NONLINEAR TIME-DEPENDENT ONE-DIMENSIONAL SCHröDINGER EQUATION WITH DOUBLE WELL POTENTIAL

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ABSTRACT. We consider time-dependent Schrödinger equations in one dimension with double well potential and an external nonlinear perturbation. If the initial state belongs to the eigenspace spanned by the eigenvectors associated to the two lowest eigenvalues then, in the semiclassical limit, we show that the reduction of the time-dependent equation to a 2-mode equation gives the dominant term of the solution with a precise estimate of the error. By means of this stability result we are able to prove the destruction of the beating motion for large enough nonlinearity.

1. INTRODUCTION

Recently, the theoretical analysis of the nonlinear time-dependent Schrödinger equation

\[ i\hbar \dot{\psi} = H_0 \psi + \epsilon |\psi|^2 \psi, \quad \epsilon \in \mathbb{R}, \quad \dot{\psi} = \frac{\partial \psi}{\partial t}, \]

(1)

where

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

has attracted an increasing interest (see [4] for a review and [10] for a rigorous derivation of the Gross-Pitaevskii energy functional). When \( V \) is a double well potential, one of the main goal is to understand how the nonlinear perturbation with strength \( \epsilon \) affects the unperturbed beating motion (see, e.g., the review paper [4] and the paper [16] where equation (1) is proposed as a model for chiral molecules). To this end, it is crucial to study the solution \( \psi \) for times of the order of the beating period; in other words, for practical purposes the unit of time is given by the beating period \( T = \pi \hbar / \omega \) where \( \hbar \) is the Planck’s constant and \( \omega \) is one half of the energy splitting between the two lowest energies.

Here, I consider equation (1) in the semiclassical limit where, by assuming that \( d = 1 \) and under some generic assumption on the double well potential, we give the asymptotic behavior of the solution \( \psi \) with a precise estimate of the error. In particular, the main result (Theorem 3) consists in proving that the solution of the Gross-Pitaevskii equation is approximated, with a rigorous control of the error,
by means of the solution of a two-dimensional dynamical system exactly solvable. As a result it follows (Theorem 4) that the beating motion between the two wells of a state initially prepared on the two lowest eigenstates gradually disappears for increasing nonlinearity.

A similar investigation has been recently performed in [6], where the nonlinear perturbation is given by $\epsilon(\psi, g\psi)g\psi$ and $g(x)$ is a given odd function, and in [13], where, in dimension $d = 1$ and $d = 3$, we consider the limit of large barrier between the two wells. In particular, in [13] I had to assume that the discrete spectrum of the Schrödinger operator $H_0$ consists of only two non-degenerate eigenvalues and that the restriction to the continuous eigenspace of the unitary evolution operator satisfies to a priori estimate uniformly with respect to the parameters of the model.

Finally, we mention other recent results concerning the study of the existence of stationary solutions for Gross-Pitaevskii equations with double well potentials [1], [2] and, in the case of single-well type potentials, the existence of solutions asymptotically given by solitary wave functions in the case that the discrete spectrum of the linear Schrödinger operator has only one non-degenerate eigenvalue [15], [18].

Our paper is organized as follows.

In Section 2 we introduce the main notations and we state the assumptions on the potential. Moreover, we collect some semiclassical results concerning the spectrum of the linear Schrödinger operator.

In Section 3 we prove the global existence of the solution of the Gross-Pitaevskii equation, the existence of conservation laws and a priori estimate (Theorem 2). The global existence of the solution is proved for both repulsive and attractive nonlinear perturbation, where, in the second case, we have to assume that the strength of the nonlinear perturbation is small enough.

In Section 4 we introduce the two-level approximation which, roughly speaking, consists in projecting the Gross-Pitaevskii equation onto the two-dimensional space spanned by the eigenvectors of the linear Schrödinger operator associated to the two lowest eigenvalues. For practical purposes, it is more convenient to choose, as a basis of such a two-dimensional space, the two "single-well" states. The dynamical system we obtain is exactly solvable.

In Section 5 we give our main result (Theorem 3) proving the stability of the two-level approximation. Here, we make use of the comparison criterion between ordinary differential equations and of a priori estimate of the solution of the Gross-Pitaevskii equation. We underline that, in order to obtain such an estimate, the assumption $d = 1$ on the dimension plays a crucial role.

In Section 6 we give the full rigorous justification of the results by Vardi [16] proving the existence of a critical value for the nonlinearity parameter giving the destruction of the beating motion (Theorem 4).

2. Assumptions and preliminary results

Here, we consider the Cauchy problem

$$i\dot{\psi} = H_\epsilon \psi, \quad H_\epsilon = H_0 + W$$

$$\psi(0, x) = \psi^0(x) \in L^2(\mathbb{R}), \quad \|\psi^0\| = 1,$$

where $\dot{\psi}$ denotes the derivative of $\psi$ with respect to the time $t$, $H_0$ is the linear Schrödinger operator formally given by (here, $x$ denotes the spatial variable in
dimension 1)
\[
H_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V,
\]
(3)

\(V\) is a symmetric double well potential and
\[
W = \epsilon |\psi|^2,
\]
is the nonlinear perturbation with strength \(\epsilon\).

