Stationary solutions to the multi-dimensional Gross–Pitaevskii equation with double-well potential

Andrea Sacchetti

Department of Physics, Computer Sciences and Mathematics, University of Modena e Reggio Emilia, Via Campi 213/B, I-41125, Modena, Italy
E-mail: andrea.sacchetti@unimore.it

Received 6 December 2013, revised 16 June 2014
Accepted for publication 3 September 2014
Published 30 September 2014

Recommended by T Grava

Abstract

In this paper we consider a nonlinear Schrödinger equation with a cubic nonlinearity and a multi-dimensional double well potential. In the semiclassical limit the problem of the existence of stationary solutions simply reduces to the analysis of a finite dimensional Hamiltonian system which exhibits different behaviour depending on the dimension. In particular, in dimension 1 the symmetric stationary solution shows a standard pitchfork bifurcation effect, while in dimensions 2 and 3 new asymmetrical solutions associated with saddle points occur. These last solutions are localized on a single well and this fact is related to the phase transition effect observed in Bose–Einstein condensates in periodical lattices.

Keywords: nonlinear Schrödinger equations, semiclassical approximation, Bose–Einstein condensates in lattices
Mathematics Subject Classification: 35Q55; 81Q20

1. Introduction

Atomic Bose–Einstein condensates (BECs) are described by means of nonlinear Schrödinger equations where the nonlinear term of the form $|\psi|^{2\sigma} \psi$, $\sigma = 1, 2, \ldots$, represents the $(\sigma + 1)$-body contact potential [12], where $\psi$ is the condensate’s wavefunction. In fact, BECs strongly depend on interatomic forces and the binary coupling term $|\psi|^2 \psi$ usually represents the dominant nonlinear term, the nonlinear Schrödinger equation obtained for $\sigma = 1$ takes the usual form of the well-known Gross–Pitaevskii equation [13].
The analysis of the time-dynamic of BECs is, in general, an open problem and few rigorous results have been given. Among the basic models for BECs the model with a symmetric external double-well potential plays an important role. Indeed, the explanation of some basic properties in such a relatively simple model will enable us to understand the fundamental mechanisms for a large family of BECs. For instance, the phase transition phenomenon we can observe for BECs in a periodic lattice can be explained as a result of the bifurcation effects we can already see in the relatively simple double well model. In particular, for BECs in a periodic lattice a transition from the superfluidity phase to the Mott-insulator phase has been seen when the effective nonlinearity parameter becomes larger than a critical value \[3, 6, 8\]. In particular, it turns out that such a transition is quite slow in one-dimensional lattice, while it becomes very sharp in three-dimensional lattices.

We consider here the case where the external potential of the linear part of the Schrödinger equation has a double well shape. If the nonlinear term is absent then the linear Schrödinger equation has symmetric and antisymmetric eigenstates. However, the introduction of a nonlinear term, which usually models in quantum mechanics an interacting many-particle system, may give rise to asymmetrical states related to spontaneous symmetry breaking phenomenon. It has been already proved that for one-dimensional nonlinear Schrödinger equations with double-well potentials (see \[7, 15\] for the result obtained in the semiclassical limit, see also \[11\] in the limit of large barrier between the two wells) then the symmetric/antisymmetric stable stationary state bifurcates when the adimensional effective nonlinear parameter takes absolute value equal to a critical value. We would also mention the recent papers \[1\], where a sort of renormalized multiple well case with a singular scaling has been considered and where a bifurcation effect is also present \[10\], where general results on symmetry breaking bifurcation with double well potential are given, and finally \[16\] where a more thorough investigation on symmetry breaking effect is given.

In this paper we explore in detail the different pictures that may occur in dimensions 1, 2 and 3 for the stationary solutions of the Gross–Pitaevskii equation associated with the linear ground state. In dimension 1 the only situation can occur is the bifurcation of the symmetric stationary solution, where a branch of asymmetrical solutions appears and where these asymmetrical solutions are going to be gradually localized on a single well when the nonlinearity strength increases. In dimension 2 we have different kinds of bifurcations. One kind of bifurcations is similar to the one already seen in dimension 1. Furthermore, new families of bifurcations appear, they are associated with the spontaneous symmetry breaking effect where a saddle point appears for a critical value of the nonlinearity strength. The stationary solutions on the branches raising from such a saddle point have the following peculiarity: they are mostly localized on just one well and thus the localization effect suddenly occurs when the nonlinearity parameter is around its critical value. A similar picture, with a more intricate sequence of bifurcations, occurs also in dimension 3.

The different behaviour between models in dimension 1 and in dimensions higher than 1 has an important physical consequences when we consider BECs in lattices. Indeed, it has been observed that for BECs in lattices a transitions from a superfluidity phase to a Mott-insulator phase occurs when the nonlinearity strength reaches a critical values; in particular in dimension 1 the transition is smooth, while in dimension 3 the transition is sharp. In fact, such a different behaviour is expected to be connected to the appearance, in dimensions 2 and 3, of stationary solutions localized on a single lattice site as we have seen for double-well models.

In this paper we make use of the semiclassical limit in order to reduce the nonlinear Schrödinger equation to a finite dimensional Hamiltonian system. This technique has been developed by \[14\] and it has the advantage to reduce the problem of the analysis of the stationary solutions and of the time-dynamics of the wavefunction to a rather simple dynamical system,
even for nonlinear Schrödinger equations in dimensions 2 and 3. A different approach has been proposed by [17], where they make use of some kind of Galerkin approximation for double-well models in dimension 2.

The paper is organized as follows. In section 2 we introduce the model. In section 3 we consider the $N$-mode approximation for nonlinear Schrödinger operator with a lattice potential in any dimension $d$. In section 4 we consider in more detail the $N$-mode approximation for double-well potential in any dimension. Finally, in section 5 we numerically compute the stationary solutions of the $N$-mode approximation in dimension $d = 1$, $d = 2$ and $d = 3$ associated with the linear ground state.

Concerning notation $w = O(\bar{h}^\infty)$ means that for any $n \in \mathbb{N}$ there exists $C_n > 0$ such that $|w| \leq C_n \bar{h}^n$.

2. Double-well model

Here, we consider the nonlinear Schrödinger (hereafter NLS) equation in the $d$-dimensional space $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$

$$\begin{cases}
\hbar \frac{\partial \psi}{\partial t} = H_0 \psi + \epsilon |\psi|^{2\sigma} \psi, \quad \psi(\cdot, t) \in L^2(\mathbb{R}^d, dx), \quad \|\psi(\cdot, t)\| = 1,
\psi_0(x) = \psi(x, 0)
\end{cases}$$

(1)

where $\epsilon \in \mathbb{R}$ and $\|\cdot\|$ denotes the $L^2(\mathbb{R}^d, dx)$ norm;

$$H_0 = -\hbar^2 \frac{\Delta}{2m} + V, \quad \Delta = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2}$$

(2)

is the linear Hamiltonian with a lattice potential $V(x)$. In the case of cubic nonlinearity where $\sigma = 1$ then (1) is usually called Gross–Pitaevskii equation. For the sake of definiteness we assume the units such that $2m = 1$. The semiclassical parameter $\bar{h} > 0$ is such that $\bar{h} \ll 1$.

Let us introduce the assumptions on the lattice potential $V(x)$.

