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Nonlinear Schrödinger equations with multiple-well potential

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ABSTRACT

We consider the stationary solutions for a class of Schrödinger equations with a N-well potential and a nonlinear perturbation. By means of semiclassical techniques we prove that the dominant term of the ground state solutions is described by a N-dimensional Hamiltonian system, where the coupling term among the coordinates is a tridiagonal Toeplitz matrix. In particular, in the limit of large focusing nonlinearity we prove that the ground state stationary solutions consist of N wavefunctions localized on a single well. Furthermore, we consider in detail the case of $N = 4$ wells, where we show the occurrence of spontaneous symmetry-breaking bifurcation effect.

1. Introduction

For a quantum system with $\mathcal{N}$ particles the Schrödinger equation is defined in a space with dimension $3\mathcal{N}+1$ and typically it is impossible to solve, neither analytically nor numerically even with today's supercomputers. However, assuming a mean field hypothesis, the $3\mathcal{N}+1$ dimensions linear system of Schrödinger equation is approximated by a $3+1$ dimensions nonlinear Schrödinger equation. Although nonlinearity typically implies some new technical difficulties, the dimension is significantly reduced when compared with the original problem and this fact simplifies the study of dynamics of quantum systems, independently of the total number $\mathcal{N}$ of particles.

One of the most successful application of such an approach is the derivation of nonlinear Schrödinger equation for a Bose–Einstein condensate (BEC). Since its realization in diluted bosonic atomic gases [1–3] the interest in studying the collective dynamics of macroscopic ensembles of atoms occupying the same quantum state is largely increased. The condensate typically consists of a few thousands to millions of atoms which are confined by a trapping potential and at temperature much smaller than some critical value, and a BEC is well described by the macroscopic wave function $\psi = \psi(x, t)$ whose time evolution is governed by a self-consistent mean field nonlinear Schrödinger equation [4].

For such a reason, in these last years the study of the nonlinear Schrödinger equation with an external potential has attracted an increasing interest. In fact, many other interesting physical problems may be described by means of such a model, e.g. nonlinear optics [5], semiconductors [6], and quantum chemistry [7,8], just to mention the most relevant.

The mathematical research recently focused on the nonlinear Schrödinger equation (hereafter NLS) with double well potential. One of the most interesting feature of such a model is the spontaneous symmetry breaking phenomenon [9–12], and recently a general rule in order to classify the kind of bifurcation has been obtained [13,14] (see also [15]).

In NLS problems with *multi-well* potentials the *effective nonlinearity parameter* is usually given by the ratio between the strength of the nonlinear term and hopping matrix element between neighbor sites. The spontaneous symmetry breaking effect, and the associated localization phenomena, occurs when such a ratio is equal to a (finite) critical value. This fact has been seen, for instance, in the study of the Mott insulator-superfluid quantum phase transition [16,17]; in fact, multiple-well potential represents the effect of *small lattice* on, e.g., Bose–Einstein condensates. Furthermore, this model is also interesting in order to understand the transition to a lattice with infinitely many wells.

So far, few models with multiple-well potentials have been studied in detail from a rigorous point of view, e.g. the model with three wells on a regular lattice [18] (where a lattice means a sequence of points displaced along a straight line), and the model with four wells centered on the four points of a regular square grid [19]. The generic case with N wells has not yet been studied.

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In this paper we treat the problem of the validity of the N-mode approximation (where N is the number of wells displaced on a regular lattice), obtained by restricting our analysis to the N-dimensional space associated to the first N eigenvectors of the linear problem; in our approach we solve this problem considering the semiclassical limit, instead of using some kind of Galerkin decomposition as in [18]. Since the hopping matrix element between neighbor sites is not fixed, but it is exponentially small as the semiclassical parameter goes to zero, then, in order to have a finite value for the effective nonlinearity parameter (if not then we simply have localization), we have to require that the strength of the nonlinear term should be exponentially small, too. Hence, in our model we introduce a multi-scale limit in order to observe the bifurcation phenomena. We point out that other multi-scale limits may be considered in order to obtain the validity of the N-mode approximation, e.g. one can consider the simultaneous limit of large distance between the wells and small nonlinear term as in [15,10]. The assumption of small semiclassical parameter has the great advantage that, from a technical point of view, all the powerful semiclassical results developed by Helffer and Sjöstrand in the 80' (see e.g. the review [20]) are easily available when we consider the interaction between neighbor wells. We point out that our analysis can be easily extended to the case of wells displaced on a regular grid, as discussed in an explicit example in Remark 3.

