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STATIONARY SOLUTIONS FOR MULTI-DIMENSIONAL GROSS-PITAEVSKII EQUATION WITH DOUBLE-WELL POTENTIAL

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ABSTRACT. In this paper we consider a non-linear 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 behavior depending on the dimension. In particular, in dimension 1 the symmetric stationary solution shows a standard pitchfork bifurcation effect, while in dimension 2 and 3 new asymmetrical solutions associated to 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.

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1. INTRODUCTION

Atomic Bose-Einstein condensates (BECs) are described by means of nonlinear Schrödinger equations where the nonlinear term of the form $|\psi|^{2\sigma}\psi$, $\sigma = 1, 2, \dots$, represents the $(\sigma + 1)$ -body contact potential [10], where ψ is the condensate's wavefunction. In fact, BECs strongly depend by 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 [11].

The analysis of the time-dynamic of BECs is, in general, an open problem and few rigorous results has 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 has been seen a transition from the *superfluidity phase* to the *Mott-insulator phase* when the effective nonlinearity parameter becomes larger than a critical value [2, 5, 7]. 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 [6, 13] for the result obtained in the semiclassical limit, see also [9] 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.

In this paper we explore in detail the different pictures may occur in dimension 1, 2 and 3 for the stationary solutions of the Gross-Pitaevskii equation associated to 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 kind 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 to 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 in dimension 3, too.

The different behavior between models in dimension 1 and in dimensions higher than 1 has an important physical consequences when we consider BECs in lattices. Indeed 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 behavior is expected to be connected to the appearance, in dimension 2 and 3, of stationary solutions localized on a single lattice site as we have seen for double-well models.

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 to the linear ground state.

2. DOUBLE-WELL MODEL

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

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

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

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

is the linear Hamiltonian with a *lattice potential* $V(x)$. In the case of cubic non-linearity 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 $\hbar > 0$ is such that $\hbar \ll 1$.

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 $x = 0$:*

$$v(x) > v_{\min} = f(0), \quad \forall x \in \mathbb{R}^d, \quad x \neq 0. \quad (3)$$

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

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

We then define a lattice potential as

$$V(x) = \sum_{j \in J} v(x - x_j), \quad x_j = jb = (j_1 b, \dots, j_d b), \quad (4)$$

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

$$N := \prod_{m=1}^d [K_m - J_m + 1] \quad (5)$$

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

It is a well known fact ([3] and Thm. 6.2.1 [4]) 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

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

follows.

3. REDUCTION TO THE N -MODE APPROXIMATION

Now, making use of the semiclassical analysis [8] 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 the papers [1, 12] and adapted here to the case of a lattice potential (4). Since the reduction method is similar to the one already exploited in [1, 12] then we don't 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 $E \geq v_{min}$ be fixed, then the Agmon (pseudo-)distance, associated to 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 γ connecting the two points x and y and where $[V - E]_+ = \frac{|V-E|+V-E}{2}$. Let us consider the Agmon distance associated to the ground state energy, since the difference between the ground state energy and the minimum of the potential is of order $O(\hbar)$ then in the semiclassical limit we can choose $E = v_{min}$; in the following, for the sake of simplicity, let us denote

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

We then define the following two quantities

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

and

$$S_1 = \inf_{|j-\ell|>1, j, \ell \in J} d_A(x_j, x_\ell), \quad \text{where } |j - \ell| = \sum_{m=1}^d |j_m - \ell_m|;$$

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*

$$S_0 = d_A(x_j, x_\ell) = 2 \int_0^{b/2} \sqrt{f(r) - f(0)} dr \quad (6)$$

is independent of j and ℓ , and

$$S_0 < S_1. \quad (7)$$

Proof. If $|j - \ell| = 1$ then all the components of x_j and x_ℓ are equal, but one: e.g. $j_m = \ell_m$ for $m = 2, \dots, d$ and $j_1 - \ell_1 = 1$. Then, by construction it turns out that

$$\begin{aligned} d_A(x_j, x_\ell) &= \int_0^b \sqrt{V[x_j + r(1, 0, \dots, 0)] - v_{min}} dr \\ &= 2 \int_0^{b/2} \sqrt{v[r(1, 0, \dots, 0)] - v_{min}} dr \\ &= 2 \int_0^{b/2} \sqrt{f(r) - v_{min}} dr \end{aligned}$$