**Hypothesis 1.** Let $v(x) \in C_0^\infty(\mathbb{R}^d)$ be a spherically symmetric single well potential, that is $v(x) = f(|x|)$ where $f(r) \in C_0^\infty(\mathbb{R}^+)$ is a smooth non-positive monotone not decreasing function with compact support and such that $f(0) < 0$. In particular, we assume that $f'(0+0) = 0$ and $f''(0+0) > 0$. Then $v(x)$ is a smooth function with compact support and with a non-degenerate minimum value at $x = 0$:

$$v(x) > v_{\text{min}} = f(0), \quad \forall x \in \mathbb{R}^d, \ x \neq 0.$$  

(3)

By construction the support of $v(x)$ is a $d$-dimensional ball with centre at $x = 0$ and radius $a$, for some $a > 0$. Let $J_m \in \mathbb{Z}$ and $K_m \in \mathbb{Z}$, $m = 1, 2, \ldots, d$ be fixed and such that $J_m \leq K_m$; let

$$J = \{ j = (j_1, \ldots, j_d) \in \mathbb{Z}^d : J_m \leq j_m \leq K_m, \ m = 1, 2, \ldots, d \}.$$  

We then define a lattice potential as

$$V(x) = \sum_{j \in J} v(x - x_j), \quad x_j = jb = (j_1 b, \ldots, j_d b),$$

(4)

where $b > 0$ is such that $b > 2a$. Hence, by construction, the lattice potential $V(x)$ has exactly

$$N := \prod_{m=1}^{d} [K_m - J_m + 1]$$

(5)

similar wells with non-degenerate minima at $x = x_j$, $j \in J$. 


It is a well-known fact ([4] and theorem 6.2.1 [5]) that the Cauchy problem (1) is globally well-posed for any $\epsilon \in \mathbb{R}$ small enough provided that

$$\sigma < \begin{cases} +\infty & \text{if } d \leq 2 \\ \frac{2}{d-2} & \text{if } d > 2 \end{cases}.$$ 

In such a case the conservation of the norm of $\psi(x, t)$ and of the energy

$$E(\psi) = \langle \psi, H_0 \psi \rangle + \frac{\epsilon}{\sigma + 1} \langle \psi^{\sigma+1}, \psi^{\sigma+1} \rangle$$

follows.

3. Reduction to the $N$-mode approximation

Now, making use of the semiclassical analysis [9] we reduce the NLS equation (1) to a $N$-dimensional Hamiltonian system, usually denoted $N$-mode approximation, where $N$ is the total number of lattice sites defined in (5). We make use of the ideas already developed in [2, 14] and adapted here to the case of a lattice potential (4). Since the reduction method is similar to the one already exploited in [2, 14] then we do not dwell here on the details of the proof of the validity of the reduction to the $N$-mode approximation and simply we state the main results.

3.1. Semiclassical results

One of the main tools in semiclassical analysis is the notion of Agmon distance. Let $E \geq v_{\text{min}}$ be fixed, then the Agmon (pseudo-)distance, associated with the energy $E$, between two points $x$ and $y$ is defined as

$$d_A(x, y; E) = \inf_{\gamma} \int_{\gamma} \sqrt{[V(x) - E]^+] \, dx,$$

where the inf is taken on the set of all regular paths $\gamma$ connecting the two points $x$ and $y$ and where $[V - E]^+ = |V - E| + V - E$. Let us consider the Agmon distance associated with the ground state energy, since the difference between the ground state energy and the minimum of the potential is of order $O(\bar{h})$ then in the semiclassical limit we can choose $E = v_{\text{min}}$; in the following, for the sake of simplicity, let us denote

$$d_A(x, y) := d_A(x, y; v_{\text{min}}).$$

We then define the following two quantities

$$S_0 = \inf_{j \neq \ell, j, \ell \in J} d_A(x_j, x_\ell)$$

and

$$S_1 = \inf_{|j - \ell| > 1, j, \ell \in J} d_A(x_j, x_\ell),$$

where $|j - \ell| = \sum_{m=1}^{d} |j_m - \ell_m|$. Then, by construction of the lattice potential $V(x)$, the following result holds true.

**Lemma 1.** Let $j \in J$ and let $\ell \in J$ be such that $|j - \ell| = 1$, then

$$S_0 = d_A(x_j, x_\ell) = 2 \int_0^{b/2} \sqrt{f(r) - f(0)} \, dr$$

is independent of $j$ and $\ell$, and

$$S_0 < S_1.$$
Proof. If |j − ℓ| = 1 then all the components of x_j and x_ℓ are equal, but one: e.g. j_m = ℓ_m for m = 2, . . . , d and j_1 − ℓ_1 = 1. Then, by construction it turns out that

\[ d_A(x_j, x_\ell) = \int_0^b \sqrt{V[x_j + r(1, 0, \ldots, 0)] - v_{\text{min}}} \, dr = 2 \int_0^{b/2} \sqrt{v[r(1, 0, \ldots, 0)] - v_{\text{min}}} \, dr = 2 \int_0^{b/2} \sqrt{f(r) - v_{\text{min}}} \, dr \]

proving (6). Now, in order to prove (7) let

\[ B_{x_j}(S_0/2) = \{ x \in \mathbb{R}^d : d_A(x_j, x) \leq \frac{1}{2} S_0 \} ; \]

then, by construction, it follows that

\[ B_{x_j}(S_0/2) = \{ x \in \mathbb{R}^d : |x_j - x| \leq \frac{1}{2} b \}, \]

where |x − x_j| denotes here the usual distance in \( \mathbb{R}^d \) between two points x and x_j. Hence, if |j − ℓ| > 1 then

\[ B_{x_j}(S_0/2) \cap B_{x_\ell}(S_0/2) = \emptyset \]

and thus (7) follows.

Lemma 2. Let \( j = (j_1, \ldots, j_d) \in \mathbb{Z}^d \), let

\[ \lfloor j \rfloor := \max_{m=1,\ldots,d} |j_m| . \]

Then

\[ d_A(x_j, x_\ell) \geq \lfloor j - \ell \rfloor S_0. \]  

Proof. Assume that s := \lfloor j - \ell \rfloor \neq 0, otherwise j = \ell and (9) immediately follows. Assume also, for argument’s sake, that \lfloor j_1 - \ell_1 \rfloor = s and that \( J_m \leq 0 \leq K_m \) for any m. By construction of the lattice potential it turns out that

\[ \sqrt{V(x_1, x_2, \ldots, x_d) - v_{\text{min}}} \geq \sqrt{V(x_1, 0, \ldots, 0) - v_{\text{min}}} , \]

hence, for any regular path \( \gamma \) connecting the two points x_j and x_\ell, it follows that

\[ d_A(x_j, x_\ell) \geq \int_\gamma \sqrt{V(x_1, x_2, \ldots, x_d) - v_{\text{min}}} \, dx \geq \int_\gamma \sqrt{V(x_1, 0, \ldots, 0) - v_{\text{min}}} \, dx \geq \int_0^s \sqrt{V(x_1, 0, \ldots, 0) - v_{\text{min}}} \, dx_1 = s \cdot S_0. \]
3.2. $N$-mode approximation

Now, let $H_D$ be the Dirichlet realization of the Schrödinger operator formally defined on $L^2(B_0(S), \text{d}x)$ by

$$H_D = -\hbar^2 \Delta + v$$

(10)

where $B_0(S)$ is the ball with centre at $x = 0$ and radius $S > 2S_0$, as defined in (8). Since Hess $v(0) > 0$, i.e. the bottom of $v(x)$ is not degenerate, then the Dirichlet problem associated with the single-well trapping potential $v(x)$ has spectrum $\sigma(H_D)$ with ground state

$$\lambda_D = \frac{v_{\min} + d \sqrt{\mu} h + O(h^2)}{\hbar}, \quad \mu = \frac{1}{2} f''(0),$$

such that

$$\text{dist}[\lambda_D, \sigma(H) \setminus \{\lambda_D\}] \geq 2Ch$$

for some $C > 0$. The normalized eigenvector $\psi_D(x)$ associated with $\lambda_D$ is localized in a neighbourhood of $x = 0$ and it exponentially decreases as $O(\hbar^{-m} e^{-d_A(x)/\hbar})$ for some $m > 0$, and where $d_A(x) := d_A(x, 0)$ is the Agmon distance between $x$ and the point $x = 0$. In particular, in a neighbourhood of $x = 0$ then $\psi_D(x) \sim \mu_{d/8}(\pi h)^{-d/2} e^{-\sqrt{\mu} x^2}/2h$.