In the following, for the sake of definiteness, we denote by \(C\) any positive constant independent of \(\epsilon, \hbar\) and \(t\), we assume \(\hbar\) small enough, that is \(\hbar \in (0, \hbar^*]\) for some \(\hbar^*\), and we denote
\[
\|\varphi\|_p = \|\varphi\|_{L^p} = \left\{ \int |\varphi(x)|^p dx \right\}^{1/p} \quad \text{and} \quad \|\varphi\| = \|\varphi\|_2.
\]
Moreover, given \(y = (y_1, \ldots, y_m) \in \mathbb{R}^m\) for some \(m \geq 1\), we denote
\[
|y| = \max_{1 \leq j \leq m} |y_j|.
\]

\[2.1. \textbf{Assumptions on the potential.} \]

Here, we assume that the potential \(V\) is a regular symmetric function which admits two non-degenerate minima and it is bounded from below. More precisely:

**Hypothesis 1.** The potential \(V(x)\) is a real valued function such that:

i. \(V(-x) = V(x), \forall x \in \mathbb{R}\);

ii. \(V \in C^2(\mathbb{R})\);

iii. \(V(x)\) admits two non-degenerate minima at \(x = \pm a\), for some \(a > 0\), such that
\[
V(x) > V_{\min} = V(\pm a), \quad \forall x \in \mathbb{R}, \; x \neq \pm a;
\]
in particular, for the sake of definiteness, we assume that
\[
\frac{dV(\pm a)}{dx} = 0 \quad \text{and} \quad \frac{d^2V(\pm a)}{dx^2} > 0;
\]
iv. finally we assume that
\[
\liminf_{|x| \to \infty} V(x) = V_{\infty} > V_{\min}.
\]

It follows that the operator formally defined in (3) admits a self-adjoint realization (still denoted by \(H_0\)) on \(L^2(\mathbb{R})\) (see, for instance, Theorem III.1.1 in [3]). Let \(\sigma(H_0) = \sigma_d \cup \sigma_{\text{ess}}\) be the spectrum of the self-adjoint operator \(H_0\) where \(\sigma_d\) denotes the discrete spectrum and \(\sigma_{\text{ess}}\) denotes the essential spectrum. From Hyp. 1-iv it follows that \(\sigma_d \subset (V_{\min}, V_{\infty}), \sigma_{\text{ess}} = \emptyset\) if \(V_{\infty} = +\infty\) (see Theorem XIII.67 in [12]) and that \(\sigma_{\text{ess}} \subseteq [V_{\infty}, +\infty)\) if \(V_{\infty} < \infty\) (see Theorem III.3.1 in [3]). Furthermore, the following two Lemmas hold:

**Lemma 1.** Let \(\sigma_d\) be the discrete spectrum of \(H_0\). Then, for any \(\hbar \in (0, \hbar^*)\) it follows that:

i. \(\sigma_d\) is not empty and, in particular, it contains two eigenvalues at least;

ii. let \(\lambda_{1,2}\) be the lowest two eigenvalues of \(H_0\), they are non-degenerate, in particular \(\lambda_1 < \lambda_2\) and there exists \(C > 0\), independent of \(\hbar\), such that
\[
\inf_{\lambda \in \sigma(H_0) - \{\lambda_{1,2}\}} |\lambda - \lambda_2| \geq C\hbar.
\]
Proof. The proof is an immediate consequence of the above assumptions and standard WKB arguments. □

Lemma 2. Let \( \varphi_{1,2} \) be the normalized eigenvectors associated to \( \lambda_{1,2} \), then:

i. \( \varphi_j, j = 1, 2 \), can be chosen to be real-valued functions such that \( \varphi_j(-x) = (-1)^{j-1}\varphi_j(x) \);

ii. \( \varphi_j \in H^1(\mathbb{R}) \);

iii. \( \varphi_j \in L^p(\mathbb{R}) \) for any \( p \in [1, +\infty] \);

iv. there exists a positive constant \( C \) such that

\[
\|\varphi_j\|_{L^p} \leq C \hbar^{-\frac{p-2}{4p}}, \quad \forall p \in [2, +\infty], \quad \forall \hbar \in (0, \hbar^*].
\] (6)

Proof. Property i. immediately follows from assumption Hyp. 1-i. Property ii. follows from Lemma III.3.1 in [3]. Property iii. follows from Theorem III.3.2 in [3]. Finally, property iv. follows for \( p = +\infty \) by means of standard WKB arguments.

From this fact, from the normalization of the eigenvectors and from the Hölder inequality then property iv. follows for any \( p \in [2, +\infty] \):

\[
\|\varphi_j\|_p = \left[\|\varphi_j^2\|_1^{1/p} \right]^{1/p} \leq \|\varphi_j\|_2 \|\varphi_j\|_\infty^{(p-2)/p} = \|\varphi_j\|_\infty^{(p-2)/p}.
\]

2.2. Splitting and single-well states. It is well known that the splitting between the two lowest eigenvalues vanishes as \( \hbar \) goes to zero. In particular, we have that:

Lemma 3. Let

\[
\omega = \frac{\lambda_2 - \lambda_1}{2} \quad \text{and} \quad \Omega = \frac{\lambda_2 + \lambda_1}{2}
\]

and

\[
\varphi_R = \frac{1}{\sqrt{2}} [\varphi_1 + \varphi_2] \quad \text{and} \quad \varphi_L = \frac{1}{\sqrt{2}} [\varphi_1 - \varphi_2]
\]

where \( \varphi_{1,2} \) are the normalized eigenvectors associated to \( \lambda_{1,2} \). Then there exist two positive constants \( C \) and \( \Gamma \), independent of \( \hbar \), such that

\[
\|\varphi_R \varphi_L\|_\infty \leq C \omega
\] (7)

and

\[
\omega \leq C e^{-\Gamma/\hbar}, \quad \forall \hbar \in (0, \hbar^*].
\] (8)

As a result it follows that

\[
\lim_{\hbar \to 0} \omega = 0
\] (9)

and

\[
\lim_{\hbar \to 0} \frac{\Omega - V_{\min}}{\hbar} = c
\] (10)

for some \( c > 0 \).