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

$$B_{x_j}(S_0/2) = \left\{ x \in \mathbb{R}^d : d_A(x_j, x) \leq \frac{1}{2} S_0 \right\}; \quad (8)$$

then, by construction, it follows that

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

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

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

and thus (7) follows. \square

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

$$\lceil j \rceil := \max_{m=1, \dots, d} |j_m|.$$

Then

$$d_A(x_j, x_\ell) \geq \lceil j - \ell \rceil S_0. \quad (9)$$

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

$$\sqrt{V(x_1, x_2, \dots, x_d) - v_{min}} \geq \sqrt{V(x_1, 0, \dots, 0) - v_{min}},$$

hence, for any regular path γ connecting the two points x_j and x_ℓ , it follows that

$$\begin{aligned} d_A(x_j, x_\ell) &\geq \int_\gamma \sqrt{V(x_1, x_2, \dots, x_d) - v_{min}} dx \\ &\geq \int_\gamma \sqrt{V(x_1, 0, \dots, 0) - v_{min}} dx \\ &\geq \int_0^s \sqrt{V(x_1, 0, \dots, 0) - v_{min}} dx_1 \\ &= s \cdot S_0. \end{aligned}$$

\square

3.2. N -mode approximation. Now, let H_D be the Dirichlet realization of the Schrödinger operator formally defined on $L^2(B_S(0), dx)$ by

$$H_D = -\hbar^2 \Delta + v \quad (10)$$

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

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

such that

$$\text{dist}[\lambda_D, \sigma(H_D) \setminus \{\lambda_D\}] \geq 2C\hbar$$

for some $C > 0$. The normalized eigenvector $\psi_D(x)$ associated to λ_D is localized in a neighborhood of $x = 0$ and it exponentially decreases as $\mathcal{O}(\hbar^{-m} e^{-d_A(x)/\hbar})$ 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 neighborhood of $x = 0$ then $\psi_D(x) \sim \mu^{d/8} (\pi\hbar)^{-d/4} e^{-\sqrt{\mu}|x|^2/2\hbar}$.

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

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

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

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

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

$$\phi_j(x) - \varphi_j(x) = \mathcal{O}(e^{-\rho/\hbar}) \quad \text{where} \quad \varphi_j(x) = \psi_D(x - x_j); \quad (11)$$

hence, the vector $\phi_j(x)$ is localized in a neighborhood of the minima point x_j . More precisely, in the semiclassical limit it follows that (for the proof we refer to Theorem 4.3.4 and Theorem 4.4.6 by [8]).

Lemma 3. *Up to an error of order $\mathcal{O}(\hbar^\infty e^{-S_0/\hbar})$ 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*

$$T_{j,\ell} = \begin{cases} \lambda_D & \text{if } |j - \ell| = 0 \\ -\beta & \text{if } |j - \ell| = 1 \\ 0 & \text{if } |j - \ell| > 1 \end{cases}, \quad (12)$$

where β is a quantity independent on the indexes and such that

$$\frac{1}{C}\hbar^{1/2} \leq \beta e^{S_0/\hbar} \leq C\hbar^{1-d/2}. \quad (13)$$

Let ψ be the normalized solution of the NLS equation (1). Then ψ may be written in the following form. Let Π 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 [1, 12], that $\psi_c(x, t)$ is exponentially small for times of order β^{-1} , that is

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

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

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

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

$$i\hbar \dot{d}_j = \sum_{\ell \in J} T_{j,\ell} d_\ell + \epsilon c |d_j|^{2\sigma} d_j, \quad j \in J, \quad (14)$$

with the normalization condition

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

where

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

is a real valued constant independent of j .

3.3. Hamiltonian form of the N -mode approximation. If we set

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

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

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

with Hamiltonian function

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

The normalization condition (15) takes the form

$$\sum_j q_j = 1 \quad (18)$$

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 $\psi(\mathbf{x}, t) = e^{i\omega t} \psi(\mathbf{x})$. Concerning the study of the stationary solutions has been proved by [6] that for 1-dimensional double-well models then the 2-mode approximation gives the stationary solutions for 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 $\mathcal{O}(e^{-\rho/\hbar})$, 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 of the system of equations

$$-\omega \hbar d_j = \sum_{\ell \in J} T_{j,\ell} d_\ell + \epsilon c |d_j|^{2\sigma} d_j, \quad j \in J. \quad (19)$$

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

$$\begin{cases} 0 &= \frac{\partial \mathcal{H}}{\partial \theta_j} \\ -\hbar \omega &= -\frac{\partial \mathcal{H}}{\partial q_j} \end{cases}. \quad (20)$$

