E_{2k}. which survive for all η; these are for the symmetry-preserving states. As we said in section 3, for the ground state we have to include one more level u_4, then in figure 2(*a*) γ represents the corresponding coefficient. Similarly, in figure 2(*b*) for the first excited state, γ corresponds to the coefficient of u_5. Here also, we find $0 < \beta, \gamma \ll 1$, as shown in figure 2 justifying our approximation in equation (9).

The coefficients α, β and γ thus determined give, by equations (10)–(13), the energy eigenvalues E_{2k} for the states, symmetry-breaking as well as symmetry-preserving. In figure 3, the results are compared with the exact results from numerical solution of the GPE [10]; the agreement is very good for $|\eta| \leqslant 10$, and not very bad even for $10 < |\eta| < 40$ for most of the states. In figure 3, one sees also the bifurcations very clearly.

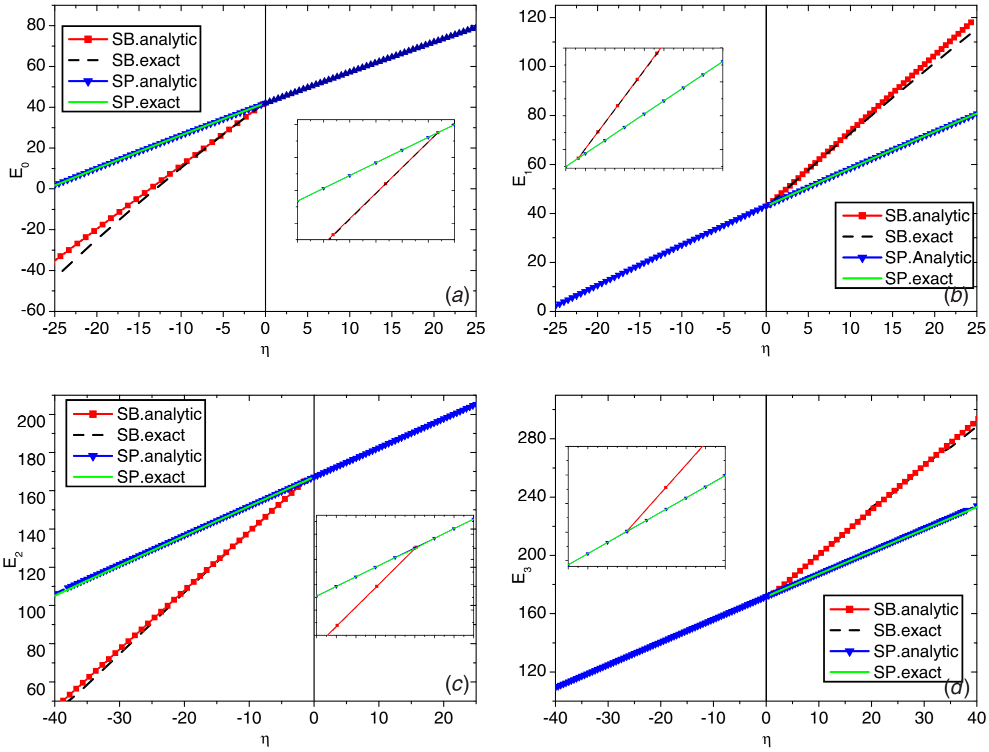

Figure 3. The energy eigenvalues of (1). Those for the symmetry-breaking states (SB) bifurcate from those for the symmetry-preserving states (SP). (*a*) $m = 0$, (*b*) $m = 1$, (*c*) $m = 2$, (*d*) $m = 3$.

5. Conclusion

An approximation method to clarify the symmetry-breaking stationary solutions of GPE (1) with symmetric double-well external potential was presented. It was shown that each symmetry-breaking solution $\Phi_n(x)$ arises from a symmetry-preserving one if η, the coupling constant of the nonlinear interaction, starting from 0, exceeds a certain value η_n^{c}, the bifurcation. η_n^{c} was determined in good approximation for each symmetry preserving solution, the result being $\eta_{2k}^{\mathrm{c}} < 0$ for symmetric states and $\eta_{2k+1}^{\mathrm{c}} > 0$ for anti-symmetric states. The lower energy eigenvalues E_n for the states, symmetry-preserving as well as symmetry-breaking, were also determined in very good approximation for $|\eta| < 10$, and in a not bad approximation for $10 \leqslant |\eta| < 40$. This success of our approximation depends on the condition, equation (5), which is satisfied well by our touchstone model, equation (3) with equation (35).

When the nonlinear interaction is larger, a natural way to keep the approximation good is to include more eigenstates of the linear Schrödinger equation in the expansions, equations (6) and (7). Another possible method is to construct the symmetry-preserving states somehow and use their linear combination to represent the symmetry-breaking states. Since the solutions to GPE need not be orthogonal to each other, we should orthogonalize them before expansion.

The present work is a model calculation to illustrate our method, and cannot be compared with experiments directly beyond the qualitative aspects, the bifurcation of the symmetry breaking states from the symmetry preserving states. In place of checking our results with experiments, we have compared the results from our approximation with those from exact numerical calculations [9, 10], finding that their agreement is very good.

In view of the experimental condition of today in which quasi-one-dimensional double well for trapping atoms has been realized and is well controllable [4, 13], we would like to mention that our results are closely related to one recent experiment on the so-called macroscopic quantum self-trapping effect [4, 6, 7]. We hope that our approximation method may be helpful in understanding this effect, clarifying the time evolution of nonlinear systems. This project is now in progress and the results will be reported in the near future.

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References

[1] Anker Th *et al* 2004 *Preprint* cond-matt/0410176
[2] Buljan H, Segev M and Vardi A 2004 *Preprint* cond-matt/0410421
[3] Shin Y *et al* 2004 *Phys. Rev. Lett.* **92** 050405
[4] Albiez M, Gati R, Folling J, Hunsmann S, Cristiani M and Oberthaler M K 2005 *Phys. Rev. Lett.* **95** 010402 (*Preprint* cond-matt/0411757)
[5] Dalfovo F, Giorgini S, Pitaevskii L P and Stringari S 1999 *Rev. Mod. Phys.* **71** 463
[6] Smerzi A, Fantoni S, Giovanazzi S and Shenory S R 1997 *Phys. Rev. Lett.* **79** 4950
[7] Raghavan S, Smerzi A, Fantoni S and Shenoy S R 1999 *Phys. Rev.* A **59** 620
[8] Mahmud K W, Kuttz J N and Reinhardt W P 2002 *Phys. Rev.* A **66** 063607
[9] D'Agosta R and Presilla C 2002 *Phys. Rev.* A **65** 043609
[10] Wei-Dong Li 2006 *Phys. Rev.* A **74** 063612
[11] Ain P, Infeld E, Matuszewski M, Rowlands G and Trippenbach M 2006 *Phys. Rev.* A **73** 022105
Infeld E, Ain P, Gocalek J and Trippenbach M 2006 *Phys. Rev.* E **74** 026610
[12] Olshanii M 1998 *Phys. Rev. Lett.* **81** 938
Astrakharchik G E, Blume D, Giorgini S and Granger B E 2004 *Phys. Rev. Lett.* **92** 030402
[13] Inouye S *et al* 1998 *Nature (London)* **392** 151
Cornish S L *et al* 2000 *Phys. Rev. Lett.* **85** 1795
Greiner M *et al* 2001 *Phys. Rev. Lett.* **87** 160405