Proof. In order to prove this Lemma we observe that \( V \) is a symmetric double well potential with non-zero barrier between the wells. That is, let \( \delta > 0 \) be small enough and let us define the two sets

\[
B_R = \left\{ x \in \mathbb{R}^+ : V(x) \leq V_{\min} + \delta \right\} \quad \text{i.e.} \quad x \in B_R \Leftrightarrow -x \in B_L.
\]

\[
B_L = \left\{ x \in \mathbb{R}^- : V(x) \leq V_{\min} + \delta \right\}
\]
From condition (5) it follows also that
\[ B_R = [b, c] \quad \text{and} \quad B_L = [-c, -b] \]
for some \( c > a > b > 0 \). The sets \( B_{R,L} \) are usually called "wells". Let
\[ \Gamma_\delta = \int_{-b}^{b} \sqrt{\max[V(x) - (V_{\min} + \delta), 0]} \, dx > 0, \]
be the Agmon distance between the two wells. From these facts and from standard WKB arguments (see [7] and [8]) then (7)–(10) follow for some \( \Gamma \in [\Gamma_0, \Gamma_\delta] \). □

**Remark 1.** By definition it follows that \( \varphi_R(-x) = \varphi_L(x) \); moreover, from (7), it follows that these functions are localized on only one of the "wells" \( B_R \) and \( B_L \), e.g.:
\[ \int_{B_R} |\varphi_R(x)|^2 \, dx = 1 + O(e^{-C/\hbar}) \]
for some \( C > 0 \). For such a reason we call them "single-well" (normalized) states.

**Remark 2.** We underline that, by assuming some regularity properties on the potential \( V \), then it is possible to obtain the precise asymptotic behavior of the splitting as \( \hbar \) goes to zero [8].

### 2.3. Assumptions on the parameter

We assume that the two parameters \( \omega \) and \( \epsilon \) are such that
\[ \omega \to 0 \quad \text{and} \quad \epsilon \to 0 \quad \text{as} \quad \hbar \to 0 \]
and there exists a positive constant \( C \) such that
\[ \frac{c\epsilon}{\omega} \leq C, \quad c = \|\varphi_R^2\|, \quad \forall \hbar \in (0, \hbar^*]. \quad (11) \]

### 2.4. Assumption on the initial state

Let
\[ \Pi_c = 1 - \langle \varphi_R, \cdot \rangle \varphi_R - \langle \varphi_L, \cdot \rangle \varphi_L \quad (12) \]
be the projection operator onto the eigenspace orthogonal to the 2-dimensional eigenspace associated to the doublet \( \{\lambda_{1,2}\} \). Let \( \psi^0 \) be the initial wavefunction, we assume that:

**Hypothesis 2.** \( \Pi_c \psi^0 = 0 \).

### 3. Global existence of the solution and conservation laws

Here, we prove that the Cauchy problem (2) admits a solution for all time provided that assumptions Hyp.1–2 are satisfied and the strength \( \epsilon \) of the nonlinear perturbation is small enough. Moreover, we prove a "priori" estimate of the solution \( \psi \).

The following results hold.

**Theorem 1.** There exist \( h^* > 0 \) and \( \epsilon_0 > 0 \) such that for any \( \hbar \in (0, h^*] \) and \( \epsilon \in [-\epsilon_0, \epsilon_0] \) then the Cauchy problem (3) admits a unique solution \( \psi(t,x) \in H^1 \) for any \( t \in R \). Moreover, the following conservation laws hold:
\[ \|\psi(t,\cdot)\| = \|\psi^0(\cdot)\| = 1 \quad (13) \]
and
\[ E(\psi) = \frac{\hbar^2}{2m} \left\| \frac{\partial \psi}{\partial x} \right\|^2 + \langle V \psi, \psi \rangle + \frac{1}{2} \left\| \psi \right\|^2 = E(\psi_0). \] (14)

Proof. From Hyp.2 it follows that
\[ \psi_0 = c_1 \varphi_1 + c_2 \varphi_2, \quad c_{1,2} = \langle \psi_0, \varphi_{1,2} \rangle. \]

From this fact and from Lemma 2 then \( \psi_0 \in H^1 \). Therefore, existence of the global solution \( \psi \in C(\mathbb{R}, H^1) \) and the conservation laws (13) and (14) follow from known results (see, e.g., the papers quoted in [14] and [15]) for any \( \epsilon > 0 \) (repulsive nonlinear perturbation) and for any \( \epsilon \in (-\epsilon_0, 0) \) for some \( \epsilon_0 > 0 \) (attractive nonlinear perturbation).

\[ \square \]

Remark 3. There exists a positive constant \( C \) independent of \( \hbar \) and \( \epsilon \) such that
\[ |E(\psi) - V_{\min}| \leq C(\omega + \hbar + \epsilon \hbar^{-1/2}), \quad \forall h \in (0, h^*), \quad \forall \epsilon \in [-\epsilon_0, \epsilon_0]. \] (15)

This estimate immediately follows from (13), from the assumption Hyp.2 and from Lemmas 1 and 2. Indeed, from Hyp.2 it follows that
\[ E(\psi_0) = \langle H_0(c_1 \varphi_1 + c_2 \varphi_2), (c_1 \varphi_1 + c_2 \varphi_2) \rangle + \frac{1}{2} \epsilon \left\| \psi_0 \right\|^4 \]
where \( \left\| \psi_0 \right\|_4 \leq C \hbar^{-1/8} \) from (3) and where
\[ \langle H_0(c_1 \varphi_1 + c_2 \varphi_2), (c_1 \varphi_1 + c_2 \varphi_2) \rangle = \lambda_1 |c_1|^2 + \lambda_2 |c_2|^2 = \Omega - \omega + 2 \omega |c_2|^2. \]

From these facts and from (3), then (15) follows.