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

$$\begin{cases} 0 &= \sum_{\ell \in J: |j-\ell|=1} \sqrt{q_j q_\ell} \sin(\theta_\ell - \theta_j) \\ -\Omega &= \sum_{\ell \in J: |j-\ell|=1} \sqrt{\frac{q_\ell}{q_j}} \cos(\theta_\ell - \theta_j) - \eta q_j^\sigma \end{cases} \quad (21)$$

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 $L_m = 0$ and $K_m = 1$ for any $m = 1, \dots, d$. 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 $V(\mathbf{x})$ is a simply double-well potential with minima points \mathbf{x}_0 and \mathbf{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 $v_2 = \left(\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right)$.

4.2. Two-dimensional model. In such a case the potential $V(\mathbf{x})$ has 4 wells with minima points

$$\mathbf{x}_{(0,0)}, \mathbf{x}_{(0,1)}, \mathbf{x}_{(1,0)}, \mathbf{x}_{(1,1)}$$

and the matrix $T := T_2$ reduces to

$$T_2 = \begin{pmatrix} \lambda_D & -\beta & -\beta & 0 \\ -\beta & \lambda_D & 0 & -\beta \\ -\beta & 0 & \lambda_D & -\beta \\ 0 & -\beta & -\beta & \lambda_D \end{pmatrix} = \begin{pmatrix} T_1 & -\beta \mathbf{1}_2 \\ -\beta \mathbf{1}_2 & T_1 \end{pmatrix}$$

where $\mathbf{1}_2$ is the 2×2 identity matrix. The matrix T_2 has eigenvalues μ_r and associated normalized eigenvectors v_r , $r = 1, \dots, 4$, given by

$$\begin{aligned} \mu_1 &= \lambda_D - 2\beta & v_1 &= \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) \\ \mu_2 &= \lambda_D & v_2 &= \left(0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\right) \\ \mu_3 &= \lambda_D & v_3 &= \left(-\frac{1}{\sqrt{2}}, 0, 0, \frac{1}{\sqrt{2}}\right) \\ \mu_4 &= \lambda_D + 2\beta & v_4 &= \left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right) \end{aligned} \tag{22}$$

4.3. Three-dimensional model. In the case of $d = 3$ then the potential $V(\mathbf{x})$ has 8 wells with minima points

$$\mathbf{x}_{(0,0,0)}, \mathbf{x}_{(0,0,1)}, \mathbf{x}_{(0,1,0)}, \mathbf{x}_{(0,1,1)}, \mathbf{x}_{(1,0,0)}, \mathbf{x}_{(1,0,1)}, \mathbf{x}_{(1,1,0)}, \mathbf{x}_{(1,1,1)},$$

and the matrix $T := T_3$ reduces to

$$T_3 = \begin{pmatrix} T_2 & -\beta \mathbf{1}_4 \\ -\beta \mathbf{1}_4 & T_2 \end{pmatrix}$$

where 1_4 is the 4×4 identity matrix. The matrix T_3 has eigenvalues μ_r and associated normalized eigenvectors v_r , $r = 1, \dots, 8$, given by

$$\begin{aligned}
\mu_1 &= \lambda_D - 3\beta & v_1 &= \left(\frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}} \right) \\
\mu_2 &= \lambda_D - \beta & v_2 &= \left(0, 0, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, 0 \right) \\
\mu_3 &= \lambda_D - \beta & v_3 &= \left(0, -\frac{1}{2}, 0, -\frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}, 0 \right) \\
\mu_4 &= \lambda_D - \beta & v_4 &= \left(-\frac{1}{2}, 0, 0, \frac{1}{2}, -\frac{1}{2}, 0, 0, \frac{1}{2} \right) \\
\mu_5 &= \lambda_D + \beta & v_5 &= \left(0, \frac{1}{2}, 0, -\frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, 0 \right) \\
\mu_6 &= \lambda_D + \beta & v_6 &= \left(\frac{1}{2}, 0, 0, -\frac{1}{2}, -\frac{1}{2}, 0, 0, \frac{1}{2} \right) \\
\mu_7 &= \lambda_D + \beta & v_7 &= \left(0, 0, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, 0, 0 \right) \\
\mu_8 &= \lambda_D + 3\beta & v_8 &= \left(-\frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, -\frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, -\frac{1}{\sqrt{8}}, -\frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}} \right)
\end{aligned} \tag{23}$$