The bottom of the spectrum $\sigma(H_0)$ of $H_0$ contains exactly $N$ eigenvalues $\lambda_j, j \in J$, such that

$$\lambda_j - \lambda_D = O(e^{-\rho/\hbar})$$

for any $0 < \rho < S_0$; this result is a consequence of the fact that the multiple well potential $V(x)$ is given by a superposition of $N$ exactly equal wells displaced on a regular lattice. Furthermore,

$$\text{dist}[(\lambda_j)_{j \in J}, \sigma(H_0) \setminus \{\lambda_j\}_{j \in J}] > Ch.$$

Let $F$ be the eigenspace spanned by the eigenvectors $\psi_j$ associated with the $N$ eigenvalues $\lambda_j$. Then, the restriction $H_0|_F$ of $H_0$ to the subspace $F$ can be represented in the basis of orthonormalized vectors $\phi_j, j \in J$, such that

$$\phi_j(x) - \psi_j(x) = O(e^{-\rho/\hbar}) \quad \text{where} \quad \psi_j(x) = \psi_D(x - x_j);$$

(11)

hence, the vector $\phi_j(x)$ is localized in a neighbourhood of the minimum point $x_j$. In particular, as a result of lemma 1 in the semiclassical limit the following holds (for the proof we refer to theorem 4.3.4 and theorem 4.4.6 by [9]).

**Lemma 3.** Up to an error of order $O(\hbar^\infty) e^{-S_0/\hbar}$ the restriction $H_0|_F$ of $H_0$ to the subspace $F$ is represented in the basis $\phi_j(x), j \in J$, by the square matrix $T$ defined as

$$T_{j,\ell} = \begin{cases} 
\lambda_D & \text{if } |j - \ell| = 0 \\
-\beta & \text{if } |j - \ell| = 1 \\
0 & \text{if } |j - \ell| > 1
\end{cases}$$

(12)

where $\beta$ is a quantity independent of the indexes and such that

$$\frac{1}{C^h^{1/2}} \leq \beta e^{S_0/\hbar} \leq C h^{1-d/2}.$$ 

(13)

Let $\psi$ be the normalized solution to the NLS equation (1). Then $\psi$ may be written in the following form. Let $\Pi$ be the projection operator on the space $F$, and let $\Pi_c = 1 - \Pi$. If the initial state $\psi_0(x) = \psi(x, 0)$ is prepared on the space $F$ spanned by the $N$ ground state linear eigenvectors, that is

$$\psi_c(x, 0) = 0, \quad \text{where} \quad \psi_c = \Pi_c \psi,$$
then it is possible to prove, by making use of ideas similar to the ones developed by [2, 14], that $\psi_c(x, t)$ is exponentially small for times of order $\beta^{-1}$, that is

$$\|\psi_c(\cdot, t)\|_{L^2(\mathbb{R}^d)} = \mathcal{O}(e^{-S_0/\bar{h}}), \ \forall t \in [0, \beta^{-1}],$$

and that $\Pi \psi$ can be written in the form

$$\Pi \psi(x, t) = \sum_{j \in J} d_j(t)\psi_j(x) + \mathcal{O}(h^{\infty}) e^{-S_0/\bar{h}},$$

where $d_j(t), \ j \in J$, satisfy to the $N$-mode approximation for the NLS equation (1), which consists of the following system of ODEs

$$i\bar{h}d_j = \sum_{\ell \in J} T_{j,\ell}d_\ell + \epsilon c|d_j|^{2\sigma}d_j, \ j \in J,$$  \hspace{1cm} (14)

with the normalization condition

$$\sum_{j \in J}|d_j(t)|^2 = 1;$$  \hspace{1cm} (15)

where

$$c = \|\psi_j\|_{L^{2\sigma+2}}^2 = \|\psi_D\|_{L^{2\sigma+2}}^2$$

is a real valued constant independent of $j$.

### 3.3. Hamiltonian form of the N-mode approximation

If we set

$$d_j = \sqrt{q_j}e^{i\theta_j}, \ q_j \in [0, 1], \ \theta_j \in [0, 2\pi),$$

then, by means of a straightforward calculation, it follows that (14) takes the Hamiltonian form

$$\begin{cases}
\hbar \dot{q}_j = \frac{\partial \mathcal{H}}{\partial \theta_j} = -2\beta \sum_{\ell \in J, |j-\ell|=1}^{\sqrt{q_jq_\ell} \sin(\theta_\ell - \theta_j)} \\
\hbar \dot{\theta}_j = \frac{\partial \mathcal{H}}{\partial q_j} = -\lambda_D + \beta \sum_{\ell \in J, |j-\ell|=1}^{\sqrt{q_jq_\ell} \cos(\theta_\ell - \theta_j)} - \epsilon c q_j^\sigma
\end{cases}$$  \hspace{1cm} (16)

with Hamiltonian function

$$\mathcal{H} := \mathcal{H}(q, \theta) = \lambda_D \sum_j q_j - \beta \sum_{j, \ell \in J, |j-\ell|=1}^{\sqrt{q_jq_\ell} \cos(\theta_\ell - \theta_j)} + \frac{\epsilon c}{\sigma + 1} \sum_{j \in J} q_j^{\sigma+1}. \hspace{1cm} (17)$$

The normalization condition (15) takes the form

$$\sum_j q_j = 1$$  \hspace{1cm} (18)

and the Hamiltonian function is a constant of motion, i.e.

$$\mathcal{H}[q(t), \theta(t)] = \mathcal{H}[q(t_0), \theta(t_0)]$$

for any $t, t_0 = 0$ is the initial instant.
### 3.4. Stationary solutions

Stationary solutions are the normalized solutions of (1) of the form \( \psi(x, t) = e^{i\omega t} \psi(x) \). Concerning the study of the stationary solutions has been proved by [7] that for one-dimensional double-well models then the 2-mode approximation gives the stationary solutions to the NLS (1), up to an exponentially small error; furthermore, the orbital stability of the stationary solutions is proved. The same arguments may be applied to the general \( d \)-dimensional problem with lattice potential; that is the stationary solutions of \( N \)-mode approximation (14) and (15), for any \( N \geq 2 \), give, up to an exponentially small error \( O(e^{-\rho/\bar{\hbar}}) \), for any \( 0 < \rho < S_0 \), the stationary solutions of the NLS (1).