The finite-dimensional system we obtain is almost decoupled, in the sense that the coupling term which represents the interaction among the adjacent wells is associated to a tridiagonal Toeplitz matrix. Furthermore, it can be written in Hamiltonian form, where one of the coordinates is a cyclic coordinate.

We then consider in details the case of $N = 4$ wells and we study the bifurcation picture when the strength of the nonlinear perturbation increases. As in the double well model we can see that the ground state stationary symmetric solution bifurcates giving rise to 4 stationary solutions fully localized on a single well, and the kind of bifurcation satisfies the same rule as in the double well model. Actually, such a result may be generalized to any number N of wells by means of a simple asymptotics argument. In particular, we focus our attention on the value of the *effective nonlinearity parameter* at the bifurcation point in the case of $N = 2, 4, 6$ and 8 wells; indeed bifurcation phenomena is associated to the phase transition and we'll see that the results obtained by our model agree with the numerical experiment on the Bose–Hubbard model [17].

2. Description of the model

Here, we consider the nonlinear Schrödinger (hereafter NLS) equations

$$i\hbar\frac{\partial\psi}{\partial t} = H_0\psi + \epsilon g(x)|\psi|^{2\sigma}\psi,$$
$$\psi(\cdot,t)\in L^2(\mathbb{R}^d,dx),\ \|\psi(\cdot,t)\| = 1, \tag{1}$$

where $\epsilon\in\mathbb{R}$ is a small parameter which represents the strength of the nonlinear perturbation and $\|\cdot\|$ denotes the $L^2(\mathbb{R}^d,dx)$ norm,

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

is the linear Hamiltonian with a multiple-well potential $V(x)$, and $g(x)|\psi|^{2\sigma}$ is a nonlinear perturbation. For the sake of definiteness we assume the units such that $2m = 1$. The semiclassical parameter $\hbar$ is such that $\hbar \ll 1$. In the following we will consider the multi-scale limit where *both* $\hbar$ and ϵ simultaneously go to zero in order that the *effective nonlinearity parameter* η, defined below in Eq. (34), goes to a finite value.

Here, we introduce the assumptions on the multiple-well potential V and we collect some semiclassical results on the linear operator H_0.

Hypothesis 1. Let $v(x)\in C_0^\infty(\mathbb{R}^d)$ be a smooth compact support function with a non degenerate minimum value at $x = 0$:

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

We consider multiple-well potentials of the kind

$$V(x) = \sum_{j=1}^N v(x-x_j) \tag{4}$$

for some $N > 1$, where

$$x_j = \left(j\ell - \frac{N+1}{2}\ell, 0, \dots, 0\right)$$

and $\ell > 2r$, where $r > 0$ is such that

$$\mathcal{C}\subseteq[-r,+r]\times\mathbb{R}^{d-1}$$

and where $\mathcal{C}$ is the compact support of $v(x)$.

Hence, the multi-well potential $V(x)$ has exactly N non degenerate minima at $x = x_j$, $j = 1, 2, \dots, N$.

Remark 1. It is a well known fact [13] that the Cauchy problem (1) is globally well-posed for any $\epsilon\in\mathbb{R}$ small enough provided that

$$\sigma < \begin{cases} +\infty & \text{if } d < 2 \\ \dfrac{1}{d-2} & \text{if } d > 2. \end{cases}$$

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

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

follows; furthermore we also have a priori estimate

$$\|\psi(\cdot,t)^{2\sigma}\| \le C\hbar^{-m} \tag{5}$$

for some positive constants C and m.

3. Analysis of the linear Schrödinger equation

Now, making use of semiclassical analysis [20] we look for the ground state of the linear Schrödinger equation

$$H_0\psi = \lambda\psi,\quad \psi\in L^2(\mathbb{R}^d).$$

Let $d_A(x,y)$ be the Agmon distance between two points x and y, let

$$S_0 = \inf_{i\neq j} d_A(x_j,x_i);$$

then, by construction of the potential $V(x)$, it turns out that

$$S_0 = d_A(x_j,x_{j+1}),\quad j = 1,2,\dots,N-1, \tag{6}$$

and

$$S_0 < d_A(x_j,x_i)\quad \text{if } |i-j| > 1. \tag{7}$$

Now, let H_D be the Dirichlet realization of

$$H_D = -\hbar^2\Delta + v \tag{8}$$

on the ball $B_S(0)$ with center at $x = 0$ and radius $S > 2S_0$. 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

$$\lambda_D = v(0) + \hbar\sum_{j=1}^d\sqrt{v_j} + \mathcal{O}(\hbar^2),$$