4.4. Any dimension. In dimension $d + 1$, for $d \geq 1$, the potential $V(x)$ has 2^{d+1} wells with minima points

$$x_{(0,j')}, x_{(1,j')}$$

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

$$T_{d+1} = \begin{pmatrix} T_d & -\beta 1_{2^d} \\ -\beta 1_{2^d} & T_d \end{pmatrix} \tag{24}$$

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:

$$\begin{aligned}
\Sigma_{2d} &= \{\lambda_D, \lambda_D \pm 2\beta, \dots, \lambda_D \pm 2(d-1)\beta, \lambda_D \pm 2d\beta\} \\
\Sigma_{2d+1} &= \{\lambda_D \pm \beta, \lambda_D \pm 3\beta, \dots, \lambda_D \pm (2d-1)\beta, \lambda_D \pm (2d+1)\beta\}
\end{aligned}$$

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

$$0 = |T_{d+1} - \lambda 1_{2^{d+1}}| = \begin{vmatrix} T_d - \lambda 1_{2^d} & -\beta 1_{2^d} \\ -\beta 1_{2^d} & T_d - \lambda 1_{2^d} \end{vmatrix}. \tag{25}$$

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

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

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 Σ^d has cardinality (counting multiplicity) 2^d and, by induction, we have that if $\lambda \in \Sigma^d$, then $\lambda \notin \Sigma^{d+1}$. \square

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

5. ANALYSIS OF THE BIFURCATION OF THE GROUND STATE

Now, we are going to discuss in dimension 1, 2 and 3 how the ground state stationary solutions of the linear problem bifurcate when we introduce the nonlinear term.

5.1. One-dimensional model. The model in dimension 1 has been largely discussed in previous papers (see, e.g., [6]), thus let us omit the details. In dimension $d = 1$ then (21) takes the form

$$\begin{cases} \sqrt{q_1 q_2} \sin(\theta_2 - \theta_1) & = 0 \\ -\sqrt{q_2/q_1} \cos(\theta_2 - \theta_1) + \eta q_1^\sigma & = \Omega \\ -\sqrt{q_1/q_2} \cos(\theta_1 - \theta_2) + \eta q_2^\sigma & = \Omega \\ q_1 + q_2 & = 1 \end{cases} \quad (26)$$

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

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

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 of (26) such that, for instance, $q_1 = 0$ and $q_2 = 1$ (or $q_1 = 1$ and $q_2 = 0$) at some η 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

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

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

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

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

$$\chi = \frac{\eta}{2^\sigma}$$

then equation (28) reduces to the form

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

and its solutions are given by

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

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

η	q_1	q_2	Ω
-2.01	0.45	0.55	-2.01
-2.1	0.35	0.65	-2.1
-2.5	0.2	0.8	-2.5

TABLE 1. Values of the coefficients q_1 and q_2 of the asymmetrical stationary solutions for the cubic one-dimensional double-well model for some values of the parameter η .

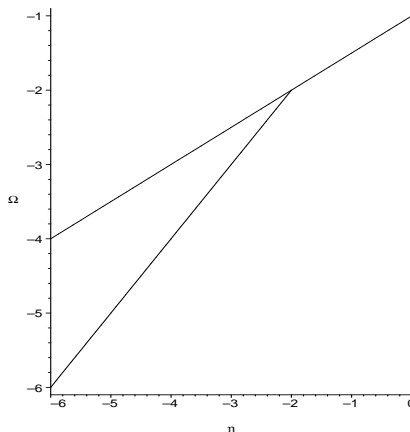


FIGURE 1. Bifurcation picture of the energy Ω as function of η for the cubic one-dimensional double-well model.

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 asymmetrical 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 Fig. 2).