Theorem 2. Let \( \epsilon_0(h) \) be a function such that
\[ \lim_{h \to 0} \epsilon_0(h)/\hbar^2 = 0. \] (16)

The solution \( \psi \) of equation (2) satisfies to the following uniform estimate: there exists a positive constant \( C \) independent of \( t, \hbar \) and \( \epsilon \), such that
\[ \left\| \psi \right\|_p \leq C \left[ \frac{|E(\psi_0) - V_{\min}|}{\hbar^2} \right]^{\frac{p-2}{4p}}, \quad \forall p \in [2, +\infty], \] (17)
and
\[ \left\| \frac{\partial \psi}{\partial x} \right\| \leq C \left[ \frac{|E(\psi_0) - V_{\min}|}{\hbar^2} \right]^{\frac{1}{4}}, \]
for all time and \( \forall h \in (0, h^*), \forall \epsilon \in [-\epsilon_0(h), \epsilon_0(h)]. \)

Proof. In order to prove the estimate (17) let
\[ k = \frac{\hbar}{\sqrt{2m}}, \quad \Lambda = \frac{E(\psi_0) - V_{\min}}{k^2}. \]

Then, the conservation laws (13) and (14) imply that
\[ \left\| \frac{\partial \psi}{\partial x} \right\|^2 + \frac{1}{2} \left[ \text{sign}(\epsilon) \right] \rho^2 \left\| \psi \right\|^2 \leq \Lambda, \]
where
\[ \rho = |\epsilon|^{1/2}/k \ll 1, \]
since (16). In particular, if we set
\[ \chi = \rho \psi \]
then the above equation takes the form
\[ \left\| \frac{\partial \chi}{\partial x} \right\|^2 + \frac{1}{2} [\text{sign}(\epsilon)] \| \chi \|^2 \leq \Lambda \rho^2 \]
from which it follows that
\[ \left\| \frac{\partial \chi}{\partial x} \right\|^2 \leq \rho^2 |\Lambda| + \frac{1}{2} \| \chi \|^2 \]
\[ \| \chi \|^2 \leq \Lambda \rho^2 \]
From the Gagliardo-Niremberg inequality (see, for instance, [5] and [17], where the dimension is here equal to 1)
\[ \| \chi \|_{2\sigma+2}^2 \leq C \left\| \frac{\partial \chi}{\partial x} \right\|^\sigma \| \chi \|^{2+\sigma}, \quad \forall \sigma \geq 0, \] (19)
where we choose \( \sigma = 1 \), it follows that
\[ \| \chi \|_4^4 \leq C \left\| \frac{\partial \chi}{\partial x} \right\|^3 \| \chi \| \rho^3 \]
since \( \| \chi \| = \rho \| \psi \| = \rho \) and \( \| \psi \| = 1 \). By inserting this inequality in (18) it follows that
\[ \left\| \frac{\partial \chi}{\partial x} \right\|^2 \leq \rho^2 |\Lambda| + C \rho^3 \left\| \frac{\partial \chi}{\partial x} \right\| \]
\[ \| \chi \|_4^4 \leq C \rho^3 \]
for any \( t \in \mathbb{R} \). From (20) immediately follows that
\[ \left\| \frac{\partial \chi}{\partial x} \right\| \leq \sqrt{|\Lambda| \rho (1 + o(1))}, \quad \text{as } \rho \to 0. \]
Hence, \( \left\| \frac{\partial \psi}{\partial x} \right\| \leq C \sqrt{|\Lambda|} \) and, from (16), we have that
\[ \| \psi \|_p \leq C \left\| \frac{\partial \psi}{\partial x} \right\|^{\sigma/p} \leq C |\Lambda|^{(p-2)/4p} \]
where we choose now \( \sigma = \frac{p-2}{2} \), i.e. \( p = 2\sigma + 2 \).

\[ \square \]

**Remark 4.** Condition (16) is true in the semiclassical limit and under the assumption (11).

**Remark 5.** From the fact \( E(\psi_0) - V_{\text{min}} = O(\hbar) \), which follows from (8), (17) and (16), and from the bounds (21) and (11) then it follows that \( \forall t \in \mathbb{R}, \forall \hbar \in (0, \hbar^*], \forall \epsilon \in [-\epsilon_0(\hbar), \epsilon_0(\hbar)] \) then
\[ \| \psi \|_p \leq C \hbar^{-\frac{p}{4p}}, \forall p \in [2, +\infty], \quad \text{and} \quad \left\| \frac{\partial \psi}{\partial x} \right\| \leq C \hbar^{-\frac{1}{2}}. \] (21)
4. Two-level approximation

For our purposes it is more convenient to make the substitution $\psi \rightarrow e^{-i\Omega t/\hbar}\psi$, hence equation (2) takes the following form (where, with abuse of notation, we still denote the new function by $\psi$)

$$ih\dot{\psi} = (H_0 - \Omega)\psi + \epsilon|\psi|^2\psi, \quad \psi(x, 0) = \psi^0(x). \quad (22)$$

Let us write the solution of this equation in the form

$$\psi(t, x) = a_R(t)\varphi_R(x) + a_L(t)\varphi_L(x) + \psi_c(t, x), \quad (23)$$

where $a_R(t)$ and $a_L(t)$ are unknown complex-valued functions depending on time and $\psi_c = \Pi_c\psi$, $\Pi_c$, defined in (12), is the projection onto the space orthogonal to the two-dimensional space spanned by the two "single-well" states $\varphi_R$ and $\varphi_L$, i.e.:

$$\langle \psi_c, \varphi_R \rangle = \langle \psi_c, \varphi_L \rangle = 0, \quad \forall t \in \mathbb{R}.$$  