In terms of \( N \)-mode approximation (14) it consists in looking for the solution to the system of equations

\[
-\omega \hbar d_j = \sum_{\ell \in J} T_{\ell, j} d_{\ell} + \epsilon c |d_j|^{2\alpha} d_j, \quad j \in J.
\]

As before, if we set \( d_j = \sqrt{q_j} e^{i\theta_j} \), then \( q_j \) and \( \theta_j \) must be the solution to the system of equations

\[
\begin{cases}
0 = \frac{\partial H}{\partial \theta_j}, \\
-\hbar \omega = -\frac{\partial H}{\partial q_j}.
\end{cases}
\]

(20)

Finally, if we set

\[
\Omega = \frac{\hbar \omega - \lambda_D}{\beta} \quad \text{and} \quad \eta = \frac{c \epsilon}{\beta}
\]

then finally we get the equations for stationary solutions

\[
\begin{cases}
0 = \sum_{\ell \in J} |j - \ell| = 1 \sqrt{q_\ell q_j} \sin(\theta_\ell - \theta_j), \\
-\Omega = \sum_{\ell \in J} |j - \ell| = 1 \sqrt{\frac{q_j}{q_\ell}} \cos(\theta_\ell - \theta_j) - \eta q_j^\alpha.
\end{cases}
\]

(21)

### 4. Multi-dimensional double-well potential

We consider now the basic model of multi-dimensional double-well potentials, where the lattice potential has exactly \( 2^d \) wells, that is we assume that \( J_m = 0 \) and \( K_m = 1 \) for any \( m = 1, \ldots, d \). In this case the matrix \( T \) has a special form and its eigenvalues can be explicitly computed.

#### 4.1. One-dimensional model

In such a case the potential \( V(x) \) is a double-well potential with minima points \( x_0 \) and \( x_1 \) and the matrix \( T := T_1 \) simply reduces to

\[
T_1 = \begin{pmatrix}
\lambda_D & -\beta \\
-\beta & \lambda_D.
\end{pmatrix}
\]

The matrix \( T_1 \) has eigenvalues \( \mu_1 = \lambda_D - \beta \) and \( \mu_2 = \lambda_D + \beta \) with associated normalized eigenvectors \( v_1 = \left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right) \) and \( v_1 = \left( \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}} \right) \).

#### 4.2. Two-dimensional model

In such a case the potential \( V(x) \) has four wells with minima points

\[
x_{(0,0)}, \ x_{(0,1)}, \ x_{(1,0)}, \ x_{(1,1)}
\]
and the matrix $T := T_2$ reduces to
\[
T_2 = \begin{pmatrix}
\lambda_D & -\beta & -\beta & 0 \\
-\beta & \lambda_D & 0 & -\beta \\
-\beta & 0 & \lambda_D & -\beta \\
0 & -\beta & -\beta & \lambda_D
\end{pmatrix} = \begin{pmatrix}
T_1 & -\beta & 1_2 \\
-\beta & 1_2 & T_1
\end{pmatrix},
\]
where $1_2$ is the $2 \times 2$ identity matrix. The matrix $T_2$ has eigenvalues $\mu_r$ and associated normalized eigenvectors $v_r$, $r = 1, \ldots, 4$, given by
\[
\begin{align*}
\mu_1 &= \lambda_D - 2\beta & v_1 &= (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \\
\mu_2 &= \lambda_D & v_2 &= (0, -\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0) \\
\mu_3 &= \lambda_D & v_3 &= (0, 0, 0, 0) \\
\mu_4 &= \lambda_D + 2\beta & v_4 &= (\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})
\end{align*}
\]

4.3. Three-dimensional model

In the case of $d = 3$ then the potential $V(x)$ has 8 wells with minima points
\[
x_{(0,0,0)}, x_{(0,0,1)}, x_{(0,1,0)}, x_{(0,1,1)}, x_{(1,0,0)}, x_{(1,0,1)}, x_{(1,1,0)}, x_{(1,1,1)},
\]
and the matrix $T := T_3$ reduces to
\[
T_3 = \begin{pmatrix}
T_2 & -\beta 1_4 \\
-\beta 1_4 & T_2
\end{pmatrix},
\]
where $1_4$ is the $4 \times 4$ identity matrix. The matrix $T_3$ has eigenvalues $\mu_r$ and associated normalized eigenvectors $v_r$, $r = 1, \ldots, 8$, given by
\[
\begin{align*}
\mu_1 &= \lambda_D - 3\beta & v_1 &= (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \\
\mu_2 &= \lambda_D - \beta & v_2 &= (0, 0, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, 0) \\
\mu_3 &= \lambda_D - \beta & v_3 &= (0, 0, 0, 0, 0, 0, 0, 0) \\
\mu_4 &= \lambda_D - \beta & v_4 &= (-\frac{1}{2}, 0, 0, 0, \frac{1}{2}, 0, 0, \frac{1}{2}) \\
\mu_5 &= \lambda_D + \beta & v_5 &= (0, 0, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, 0) \\
\mu_6 &= \lambda_D + \beta & v_6 &= (0, 0, 0, 0, -\frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}) \\
\mu_7 &= \lambda_D + \beta & v_7 &= (0, 0, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, 0, 0) \\
\mu_8 &= \lambda_D + 3\beta & v_8 &= (-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})
\end{align*}
\]

4.4. Any dimension

In dimension $d + 1$, for $d \geq 1$, the potential $V(x)$ has $2^{d+1}$ wells with minima points
\[
x_{(0,j block, x_{(1,j block)},
\]
where $j \in \{0, 1\}^d$ are the indexes of the model in dimension $d$. Then the matrix $T_{d+1}$ has the following form:
\[
T_{d+1} = \begin{pmatrix}
T_d & -\beta 1_{2^d} \\
-\beta 1_{2^d} & T_d
\end{pmatrix}
\]
and it has $2^{d+1}$ eigenvalues (counting multiplicity). We state now a general result.
Lemma 4. Let $\Sigma^0 = \{\lambda_D\}$ and, by induction, let

$$\Sigma^{d+1} = \{\lambda \in \mathbb{R} : \exists \mu \in \Sigma^d \text{ such that } |\lambda - \mu| = \beta\};$$

that is

$$\Sigma_{2d} = \{\lambda_D, \lambda_D \pm 2\beta, \ldots, \lambda_D \pm 2(d-1)\beta, \lambda_D \pm 2d\beta\}$$

$$\Sigma_{2d+1} = \{\lambda_D \pm \beta, \lambda_D \pm 3\beta, \ldots, \lambda_D \pm (2d-1)\beta, \lambda_D \pm (2d+1)\beta\}.$$  

Then, the set of eigenvalues of $T_{d+1}$ coincides with $\Sigma^{d+1}$. Furthermore, if $\text{mult}(\lambda)$ denotes the multiplicity of the eigenvalue $\lambda$, then

$$\text{mult}(\lambda) = \sum_{\mu \in \Sigma^d : |\lambda - \mu| = \beta} \text{mult}(\mu).$$

Proof. From (24) we have that the eigenvalue equation for $T_{d+1}$ is given by

$$0 = \begin{vmatrix} T_d - \lambda 1_{2d'} & -\beta 1_{2d'} \\ -\beta 1_{2d'} & T_d - \lambda 1_{2d'} \end{vmatrix}.$$  

(25)

If we assume for a moment that $\lambda$ is not an eigenvalue of $T_d$ then from Schur’s formula it follows that equation (25) becomes

$$0 = |T_d - (\lambda + \beta)1_{2d'}| \cdot |T_d - (\lambda - \beta)1_{2d'}|$$

from which follows that $\lambda \in \Sigma^{d+1}$ if, and only if, $\lambda \pm \beta \in \Sigma^d$. Since $\Sigma^0 = \{\lambda_D\}$ has cardinality 1, then $\Sigma^d$ has cardinality (counting multiplicity) $2^d$ and, by induction, we have that if $\lambda \in \Sigma^d$, then $\lambda \notin \Sigma^{d+1}$. □

Remark 1. It is not hard to see that the ground state associated with the eigenvalues $\lambda = \lambda_D - d\beta$ of $T_d$ has normalized eigenvector $v = (2^{-d/2}, \ldots, 2^{-d/2})$.