5.2. **Two-dimensional model.** In such a case (21) takes the form

$$\left\{ \begin{array}{l}
 \sqrt{q_1 q_2} \sin(\theta_2 - \theta_1) + \sqrt{q_1 q_3} \sin(\theta_3 - \theta_1) = 0 \\
 \sqrt{q_2 q_1} \sin(\theta_1 - \theta_2) + \sqrt{q_2 q_4} \sin(\theta_4 - \theta_2) = 0 \\
 \sqrt{q_3 q_1} \sin(\theta_1 - \theta_3) + \sqrt{q_3 q_4} \sin(\theta_4 - \theta_3) = 0 \\
 \sqrt{q_4 q_2} \sin(\theta_2 - \theta_4) + \sqrt{q_4 q_3} \sin(\theta_3 - \theta_4) = 0 \\
 - \left(\sqrt{q_2/q_1} \cos(\theta_2 - \theta_1) + \sqrt{q_3/q_1} \cos(\theta_3 - \theta_1) \right) + \eta q_1^\sigma = \Omega \\
 - \left(\sqrt{q_1/q_2} \cos(\theta_1 - \theta_2) + \sqrt{q_4/q_2} \cos(\theta_4 - \theta_2) \right) + \eta q_2^\sigma = \Omega \\
 - \left(\sqrt{q_1/q_3} \cos(\theta_1 - \theta_3) + \sqrt{q_4/q_3} \cos(\theta_4 - \theta_3) \right) + \eta q_3^\sigma = \Omega \\
 - \left(\sqrt{q_2/q_4} \cos(\theta_2 - \theta_4) + \sqrt{q_3/q_4} \cos(\theta_3 - \theta_4) \right) + \eta q_4^\sigma = \Omega \\
 q_1 + q_2 + q_3 + q_4 = 1
 \end{array} \right. \quad (31)$$

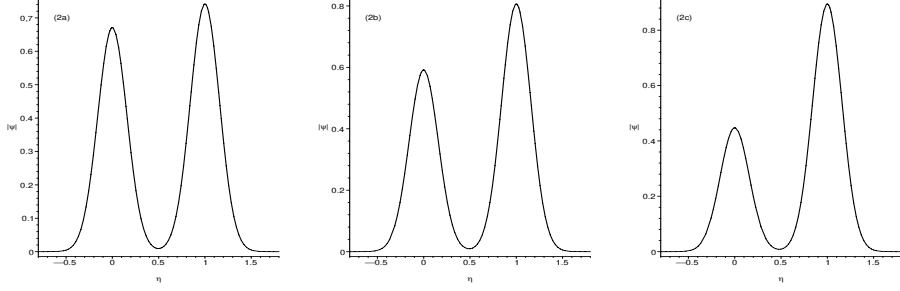


FIGURE 2. Picture of the absolute value of the asymmetrical stationary wave-function $\psi = \sqrt{q_1}\varphi_1 + \sqrt{q_2}\varphi_2$ for different values of η ($\eta = -2.01$ in panel (2a), $\eta = -2.1$ in panel (2b) and $\eta = -2.5$ in panel (2c)) where φ_j , $j = 1, 2$, are the vectors, defined in (11), localized on the single lattice cell x_j . The asymmetrical solution is, for η 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 $d_2 = -d_3$. 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 $\theta_j = \theta_\ell$ 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 $\theta_j = \theta_\ell$, 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

$$f_j = 0, \quad j = 1, \dots, 5, \quad \text{where} \quad \begin{cases} f_1 = -\left(\sqrt{q_2/q_1} + \sqrt{q_3/q_1}\right) + \eta q_1^\sigma - \Omega \\ f_2 = -\left(\sqrt{q_1/q_2} + \sqrt{q_4/q_2}\right) + \eta q_2^\sigma - \Omega \\ f_3 = -\left(\sqrt{q_1/q_3} + \sqrt{q_4/q_3}\right) + \eta q_3^\sigma - \Omega \\ f_4 = -\left(\sqrt{q_2/q_4} + \sqrt{q_3/q_4}\right) + \eta q_4^\sigma - \Omega \\ f_5 = q_1 + q_2 + q_3 + q_4 - 1 \end{cases} \quad (32)$$

which always has a symmetric solution

$$q_1 = q_2 = q_3 = q_4 = \frac{1}{4} \quad \text{with} \quad \Omega = \eta 4^{-\sigma} - 2 \quad (33)$$

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

$$\begin{cases} -\left(1 + \sqrt{q_3/q_1}\right) + \eta q_1^\sigma & = \Omega \\ -\left(1 + \sqrt{q_1/q_3}\right) + \eta q_3^\sigma & = \Omega \\ q_1 + q_3 & = \frac{1}{2} \end{cases} \quad (34)$$

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 $\chi = \frac{\eta}{4^\sigma}$, which has solutions