From the conservation law (13) it follows that

$$|a_R(t)|^2 + |a_L(t)|^2 + \|\psi_c(t, \cdot)\|^2 = 1, \forall t \in \mathbb{R}. \quad (24)$$

By substituting $\psi$ by (23) in equation (2) we obtain that $a_R$, $a_L$ and $\psi_c$ must satisfy to the system of differential equations

$$\begin{cases}
    ih\dot{a}_R &= -\omega a_L + \epsilon\langle \varphi_R, |\psi|^2\psi \rangle \\
    ih\dot{a}_L &= -\omega a_R + \epsilon\langle \varphi_L, |\psi|^2\psi \rangle \\
    ih\dot{\psi}_c &= (H_0 - \Omega)\psi_c + \epsilon\Pi_c|\psi|^2\psi
\end{cases} \quad (25)$$

By substituting again $\psi$ by (23) in the first two equations of the above system then we obtain that these equations take the form

$$\begin{cases}
    ih\dot{a}_R &= -\omega a_L + \epsilon c|a_R|^2 a_R + \epsilon r_R \\
    ih\dot{a}_L &= -\omega a_R + \epsilon c|a_L|^2 a_L + \epsilon r_L
\end{cases} \quad (26)$$

where

$$c = \|\varphi_R^2\|^2 = \|\varphi_L^2\|^2 = O(\hbar^{-1}) \quad (27)$$

and where $r_R$ and $r_L$ are given by

$$r_R = \langle \varphi_R, |\psi|^2\psi \rangle - |a_R|^2\langle \varphi_R, |\varphi_R|^2\varphi_R \rangle = \langle \varphi_R, |\psi|^2\phi_L \rangle + a_R\langle |\varphi_R|^2, |\phi_L|^2 + a_R|\varphi_R\phi_L + a_R|\varphi_R\phi_L \rangle$$

$$r_L = \langle \varphi_L, |\psi|^2\psi \rangle - |a_L|^2\langle \varphi_L, |\varphi_L|^2\varphi_L \rangle = \langle \varphi_L, |\psi|^2\phi_R \rangle + a_L\langle |\varphi_L|^2, |\phi_R|^2 + a_L|\varphi_L\phi_R + a_L|\varphi_L\phi_R \rangle$$

where

$$\phi_L = a_L\varphi_L + \psi_c \quad \text{and} \quad \phi_R = a_R\varphi_R + \psi_c.$$  

We denote two-level approximation the solutions $b_R$ and $b_L$ of the system of ordinary differential equations

$$\begin{cases}
    ib\dot{b}_R &= -\omega b_L + \epsilon c|b_R|^2 b_R \\
    ib\dot{b}_L &= -\omega b_R + \epsilon c|b_L|^2 b_L \quad , \quad b_{R,L}(0) = a_{R,L}(0). \quad (28)
\end{cases}$$

obtained by neglecting the remainder terms $r_R$ and $r_L$ in (24). It is easy to see that the solution of this system satisfies to the following conservation law

$$|b_R(t)|^2 + |b_L(t)|^2 = |b_R(0)|^2 + |b_L(0)|^2 = a_R(0)^2 + a_L(0)^2 = 1, \quad (29)$$
and, moreover, it is also possible to explicitly compute (see [11] and Appendix B in [13]) the solution of (28) by means of elliptic functions. In particular, we obtain that the imbalance function, defined as

\[ z(t) = |b_R(t)|^2 - |b_L(t)|^2, \tag{30} \]

is given by

\[ z(t) = \begin{cases} 
\text{Acn} \left[ \frac{\eta(\omega t - \tau_0)}{2k,k} \right], & \text{if } k < 1, \\
\text{Adn} \left[ \frac{\eta(\omega t - \tau_0)}{2,1/k} \right], & \text{if } k > 1,
\end{cases} \]

where \( \eta = \frac{\epsilon c}{\omega} \), \( \tau_0 \) depends on the initial condition, \( I = \sqrt{1 - z^2(0)} \cos[\theta(0)] - \eta z^2(0)/4, \) \( \theta = \text{arg}(b_R) - \text{arg}(b_L) \) is the relative phase,

\[ A = 2\sqrt{2} \frac{\eta}{\eta} \left( \sqrt{\frac{1}{4} \eta^2 + 1} + I \eta - \left( 1 + \frac{1}{2} I \eta \right)^{1/2} \right)^{1/2}, \]

and

\[ k^2 = \frac{1}{2} \left[ 1 - \frac{1 + \frac{1}{2} I \eta}{\sqrt{\frac{1}{4} \eta^2 + 1} + I \eta} \right]. \tag{31} \]

We underline that \( z(t) \) periodically assumes positive and negative values if, and only if, \( k < 1 \).

5. Stability of the two-level approximation

Our main result consists in proving the stability of the two-level approximation when we restore the remainder terms \( r_R \) and \( r_L \) in equation (28).

We prove that:

**Theorem 3.** Let \( \psi_c = \Pi \psi, a_R(t) = \langle \psi, \varphi_R \rangle \) and \( a_L(t) = \langle \psi, \varphi_L \rangle \), where \( \psi \) is the solution of equation (22), let \( b_R(t) \) and \( b_L(t) \) be the solution of the system of ordinary differential equations (28). Let \( \epsilon \in [-\epsilon_0(h), \epsilon_0(h)] \), where \( \epsilon_0(h) \) satisfies the condition (16). Then, for any \( \tau' > 0 \) there exists a positive constant \( C \) independent of \( \epsilon, h \) and \( t \) such that:

\[ |b_{R,L}(t) - a_{R,L}(t)| \leq Ce^{-Ch^{-1}} \quad \text{and} \quad \|\psi_c(\cdot,t)\| \leq Ce^{-Ch^{-1}} \tag{32} \]

for any \( h \in (0,h^*) \) and for any \( t \in [0,\tau'/\omega] \).