5. Analysis of the bifurcation of the ground state

Now, we are going to discuss in dimensions 1, 2 and 3 how the ground state stationary solutions of the linear problem bifurcate when we introduce the nonlinear term. First of all we would underline that in equation (19) we can switch from the case of attractive interaction, where $\epsilon < 0$, to the case of repulsive interaction, where $\epsilon > 0$, by means of the transformation

$$\epsilon \to -\epsilon, \omega \to -\omega, d_j \to (-1)^{j-1} \sum_{i=1}^{d} b_j,$$

which transforms a solution to the stationary equation (19) for a given sign of $\epsilon$ to another solution to the same equation with the opposite sign of $\epsilon$. Thus, for the sake of definiteness, we restrict ourselves to the case of attractive interaction $\eta < 0$ and the following results will also hold true for the case of repulsive interaction $\eta > 0$.

5.1. One-dimensional model

The model in dimension 1 has been largely discussed in previous papers (see, e.g., [7]), thus let us omit the details. In dimension $d = 1$ then (21) takes the form

$$\begin{cases}
\sqrt{q_1 q_2} \sin(\theta_2 - \theta_1) = 0 \\
-\sqrt{q_1 / q_2} \cos(\theta_2 - \theta_1) + \eta q_2^\eta = \Omega \\
-\sqrt{q_1 / q_2} \cos(\theta_1 - \theta_2) + \eta q_1^\eta = \Omega \\
q_1 + q_2 = 1
\end{cases}$$

(26)
and for $\eta = 0$ the above equation has ground state corresponding to

$$q_1 = q_2 = \frac{1}{2}, \quad \theta_1 = \theta_2 \quad \text{and} \quad \Omega = -1 + \frac{1}{2\sigma} \eta. \quad \tag{27}$$

Now, we observe that all the solutions of (26) are such that $q_1 \neq 0$ and $q_2 \neq 0$. Indeed, if there exists a solution to (26) such that, for instance, $q_1 = 0$ and $q_2 = 1$ (or $q_1 = 1$ and $q_2 = 0$) at some $\eta$ then $d_1 = 0$ and $d_2 \neq 0$ in contradiction with (19) for $d = 1$. Then stationary solutions are such that $\theta_1 = \theta_2$ or $\theta_1 - \theta_2 = \pi$ and the equation that gives the stationary solutions that bifurcate from the linear ground state simply reduces to

$$\begin{cases}
-\sqrt{q_2/q_1 + \eta q_1^\sigma} = \Omega \\
-\sqrt{q_1/q_2 + \eta q_2^\sigma} = \Omega. \\
q_1 + q_2 = 1
\end{cases} \quad \tag{28}$$

First of all we remark that the problem is invariant under the reflection

$$x_0 \leftrightarrow x_1, \text{ i.e. } q_1 \leftrightarrow q_2.$$

Hence, asymmetrical solutions, if there exists, are doubly degenerate.

If we set $z = q_1 - q_2 \in (-1, +1)$, that is

$$q_1 = \frac{1}{2} + \frac{1}{2} z \quad \text{and} \quad q_2 = \frac{1}{2} - \frac{1}{2} z$$

and if we set

$$\chi = \eta/2$$

then equation (28) reduces to the form

$$\sqrt{\frac{1 - z}{1 + z}} - \chi (1 + z)^\sigma = \sqrt{\frac{1 + z}{1 - z}} + \chi (1 - z)^\sigma = 0 \quad \tag{29}$$

and its solutions are given by

— $z = 0$, which coincides with the symmetric solution (27);
— for $\sigma = 1$, $z = \pm \frac{1}{2} \sqrt{\chi^2 - 1}$, provided that $\chi < -1$.

Therefore, for $\sigma = 1$ we have that the symmetric ground state solution bifurcates at $\eta = -2$ and the new asymmetrical solutions are such that (see figure 1)

$$z = \pm \frac{1}{\eta} \sqrt{\eta^2 - 4} \quad \text{and} \quad \Omega = \eta, \quad \text{for} \quad \eta \leq -2. \quad \tag{30}$$

In conclusion, for $\eta \geq -2$ the stationary solutions of equation (21) for the cubic (corresponding to $\sigma = 1$) one-dimensional double-well model are only given by the symmetric stationary solution (27). At $\eta = -2$ this solution bifurcates and the new solutions are asymmetrical. The transition from the symmetric stationary solution to the asymmetrical stationary solution is smooth. In particular, in table 1 we collect the values for $q_1$ and $q_2$ corresponding to the asymmetric stationary solution; it turns out that the asymmetrical stationary solutions become gradually localized on only one of the two wells when $|\eta| > 2$ increases (see also figure 2).
Figure 1. Bifurcation picture of the energy $\Omega$ as a function of $\eta$ for the cubic one-dimensional double-well model.

Table 1. Values of the coefficients $q_1$ and $q_2$ of the asymmetrical stationary solutions to the cubic one-dimensional double-well model for some values of the parameter $\eta$.

| $\eta$ | $q_1$ | $q_2$ | $\Omega$ |
|-------|-------|-------|---------|
| −2.01 | 0.45  | 0.55  | −2.01   |
| −2.1  | 0.35  | 0.65  | −2.1    |
| −2.5  | 0.2   | 0.8   | −2.5    |

5.2. Two-dimensional model

In such a case (21) takes the form

\[
\begin{align*}
\sqrt{q_1 q_2} \sin(\theta_2 - \theta_1) + \sqrt{q_3 q_1} \sin(\theta_3 - \theta_1) &= 0 \\
\sqrt{q_2 q_3} \sin(\theta_1 - \theta_2) + \sqrt{q_4 q_3} \sin(\theta_4 - \theta_2) &= 0 \\
\sqrt{q_4 q_1} \sin(\theta_1 - \theta_4) + \sqrt{q_3 q_4} \sin(\theta_3 - \theta_4) &= 0 \\
\sqrt{q_2 q_4} \sin(\theta_2 - \theta_4) + \sqrt{q_4 q_3} \sin(\theta_3 - \theta_4) &= 0 \\
- \left( \sqrt{q_2/q_1} \cos(\theta_2 - \theta_1) + \sqrt{q_3/q_1} \cos(\theta_3 - \theta_1) \right) + \eta q_1^\sigma &= \Omega \\
- \left( \sqrt{q_4/q_2} \cos(\theta_1 - \theta_2) + \sqrt{q_3/q_4} \cos(\theta_4 - \theta_2) \right) + \eta q_2^\sigma &= \Omega \\
- \left( \sqrt{q_1/q_3} \cos(\theta_1 - \theta_3) + \sqrt{q_4/q_3} \cos(\theta_4 - \theta_3) \right) + \eta q_3^\sigma &= \Omega \\
- \left( \sqrt{q_2/q_4} \cos(\theta_2 - \theta_4) + \sqrt{q_3/q_4} \cos(\theta_3 - \theta_4) \right) + \eta q_4^\sigma &= \Omega, \\
q_1 + q_2 + q_3 + q_4 &= 1
\end{align*}
\]
The asymmetrical solution is, for $\eta$ close to the bifurcation point at $\eta = -2$, delocalized between both two wells; when $|\eta| > 2$ increases then the wavefunction is going to be fully localized on just one of the two wells.