- $z = 0$, which corresponds to the case (33);
- for $\sigma = 1$, $z = \pm \frac{1}{\eta} \sqrt{\eta^2 - 16}$ 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

$$q_1 = q_4 \quad \text{and} \quad q_2 = q_3 \quad (35)$$

Then equations (32) become

$$\begin{cases} -2\sqrt{q_2/q_1} + \eta q_1^\sigma & = \Omega \\ -2\sqrt{q_1/q_2} + \eta q_2^\sigma & = \Omega \\ q_1 + q_2 & = \frac{1}{2} \end{cases} \quad (36)$$

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 $\chi = \frac{\eta}{2 \cdot 4^\sigma}$, which has solutions

- $z = 0$, which corresponds to the case (33);
- for $\sigma = 1$, $z = \pm \frac{1}{\eta} \sqrt{\eta^2 - 64}$ for $\eta \leq -8$ which gives $\Omega = +\frac{1}{2}\eta$.

Thus, at $\eta = -8$ the solution (33) bifurcates again.

5.2.3. *Partially symmetric solutions.* We consider now solutions such that

$$q_1 = q_4 \quad \text{and} \quad q_2 \neq q_3, \quad (37)$$

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 $\eta_{crit}^2 = -3.5836$ 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), Ω behaves like η (see Fig. 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 $\eta = \eta_{crit}^2$ the value of q_2 is equal to 0.571, and 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 η , see also Fig. 4 and 4).

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

$$\det \left(\frac{\partial f_i}{\partial q_h} \right)_{i,h=1,2,3,4,5} = 0, \quad (38)$$

where we denote $q_5 = \Omega$. Bifurcations of the symmetric stationary solution (33) are the solutions of equation (38) with $q_j = \frac{1}{4}$, $j = 1, 2, 3, 4$; 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:

1. At $\eta = \eta_{crit}^2 = -3.5836$ 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 to the saddle point at $\eta = \eta_{crit}^2$, and the last branch is the branch of the solutions observed in §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 §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 $\eta > \eta_{crit}^2$ there exists only one solution and it is equally distributed on the four wells; once η reaches the value η_{crit}^2 then two (families of) new solutions suddenly appears, and the solutions associated to the branch (a) of Fig. 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 the discussed in §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 $j, \ell = 1, 2, \dots, 8$. That is, in order to find the bifurcation from the ground state solution we can restrict ourselves to study the following system of equations

$$\left\{ \begin{array}{l} -\frac{1}{\sqrt{q_1}} (\sqrt{q_2} + \sqrt{q_3} + \sqrt{q_5}) + \eta q_1^\sigma = \Omega \\ -\frac{1}{\sqrt{q_2}} (\sqrt{q_1} + \sqrt{q_4} + \sqrt{q_6}) + \eta q_2^\sigma = \Omega \\ -\frac{1}{\sqrt{q_3}} (\sqrt{q_1} + \sqrt{q_4} + \sqrt{q_7}) + \eta q_3^\sigma = \Omega \\ -\frac{1}{\sqrt{q_4}} (\sqrt{q_2} + \sqrt{q_3} + \sqrt{q_8}) + \eta q_4^\sigma = \Omega \\ -\frac{1}{\sqrt{q_5}} (\sqrt{q_1} + \sqrt{q_6} + \sqrt{q_7}) + \eta q_5^\sigma = \Omega \\ -\frac{1}{\sqrt{q_6}} (\sqrt{q_2} + \sqrt{q_5} + \sqrt{q_8}) + \eta q_6^\sigma = \Omega \\ -\frac{1}{\sqrt{q_7}} (\sqrt{q_3} + \sqrt{q_5} + \sqrt{q_8}) + \eta q_7^\sigma = \Omega \\ -\frac{1}{\sqrt{q_8}} (\sqrt{q_4} + \sqrt{q_6} + \sqrt{q_7}) + \eta q_8^\sigma = \Omega \end{array} \right. \quad (39)$$

η	Branch (a)					Branch (b)				
	q_1	q_2	q_3	q_4	Ω	q_1	q_2	q_3	q_4	Ω
-3.5836						0.168	0.581	0.082	0.168	-3.159
-3.6	0.186	0.527	0.1	0.186	-3.0867	0.152	0.628	0.067	0.152	-3.24617
-3.7	0.214	0.436	0.136	0.214	-3.152	0.125	0.703	0.047	0.125	-3.445
-3.8	0.229	0.379	0.162	0.229	-2.998	0.110	0.742	0.037	0.110	-3.591
-3.9	0.241	0.329	0.189	0.241	-2.995	0.1	0.77	0.031	0.1	-3.722
-3.95	0.246	0.302	0.207	0.246	-2.997	0.095	0.781	0.029	0.095	-3.784
-4.05						0.088	0.801	0.024	0.088	-3.904
-8.1						0.016	0.967	0.001	0.016	-8.088

TABLE 2. Here we report the numerical solutions of equations $f_j = 0$, $j = 1, 2, 3, 4, 5$, associated to the two branches (a) and (b) raising from the saddle point at $\eta = \eta_{crit}^2 = -3.5836$. We can see that the solutions associated to the branch (b) are going to be fully localized on just one well (in this case it is the well with center at $x_{(0,1)}$).