**Proof.** For the sake of simplicity, hereafter, let us drop out the parameters where this does not cause misunderstanding. In order to prove the theorem we introduce the ”slow time” \( \tau = \omega t/h \) and let

\[
\begin{cases} 
A_{R,L}(\tau) = a_{R,L}(t) \\
B_{R,L}(\tau) = b_{R,L}(t)
\end{cases}, \quad \begin{cases} 
R_{R,L}(\tau) = \frac{\epsilon}{\omega} R_{R,L}(t) \quad \text{and} \quad \eta = \frac{\epsilon c}{\omega}.
\end{cases}
\]

Then (28) and (29) respectively take the form (here ’ denotes the derivative with respect to \( \tau \))

\[
\begin{align*}
A_{R}'(\tau) & = iA_L - i\eta|A_R|^2 A_R + R_R \\
A_{L}'(\tau) & = iA_R - i\eta|A_L|^2 A_L + R_L
\end{align*} \tag{33}
\]
Lemma 4. The function $A, B$ where

\[
\begin{align*}
B'_R &= iB_L - i\eta |B_R|^2 B_R \\
B'_L &= iB_R - i\eta |B_L|^2 B_L
\end{align*}
\]

satisfying to the same initial condition

$B_{R,L}(0) = A_{R,L}(0) = a_{R,L}(0)$,

since (24) and (28), they are such that

$|B_R(\tau)|^2 + |B_L(\tau)|^2 = 1, \quad |A_R(\tau)|^2 + |A_L(\tau)|^2 \leq 1$. \hfill (35)

In a more concise way, with an obvious meaning of the notation, we can write (33) and (24) as

$A' = f(A) + R$ and $B' = f(B), \quad A(0) = B(0) = a(0)$, \hfill (36)

where $A, B \in S^2$ since (33), $S^2 = \{ (z_1, z_2) \in C^2 : |z_1|^2 + |z_2|^2 \leq 1 \}$.

**Lemma 4.** The function $f : S^2 \to C^2$ satisfies to the Lipschitz condition:

$|f(A) - f(B)| \leq L|A - B|, \quad L = 1 + 3\eta$. \hfill (37)

**Proof.** According with the notation (4) we have that

$|f(A) - f(B)| = \max |f_R|, |f_L|$ \hspace{1cm}

where $|A| \leq 1$ and $|B| \leq 1$ since $A, B \in S^2$ and where

\[
\begin{align*}
f_R &= (A_L - B_L) - \eta(|A_R|^2 A_R - |B_R|^2 B_R) \\
f_L &= (A_R - B_R) - \eta(|A_L|^2 A_L - |B_L|^2 B_L)
\end{align*}
\]

Then (37) immediately follows since

$f_R = (A_L - B_L) - \eta [|B_R|^2 (A_R - B_R) + A_R(|A_R| + |B_R||(|A_R| - |B_R|))]$

where $|A_R| - |B_R| \leq |A_R - B_R|$ and where the other term $f_L$ will be treated in the same way. \hfill \Box

**Lemma 5.** Let

$\beta = \max[\kappa, \omega]$

where $c$ is defined in (23). Let $\psi_c = \Pi_c \psi$ where $\psi$ is the solution of equation (23); it satisfies to the following uniform estimate

$\|\psi_c\| \leq C\beta h^{-3/2} \left [ \exp(Ch^{-1/2}(\epsilon t)h) + 1 \right ], \quad \forall t \in R$, \hfill (38)

for some positive constant $C$ independent of $h, \epsilon$ and $t$.

**Proof.** As a first step we consider the following rough estimates:

$\|\psi_c\|_p \leq Ch^{-\frac{p-2}{2}}, \quad \forall p \in [2, +\infty], \quad \forall t \in R$, \hfill (39)

and

$|r_{R,L}| \leq Ch^{-1/2}, \quad \forall t \in R$,

Indeed, (39) immediately follows from the Minkowski inequality and from (21):

$Ch^{-\frac{p-2}{2}} \geq \|\psi\|_p \geq - (|a_R(t)||\varphi_R|_p + |a_L(t)||\varphi_L|_p) + \|\psi_c\|_p$
where $|a_{R,L}(t)| \leq 1$ and where $\varphi_{R,L}$ satisfy the bound (3). In the same way, from Lemma 2 and Theorem 2, it follows that

\[
|r_R| \leq C\|\varphi_R\|^2 \cdot \|\varphi_R\| + \|\varphi_R\|_{\infty} \\
\leq C\|\varphi_R\|_{\infty} \|\varphi\|^2 + C\|\varphi_R\|_{\infty} \\
\leq C\hbar^{-1/2}
\]

and similarly for $|r_L|$.

Now, in order to prove the estimate (38) we make use of the third equation of (25) from which it follows that

\[
\psi_c(\cdot,t) = -i\hbar \int_0^t e^{-i(H_0-\Omega)(t-s)/\hbar} \Pi_c |\psi(\cdot,s)|^2 \psi(\cdot,s) ds
\]

since $\psi_0^c = \Pi_c \psi_0 = 0$ from assumption Hyp.2.