First of all we remark that for dimension $d > 1$ equations (31) admit solutions with $q_j = 0$ for some $j = 0$; in such a case it turns out that the solutions of equations (21), or (31), with some $d_j = 0$ are necessarily of the form $d_2 = d_3 = 0$ and $d_1 = -d_4$, or $d_1 = d_4$ and $d_2 = -d_1$. Then, these solutions are the continuation of the solutions $v_2$ and $v_3$ given in (22) at $\eta = 0$. On the other side, we remark that at $\eta = 0$ then the above equation has ground state corresponding to the solution $v_1$ given in (22) where $q_j = \frac{1}{4}$ and $\theta_j = \theta_l$ for any value of the indexes $j, \ell = 1, 2, 3, 4$. By continuity, for $\eta \neq 0$ then the continuation of the solution $v_1$ will have all $q_j > 0$ and $\theta_j = \theta_l$, for any $j, \ell = 1, 2, 3, 4$. In fact, if we assume that, for instance, $\theta_2 > \theta_1$, then the first equation of (31) implies that $\theta_3 - \theta_1 < 0$ and the second one implies that $\theta_4 - \theta_2 < 0$; hence the third equation implies that $\theta_4 - \theta_3 > 0$, and, finally, we have a contradiction because of the fourth equation.

In conclusion, in order to find the bifurcations from the ground state solution we can restrict ourselves to study the following system of equations:

$$
\begin{align*}
    f_1 &= -\left(\sqrt{q_2/q_1} + \sqrt{q_3/q_1}\right) + \eta q_1^0 - \Omega \\
    f_2 &= -\left(\sqrt{q_1/q_2} + \sqrt{q_4/q_2}\right) + \eta q_2^0 - \Omega \\
    f_3 &= -\left(\sqrt{q_1/q_3} + \sqrt{q_4/q_3}\right) + \eta q_3^0 - \Omega \\
    f_4 &= -\left(\sqrt{q_2/q_4} + \sqrt{q_3/q_4}\right) + \eta q_4^0 - \Omega \\
    f_5 &= q_1 + q_2 + q_3 + q_4 - 1
\end{align*}
$$

which always has a symmetric solution

$$
q_1 = q_2 = q_3 = q_4 = \frac{1}{4} \quad \text{with} \quad \Omega = 4^{\frac{-\sigma}{4}} - 2.
$$

Let us remark that the problem is invariant under the 8 transformation of the Dihedral group of the square. Hence, asymmetrical solutions, if there exist, are degenerate.

Then we look for the symmetric and partially symmetric solutions coming from the solution (33) by bifurcation.
5.2.1. Symmetric solutions—mirror symmetry. We look for the solutions such that
\[ q_1 = q_2 \quad \text{and} \quad q_3 = q_4 \]
and similarly such that \( q_1 = q_3 \) and \( q_2 = q_4 \). Under these conditions then equations (32) become
\[
\begin{cases}
-(1 + \sqrt{q_3/q_1}) + \eta q_1^\sigma = \Omega \\
-(1 + \sqrt{q_1/q_3}) + \eta q_3^\sigma = \Omega \\
q_1 + q_3 = \frac{1}{2}
\end{cases}
\] (34)
If we set \( z = 2(q_1 - q_3) \in (-2, +2) \), that is
\[ q_1 = \frac{1}{4}(1 + z) \quad \text{and} \quad q_3 = \frac{1}{4}(1 - z) \]
then equation (34) takes the form (29), provided we set \( \chi = \eta^2 \cdot \frac{4}{c_1^2} \), which has solutions
--- \( z = 0 \), which corresponds to the case (33);
--- for \( \sigma = 1 \), \( z = \pm \frac{1}{\sqrt{2}}\eta^2 - 16 \) for \( \eta \leq -4 \) which gives \( \Omega = -1 + \frac{1}{2}\eta \).
Thus, at \( \eta = -4 \) the solution (33) bifurcates.

5.2.2. Symmetric solutions—point symmetry. We look for solutions such that
\[ q_1 = q_4 \quad \text{and} \quad q_2 = q_3 \] (35)
Then equations (32) become
\[
\begin{cases}
-2\sqrt{q_2/q_1} + \eta q_1^\sigma = \Omega \\
-2\sqrt{q_1/q_2} + \eta q_2^\sigma = \Omega \\
q_1 + q_2 = \frac{1}{2}
\end{cases}
\] (36)
If, similarly to the previous case, we set \( z = 2(q_1 - q_2) \in (-2, +2) \) then such an equation takes the form (29) provided we set \( \chi = \frac{2\eta}{z^2} \), which has solutions
--- \( z = 0 \), which corresponds to the case (33);
--- for \( \sigma = 1 \), \( z = \pm \frac{1}{\sqrt{2}}\eta^2 - 64 \) for \( \eta \leq -8 \) which gives \( \Omega = +1 \cdot \frac{1}{2}\eta \).
Thus, at \( \eta = -8 \) the solution (33) bifurcates again.

5.2.3. Partially symmetric solutions. We consider now solutions such that
\[ q_1 = q_4 \quad \text{and} \quad q_2 \neq q_3 \] (37)
or similarly such that \( q_2 = q_3 \) and \( q_1 \neq q_4 \). In such a case the numerical analysis of equation (32) shows that at \( \eta^2_{\text{crit}} = -3.5836 \) a saddle point occurs and the solution has two branches. One branch denoted as branch (a) is connected with the branch of solutions (33) at \( \eta = -4 \), while on the other branch, denoted as branch (b), \( \Omega \) behaves like \( \eta \) (see figure 3). The relevant fact is that on the branch (b) the wavefunction is going to be well localized on only one well. For instance, at \( \eta = \eta^2_{\text{crit}} \) the value of \( q_2 \) is equal to 0.571, at \( \eta = -3.95 \) the value of \( q_2 \) of the solution on the branch (b) is equal to 0.781, which means that the wavefunction is practically fully localized on the well around \( x_{0,1} \) (see table 2 for different values of \( \eta \), see also figures 4(a) and 4(b)).