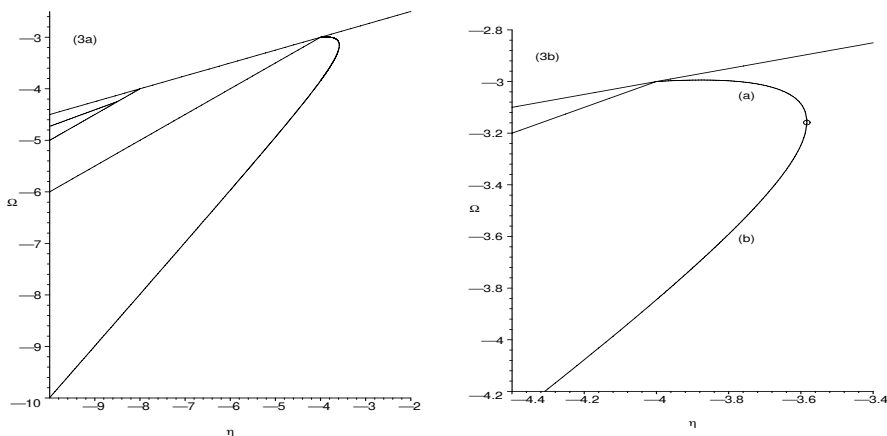


FIGURE 3. In the left panel (3a) we plot the graph of Ω as function of η , and we observe 3 bifurcation points and 1 saddle point. In the right panel (3b) we zoom the picture around the saddle point (denoted by the circle point) and we name the two branches (a) and (b). On the branch (b) the wavefunction is going to be fully localized on just one well as $|\eta|$ increases.

which always has a symmetric solution

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

As in the previous cases in dimension 1 and 2, asymmetrical solutions, if there exists, 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 $S_4 \times C_2$.