Let $\psi = \varphi + \psi_c$ where $\varphi = a_R \varphi_R + a_L \varphi_L$, then

\[
|\psi|^2 \psi = \varphi_I + \psi_c \varphi_{II} + \bar{\psi}_c \varphi_{III}, \quad \begin{cases} 
\varphi_I = |\varphi|^2 \varphi, \\
\varphi_{II} = 2|\varphi|^2 + 2\bar{\psi}_c \varphi + |\psi_c|^2 + \bar{\varphi}_c, \\
\varphi_{III} = \varphi^2
\end{cases}
\]

Therefore, we can write

\[
\psi_c = -i\frac{\epsilon}{\hbar} [I + II + III]
\]

where

\[
I = \int_0^t e^{-i(H_0-\Omega)(t-s)/\hbar} \Pi_c \varphi_1 ds \\
II = \int_0^t e^{-i(H_0-\Omega)(t-s)/\hbar} \Pi_c \psi_{II} ds \\
III = \int_0^t e^{-i(H_0-\Omega)(t-s)/\hbar} \bar{\Pi_c} \bar{\psi}_c \varphi_{III} ds
\]

For what concerns the first term we have that, by integrating by part,

\[
I = [ -i\hbar e^{-i(H_0-\Omega)(t-s)/\hbar} [H_0 - \Omega]^{-1} \Pi_c |\varphi|^2 \varphi ]_0^t + +i\hbar \int_0^t e^{-i(H_0-\Omega)(t-s)/\hbar} [H_0 - \Omega]^{-1} \Pi_c \frac{\partial |\varphi|^2 \varphi}{\partial s} ds
\]

Let us underline that from Lemma 1 it follows that the following operators, from $L^2$ into $L^2$, are bounded

\[
\left\| e^{-i(H_0-\Omega)(t-s)/\hbar} \right\| = 1, \quad \| H_0 - \Omega \|^{-1} \Pi_c \leq C,
\]

and, from Lemma 2 and equations (24) and (26) we have the following uniform estimate for any $t \in \mathbb{R}$

\[
\|\varphi\|_p \leq (|a_r| + |a_L|) (\|\varphi_R\|_p + \|\varphi_L\|_p) \leq C\hbar^{-1} \max\{c, \omega, \epsilon \hbar^{-\frac{3}{2}}\} \hbar^{-\frac{p-2}{2p}} \\
\leq C\hbar^{-1} \beta \hbar^{-\frac{p-2}{2p}}.
\]
Then we have that
\[ \| I \| \leq C \max_{s \in [0, t]} \left\{ \| \phi^3(s, \cdot) \| + t \| \dot{\phi}(s, \cdot) \phi^2(s, \cdot) \| \right\} \]
\[ \leq C \max_{s \in [0, t]} \left\{ \| \phi(s, \cdot) \|_3 + t \| \dot{\phi}(s, \cdot) \| \cdot \| \phi(s, \cdot) \|_\infty^2 \right\} \]
\[ \leq C \left\{ h^{-1/2} + th^{-1} \beta h^{-1/2} \right\}. \]

For what concerns the other two terms we have that
\[ \| II \| \leq \int_0^t \| \psi_c \| \cdot \| \phi_{II} \|_\infty ds \leq C \epsilon h^{-1/2} \int_0^t \| \psi_c \| ds \]
since \( \| \phi_{II} \|_\infty \leq C h^{-1/2} \), and similarly
\[ \| III \| \leq \int_0^t \| \psi_c \| \cdot \| \phi_{III} \|_\infty ds \leq C \epsilon h^{-1/2} \int_0^t \| \psi_c \| ds. \]

Indeed, from Lemma 2 and (39) it follows that
\[ \| \phi_{II} \|_\infty \leq C \left\{ \| \varphi \|_\infty^2 + \| \psi_c \| \varphi \|_\infty + \| \psi_c \|_\infty^2 \right\} \leq C h^{-1/2} \]
and
\[ \| \phi_{III} \|_\infty \leq \| \varphi \|_\infty^2 \leq C h^{-1/2}. \]

Collecting all these results and denoting
\[ g(t) = \| \psi_c(\cdot, t) \| \]
we have that \( g(t) \) is a positive real valued function satisfying the estimate
\[ g(t) \leq C \epsilon \frac{h}{h} \left\{ h^{-1/2} \int_0^t g(s) ds + h^{-1/2} \left( 1 + th^{-1} \beta \right) \right\} \]
\[ \leq a \int_0^t g(s) ds + a + abt, \quad a = C \frac{\epsilon}{h^{3/2}}, \quad b = \frac{\beta}{h}. \]

From this estimate, since \( \psi_c(0) = 0 \) and from the Gronwall’s Lemma (see [3], pag. 19) it follows that
\[ g(t) \leq a + abt + a \int_0^t e^{at-s}(a+abs) ds = -b + ac^t + be^t \]
\[ \leq \frac{C \beta}{h^{3/2}} \left[ e^{Ct}h^{-3/2} + 1 \right] \]
proving so the result. \( \square \)

From the inequality (3) and from the assumption (14) it follows that for any fixed \( \tau’ > 0 \) then there exists \( C > 0 \) satisfying the second inequality in (33).

**Lemma 6.** For any fixed \( \tau’ > 0 \) then the remainder terms \( r_R \) and \( r_L \) satisfy to the following uniform estimate:
\[ \max \| r_R \|, \| r_L \| \leq C3h^{-2} e^{C h^{-1/2}}, \quad \forall t \in [0, \tau’ h/\omega], \]
for some positive constant \( C \) independent of \( h, \epsilon \) and \( t \).
Proof. Let us only consider the term \( |r_R| \), the other term \( |r_L| \) could be treated in the same way. By definition and since \( \max[|a_R|,|a_L|] \leq 1 \) then it follows that

\[
|r_R| \leq + |\langle \varphi_R \bar{\varphi}_L, |\psi|^2 \rangle| + |\langle \varphi_R |\psi|^2, \psi_c \rangle| + |\langle |\varphi_R|^2, |\phi_L|^2 + a_R \varphi_R \bar{\phi}_L + \bar{a}_R \varphi_R \phi_L \rangle| \tag{40}
\]

and we estimate separately each term.