Remark 2. In the case of partially symmetric solutions to the cubic nonlinearity it is possible to obtain the exact value of the bifurcation point \( \eta^2_{\text{crit}} \). In fact, a straightforward calculation lead to the following value:
\[
\eta^2_{\text{crit}} = \frac{1}{8} c_1 c_2 \left( 187 + 2464 c_1^2 - 30464 c_1^4 - 1569 c_2^2 - 12000 c_1^2 c_2^2 + 136448 c_1^4 c_2^2 \right)
\]
Figure 3. In (a) we plot the graph of $\Omega$ as a function of $\eta$, and we observe three bifurcation points and one saddle point. In (b) we zoom the picture around the saddle point (denoted by the circle point) and we name the two branches (a) and (b). On the branch (b) the wavefunction is going to be fully localized on just one well as $|\eta|$ increases.

where

$$c_2 = \frac{1}{2} \sqrt{2 - 4c_1^2 + \sqrt{2 - 6c_1^2}}$$

and

$$c_1 = \frac{1}{8} \sqrt{\frac{(2c_1^2 - 8c_3 + 24)}{c_3}}$$

$$= \frac{1}{4} \sqrt{2 + 2\sqrt{3} \sin \left( -\frac{1}{3} \arctan \left( \sqrt{2} \right) + \frac{1}{6} \pi \right)}$$

since

$$c_3 = \left[ -3 + 3i\sqrt{2} \right]^{1/3} (1 + i\sqrt{3}).$$

5.2.4. Classification of the bifurcations. Bifurcation points are the solutions $(q_1, q_2, q_3, q_4, \Omega, \eta)$ of the system of equations (32) under the condition

$$\det \left( \frac{\partial f_i}{\partial q_h} \right)_{i,b=1,2,3,4,5} = 0,$$

where we denote $q_5 = \Omega$. Bifurcations of the symmetric stationary solution (33) are the solutions of equation (38) with $q_j = \frac{1}{2}, j = 1, 2, 3, 4$; this equation has 2 solutions $\eta = -2$, with double multiplicity, and $\eta = -4$ with multiplicity one. Furthermore, we can numerically compute the other solutions of the system $f_j = 0, j = 1, 2, 3, 4, 5$; in particular, we can observe the occurrence of a saddle point and a bifurcation. That is
Table 2. Here we report the numerical solutions of equations $f_j = 0, j = 1, 2, 3, 4, 5$, associated with the two branches (a) and (b) raising from the saddle point at $\eta = \eta_{\text{crit}}^2 = -3.5836$. We can see that the solutions associated with the branch (b) are going to be fully localized on just one well (in this case it is the well with centre at $x_{(0,1)}$).

| $\eta$   | $q_1$ | $q_2$ | $q_3$ | $q_4$ | $\Omega$ |
|----------|-------|-------|-------|-------|----------|
| $-3.5836$ | 0.168 | 0.581 | 0.082 | 0.168 | $-3.159$ |
| $-3.6$    | 0.186 | 0.527 | 0.1   | 0.186 | $-3.0867$|
| $-3.7$    | 0.214 | 0.436 | 0.136 | 0.214 | $-3.152$ |
| $-3.8$    | 0.229 | 0.379 | 0.162 | 0.229 | $-2.998$ |
| $-3.9$    | 0.241 | 0.329 | 0.189 | 0.241 | $-2.995$ |
| $-3.95$   | 0.246 | 0.302 | 0.207 | 0.246 | $-2.997$ |
| $-4.05$   |       |       |       |       | $0.085$  |
| $-8.1$    |       |       |       |       | $0.016$  |

(1) At $\eta = \eta_{\text{crit}}^2 = -3.5836$ a saddle point occurs and the new stationary solutions have asymmetrical wavefunctions such that $q_1 = q_4$ and $q_2 \neq q_3$ and where the wavefunction corresponding to the branch (b) is localized on one well.

(2) At $\eta = -4$ the solution (33) bifurcates. We have three branches, one is the branch of the solution (33), another one is the branch (a) associated with the saddle point at $\eta = \eta_{\text{crit}}^2$, and the last branch is the branch of the solutions observed in section 5.2.1.

(3) At $\eta = -8$ the solution (33) bifurcates again. We have two branches, one is the branch of the solution (33) and the other branch is the branch of the solutions observed in section 5.2.2.

(4) At $\eta = -8.4853$ the solution (35) bifurcates. We have two branches, one is the branch of the solution (35) and the other branch is a branch of solutions of the kind (37).

In conclusion, for $\eta > \eta_{\text{crit}}^2$ there exists only one solution and it is equally distributed on the four wells; once $\eta$ reaches the value $\eta_{\text{crit}}^2$, then two (families of) new solutions suddenly appear, and the solutions associated with the branch (a) of figure 3 are fully localized on a single well. This phenomenon is the opposite of the one observed in the one-dimensional model where the localization effect gradually occurs, in this case the localization effect suddenly occurs.

5.3. Three-dimensional model

By means of arguments similar to those discussed in section 5.2 for two-dimensional models it turns out that bifurcations of the continuation of the symmetric solution $v_1$ in (23) of (21) are such that $q_j > 0$ and $\theta_j = \theta_{\ell}$ for any $j, \ell = 1, 2, \ldots, 8$. That is, in order to find the bifurcation from the ground state solution we can restrict ourselves to study the following

2658
Figure 4. Pictures of the absolute value of the asymmetrical stationary wavefunction associated with the branch (b) for $\eta = \eta_{\text{crit}}^2 (a)$ and $\eta = -3.95$; in (b) we plot the absolute value of the function corresponding to a solution in the branch (a); in (c) we plot the absolute value of the function corresponding to a solution in the branch (b). At $\eta = \eta_{\text{crit}}^2$, the stationary solution is quite localized on just one well and the wavefunction corresponding to the branch (b) is going to be localized on the well around $x_{(0,1)}$ when $|\eta|$ increases; on the other side the wavefunction corresponding to the branch (a) is going to be delocalized between the four wells as $\eta$ approaches $\eta = -4$.

System of equations:

$$\begin{align*}
- \frac{1}{\sqrt{q_1}} \left( \sqrt{q_2} + \sqrt{q_3} + \sqrt{q_5} \right) + \eta q_1^\xi &= \Omega \\
- \frac{1}{\sqrt{q_2}} \left( \sqrt{q_1} + \sqrt{q_4} + \sqrt{q_6} \right) + \eta q_2^\xi &= \Omega \\
- \frac{1}{\sqrt{q_3}} \left( \sqrt{q_1} + \sqrt{q_4} + \sqrt{q_7} \right) + \eta q_3^\xi &= \Omega \\
- \frac{1}{\sqrt{q_4}} \left( \sqrt{q_2} + \sqrt{q_3} + \sqrt{q_5} \right) + \eta q_4^\xi &= \Omega \\
- \frac{1}{\sqrt{q_5}} \left( \sqrt{q_1} + \sqrt{q_6} + \sqrt{q_7} \right) + \eta q_5^\xi &= \Omega \\
- \frac{1}{\sqrt{q_6}} \left( \sqrt{q_2} + \sqrt{q_3} + \sqrt{q_8} \right) + \eta q_6^\xi &= \Omega \\
- \frac{1}{\sqrt{q_7}} \left( \sqrt{q_4} + \sqrt{q_5} + \sqrt{q_8} \right) + \eta q_7^\xi &= \Omega \\
- \frac{1}{\sqrt{q_8}} \left( \sqrt{q_4} + \sqrt{q_5} + \sqrt{q_6} \right) + \eta q_8^\xi &= \Omega
\end{align*}$$

(39)
Table 3. Here we report the numerical solutions of equations (39) under conditions (41) associated with the two branches (a) and (b) raising from the saddle point at $\eta = \eta_{\text{crit},1} = -5.0116$. We can see that the solutions associated with the branch (b) are going to be fully localized on just one well.