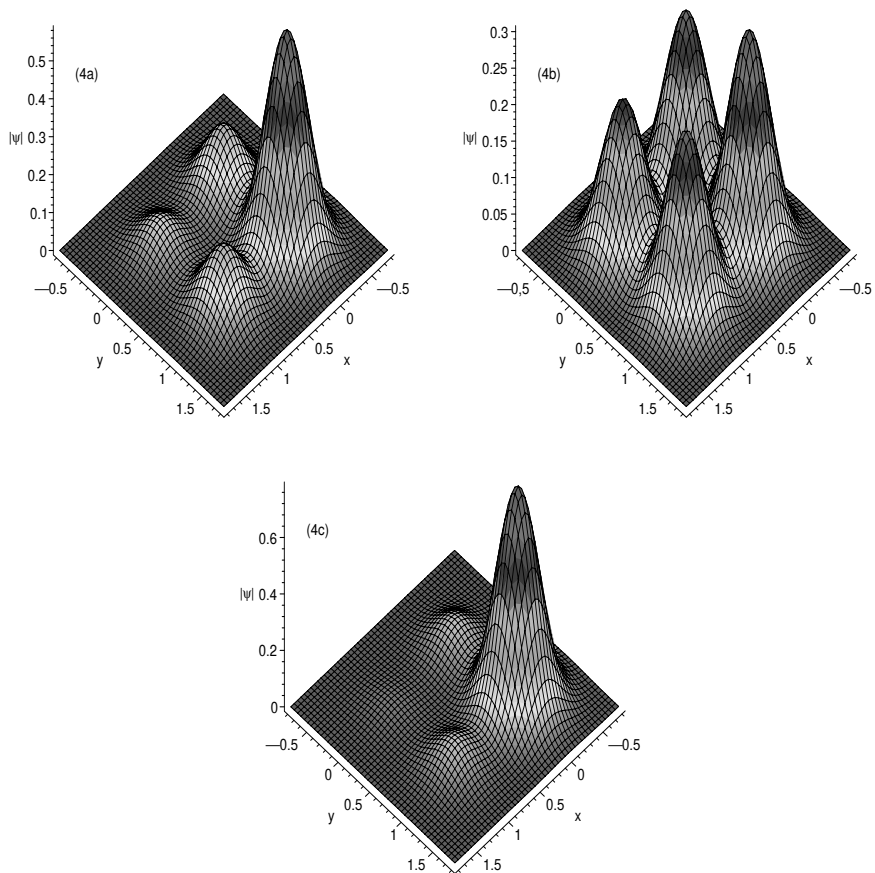


FIGURE 4. Pictures of the absolute value of the asymmetrical stationary wavefunction associated to the branch (b) for $\eta = \eta_{crit}^2$ (panel (4a)) and $\eta = -3.95$; in panel (4b) we plot the absolute value of the function corresponding to a solution in the branch (a); in panel (4c) we plot the absolute value of the function corresponding to a solution in the branch (b). At $\eta = \eta_{crit}^2$ 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 η approaches $\eta = -4$.

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

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

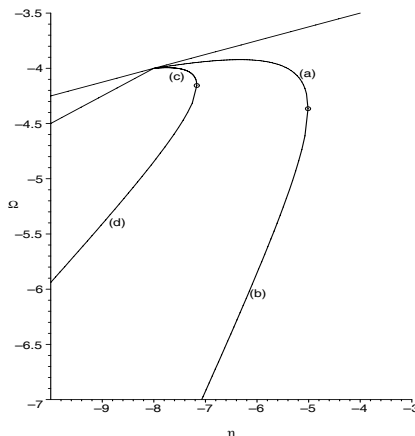


FIGURE 5. We plot the graph of Ω as function of η , and we observe 2 bifurcation points and 2 saddle point. On the branches (b) the wavefunction is going to be fully localized on just one well as $|\eta|$ increases.

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 $\eta = \eta_{crit,1}^3 = -5.0116$ a saddle point occurs and the new stationary solutions have asymmetrical wavefunctions satisfying (41), and where the wavefunction corresponding to the branch (b) of Fig. 5 is localized on just one single well (see table 3).
2. At $\eta = \eta_{crit,2}^3 = -7.1672$ a saddle point occurs and the new stationary solutions have asymmetrical wavefunctions satisfying (42), and where the wavefunction corresponding to the branch (d) of Fig. 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 4 different branches, the bifurcation point at $\eta = -24$ corresponds to 2 different branches.

5.4. Conclusion. As we can see in the 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 to branch of stationary solutions localized on a single well. This fact is the basic argument for the explanation of the phase transition from superfluidity phase to insulator phase. Indeed, in presence of stationary solutions associated to 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

η	Branch (a)					Branch (b)				
	q_1	q_2	q_4	q_8	Ω	q_1	q_2	q_4	q_8	Ω
-5.0116						0.659	0.083	0.027	0.0129	-4.3659
-5.1	0.569	0.098	0.038	0.021	-4.151	0.739	0.067	0.017	0.007	-4.674
-6	0.355	0.128	0.071	0.048	-3.928	0.873	0.037	0.005	0.001	-5.853
-7	0.240	0.136	0.094	0.071	-3.939	0.919	0.024	0.002	0.0004	-6.924
-7.9	0.150	0.131	0.117	0.105	-3.993	0.941	0.018	0.013	0.0002	-7.852
-8.1						0.945	0.017	0.001	0.0002	-8.056
-10						0.957	0.014	0.001	0.0001	-8.970

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

η	Branch (c)				Branch (d)			
	q_1	q_3	q_5	Ω	q_1	q_3	q_5	Ω
-7.1672					0.085	0.041	0.290	-4.156
-7.2	0.093	0.050	0.264	-4.087	0.076	0.034	0.314	-4.246
-7.5	0.111	0.074	0.203	-4.003	0.059	0.021	0.362	-4.521
-7.9	0.123	0.103	0.150	-3.997	0.048	0.014	0.391	-4.784
-8.1					0.044	0.012	0.400	-4.904
-9					0.032	0.007	0.429	-5.409

TABLE 4. Here we report the numerical solutions of equations (39) under conditions (42) associated to the two branches (c) and (d) raising from the saddle point at $\eta = \eta_{crit,2}^3 = -7.1672$. We can see that the solutions associated to the branch (d) are going to be fully localized on a couple of wells.

becomes gradually localized on just one well when the nonlinear strength parameter increases, then the phase transition is quite slow. In dimension 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.

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