| $\eta$  | $q_1$  | $q_2$  | $q_4$  | $q_8$  | $\Omega$  | $q_1$  | $q_2$  | $q_4$  | $q_8$  | $\Omega$  |
|---------|--------|--------|--------|--------|-----------|--------|--------|--------|--------|-----------|
| $-5.0116$ | 0.659  | 0.083  | 0.027  | 0.0129  | $-4.3659$ | 0.739  | 0.067  | 0.017  | 0.007  | $-4.674$  |
| $-5.1$   | 0.569  | 0.098  | 0.038  | 0.021   | $-4.151$ | 0.873  | 0.037  | 0.005  | 0.001  | $-5.853$  |
| $-6$     | 0.355  | 0.128  | 0.071  | 0.048   | $-3.928$ | 0.919  | 0.024  | 0.002  | 0.004  | $-6.924$  |
| $-7$     | 0.240  | 0.136  | 0.094  | 0.071   | $-3.939$ | 0.941  | 0.018  | 0.013  | 0.0002 | $-7.852$  |
| $-8.1$   | 0.945  | 0.017  | 0.001  | 0.0002  | $-8.056$ | 0.957  | 0.014  | 0.001  | 0.0001 | $-8.970$  |
| $-10$    |        |        |        |         |           |        |        |         |         |            |

which always has a symmetric solution

$$q_j = \frac{1}{8}, \quad j = 1, \ldots, 8 \quad \text{with} \quad \Omega = \eta 8^{-\sigma} - 3. \quad (40)$$

As in the previous cases in dimensions 1 and 2, asymmetrical solutions, if these exist, are degenerate because of the invariance of the model with respect to several transformations; in particular our model is invariant with respect to the 48 transformations of the achiral octahedral symmetric group isomorphic to $S_4 \times C_2$. Among the symmetric and partially symmetric solutions coming from the solution (40) by bifurcation the first one we can observe are the two families of partially symmetric solutions such that

$$q_2 = q_3 = q_5 \quad \text{and} \quad q_4 = q_6 = q_7 \quad (41)$$

and such that

$$q_1 = q_2 = q_7 = q_8, \quad q_5 = q_6 \quad \text{and} \quad q_3 = q_4. \quad (42)$$

In particular (see figure 5):

(1) At $\eta = \eta_{\text{crit},1} = -5.0116$ a saddle point occurs and the new stationary solutions have asymmetrical wavefunctions satisfying (41), and where the wavefunction corresponding to the branch (b) of figure 5 is localized on just one single well (see table 3).

(2) At $\eta = \eta_{\text{crit},2} = -7.1672$ a saddle point occurs and the new stationary solutions have asymmetrical wavefunctions satisfying (42), and where the wavefunction corresponding to the branch (d) of figure 5 is localized on a couple of adjacent wells (see table 4).

(3) At $\eta = -8$ the solution (40) bifurcates in four branches; two of them are the branches (a) and (c) connected with the two saddle points previously discussed.

(4) Solution (40) bifurcates at the value $\eta = -16$ and $\eta = -24$, too. The bifurcation point at $\eta = -16$ corresponds to four different branches, the bifurcation point at $\eta = -24$ corresponds to two different branches.

5.4. Conclusion

As we can see in the previous pictures and tables, there exists a fundamental difference between the one-dimensional model and the two- and three-dimensional models: the appearance of saddle points associated with branch of stationary solutions localized on a single well. This fact is the basic argument for the explanation of the phase transition from the superfluidity...
Figure 5. We plot the graph of $\Omega$ as a function of $\eta$, and we observe two bifurcation points and two saddle points. On the branches (b) the wavefunction is going to be fully localized on just one well as $|\eta|$ increases.

Table 4. Here we report the numerical solutions of equations (39) under conditions (42) associated with the two branches (c) and (d) raising from the saddle point at $\eta = \eta_{\text{crit}}^{1,2} = -7.1672$. We can see that the solutions associated with the branch (d) are going to be fully localized on a couple of wells.

| $\eta$   | $q_1$  | $q_3$  | $q_5$  | $\Omega$ |
|---------|--------|--------|--------|----------|
| -7.1672 | 0.093  | 0.050  | 0.264  | -4.087   |
| -7.2    | 0.111  | 0.074  | 0.203  | -4.003   |
| -7.9    | 0.123  | 0.103  | 0.150  | -3.997   |
| -8.1    | 0.044  | 0.012  | 0.400  | -4.904   |
| -9      | 0.032  | 0.007  | 0.429  | -5.409   |

phase to the insulator phase. Indeed, in the presence of stationary solutions associated with the ground state and localized in just one well we expect that the typical beating motion in symmetric potential does not work and thus the motion of the particle of the condensate between adjacent wells is forbidden. Since in dimension 1 the asymmetrical state becomes gradually localized on just one well when the nonlinear strength parameter increases, then
the phase transition is quite slow. In dimensions 2 and 3 we have the opposite situation, the asymmetrical ground states localized on just one well suddenly appear with the saddle points and then the phase transition is expected to be very sharp.

Acknowledgments

The author is indebted to Reika Fukuizumi for useful discussion on nonlinear Schrödinger equations. This work is partially supported by GNFM-INdAM.

References

[1] Adami R and Noja D 2013 Stability and symmetry breaking bifurcation for the ground states of a NLS equation with a δ′ interaction Commun. Math. Phys. 318 247–89
[2] Bambusi D and Sacchetti A 2007 Exponential times in the one-dimensional Gross–Pitaevskii equation with multiple well potential Commun. Math. Phys. 275 1–36
[3] Bloch I 2005 Ultracold quantum gases in optical lattices Nature Phys. 1 23–30
[4] Cazenave T and Weissler F B 1988 The Cauchy problem for the nonlinear Schrödinger equation in $H^1$ Manuscr. Math. 61 477–94
[5] Cazenave T 2003 Semilinear Schrödinger Equations (Providence, RI: AMS)
[6] Fisher M P A, Weichman P B, Grinstein G and Fisher D S 1989 Boson localization, the superfluid–insulator transition Phys. Rev. B 40 546–70
[7] Fukuizumi R and Sacchetti A 2011 Bifurcation and stability for Nonlinear Schrödinger equations with double well potential in the semiclassical limit J. Stat. Phys. 145 1546–94
[8] Greiner M, Mandel O, Esslinger T, Hansch T H and Bloch I 2002 Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms Nature 415 39–44
[9] Helffer B 1988 Semi-Classical Analysis for the Schrödinger Operator and Applications (Lecture Notes in Mathematics vol 1336) (Berlin: Springer)
[10] Kevrekidis G P and Pelinovsky D 2011 Symmetry breaking bifurcation in the nonlinear Schrödinger equations with symmetric potentials Commun. Math. Phys. 308 795–844
[11] Kirr E W, Kevrekidis G P, Shlizerman E and Weinstein M I 2008 Symmetry-breaking bifurcation in nonlinear Schrödinger/Gross–Pitaevskii equations SIAM J. Math. Anal. 40 566–604
[12] Kohler T 2002 Three-body problem in a dilute Bose–Einstein condensate Phys. Rev. Lett. 89 210404
[13] Pitaevskii L and Stringari S 2003 Bose–Einstein Condensation (Oxford: Clarendon)
[14] Sacchetti A 2005 Nonlinear double well Schrödinger equations in the semiclassical limit J. Stat. Phys. 119 1347–82
[15] Sacchetti A 2009 Universal critical power for nonlinear Schrödinger equations with a symmetric double well potential Phys. Rev. Lett. 103 194101
[16] Tuoc V P and Pelinovsky D E 2012 Normal form for the symmetry-breaking bifurcation in the nonlinear Schrödinger equation J. Diff. Equa 253 2796–824
[17] Wang C, Theocharis G, Kevrekidis P G, Whitaker N, Law K J H, Frantzeskakis D J and Malomed B A 2009 Two-dimensional paradigm for symmetry breaking: The nonlinear Schrodinger equation with a four-well potential Phys. Rev. E 80 046611