From Lemma 3, equation (13) and the Hölder inequality it follows that the term (40) satisfies to the following estimate:

\[
|\langle \varphi_R \bar{\varphi}_L, |\psi|^2 \rangle| \leq \| \varphi_R \bar{\varphi}_L \|_\infty \cdot \| \psi \|^2 \|_1 \leq C_\omega.
\]

From Lemma 5 and the Hölder inequality it follows that the term (41) satisfies to the following estimates:

\[
|\langle \varphi_R |\psi|^2, \psi_c \rangle| \leq \| \varphi_R \|_\infty \cdot \| \psi \|^2 \cdot \| \psi_c \| \leq C_\beta \hbar^{-2} e^{C_\hbar^{-1/2}}
\]

and that the term (42) satisfies to the estimate

\[
|\langle |\varphi_R|^2, |\phi_L|^2 + a_R \varphi_R \bar{\phi}_L + \bar{a}_R \varphi_R \phi_L \rangle| \leq C \left[ \| \varphi_R \|_\infty \cdot \| \psi \|^2 \cdot \| \psi_c \|^2 + \| \varphi_R \|_\infty \cdot \| \psi \|^2 \| \psi_c \| \right] \leq C \omega.
\]

Collecting all these estimates we obtain the proof of the Lemma.

The proof of the Theorem is almost done. Indeed, equations (36) can be rewritten in the integral form:

\[
A(\tau) = A(0) + \int_0^\tau f[A(s)]ds + \int_0^\tau Rds
\]

and

\[
B(\tau) = B(0) + \int_0^\tau f[B(s)]ds
\]

from which it follows that for any \( \tau \in [0, \tau'] \)

\[
|A(\tau) - B(\tau)| \leq \int_0^\tau |f[A(s)] - f[B(s)]| ds + \int_0^\tau |R| ds \\
\leq a \int_0^\tau |A(s) - B(s)| ds + b \tau, \quad a = L, \quad b = C \frac{\epsilon \hbar^{-2} e^{C_\hbar^{-1/2}}}{\omega}
\]

since Lemmas 4 and 5. From this inequality and by means of the Gronwall’s Lemma we finally obtain that

\[
|A(\tau) - B(\tau)| \leq b \tau + ab \int_0^\tau e^{\alpha(t-s)} ds = \frac{b}{\alpha} [e^{\alpha \tau} - 1] \\
\leq \frac{C \epsilon \hbar^{-2} e^{C_\hbar^{-1/2}}}{L} \frac{\omega + \epsilon}{\omega}
\]

proving so (32) since

\[
\frac{\omega + \epsilon}{C' \omega} \leq L = 1 + 3 \eta \leq C' \frac{\omega + \epsilon}{\omega},
\]

for some \( C' > 0 \), which implies that \( \frac{b}{\omega} \leq C \) for some \( C > 0 \).
Remark 6. Recalling that \( \omega = O(e^{-\rho/h}) \) then the above theorem implies that for any \( \alpha < 1 \) and for any \( \tau' > 0 \) there exists \( C \) such that
\[
|b_{R,L}(t) - a_{R,L}(t)| \leq C \omega^\alpha \quad \text{and} \quad \|\psi_c(\cdot, t)\| \leq C \omega^\alpha, \quad \forall t \in [0, h\tau'/\omega].
\]

6. Destruction of the beating motion for large nonlinearity

6.1. The unperturbed case \( \epsilon = 0 \). Under the assumption Hyp.2 it follows that the solution of the unperturbed equation
\[
i\hbar \dot{\psi} = H_0 \psi, \quad \psi(0, x) = \psi^0(x),
\]
is simply given by
\[
\psi(t, x) = e^{-i\Omega t/\hbar}\left[c_1 + c_2 \cos(\omega t/\hbar) + i\frac{c_2 - c_1}{\sqrt{2}} \sin(\omega t/\hbar)\right] \varphi_R(x) + e^{-i\Omega t/\hbar}\left[c_1 - c_2 \cos(\omega t/\hbar) - i\frac{c_1 + c_2}{\sqrt{2}} \sin(\omega t/\hbar)\right] \varphi_L(x)
\]
where
\[
c_{1,2} = \langle \varphi_{1,2}, \psi^0 \rangle, \quad |c_1|^2 + |c_2|^2 = 1.
\]
Hence, \( \psi(t, x) \) is, up to the phase factor \( e^{-i(\Omega - \omega)t/\hbar} \), a periodic function with period \( T = \pi\hbar/\omega \).

In particular, if \( \psi \) initially coincides with a single-well state, e.g. \( \psi^0 = \varphi_R \), then
\[
\psi(t, x) = e^{-i(\Omega - \omega)t/\hbar}\left[e^{-i\omega t/\hbar} \cos(\omega t/\hbar) \varphi_R(x) - i e^{-i\omega t/\hbar} \sin(\omega t/\hbar) \varphi_L(x)\right]
\]
and the state \( \psi(t, x) \) performs a beating motion. That is the state, initially localized on the well \( B_R \), is localized on the other well \( B_L \) after half a period and, after a whole period, it "returns" on the initial well, and so on. In particular, let us consider the motion of the "center of mass" defined here as
\[
\langle X \rangle^t = \langle X \varphi, \psi \rangle = \int_R X(x)|\psi(t, x)|^2 dx
\]
where \( X \in C(R) \cap L^2(R) \) is a given bounded function such that \( X(-x) = -X(x) \). We have that
\[
\langle X \rangle^t = \left[\cos^2(\omega t/\hbar) - \sin^2(\omega t/\hbar)\right] \int_R X(x)|\varphi_R(x)|^2 dx
\]
is a periodic function which periodically assumes positive and negative values, i.e. we have the well know beating motion for double-well problem.

6.2. The perturbed case \( \epsilon \neq 0 \). In such a case it follows that the "center of mass" is given by
\[
\langle X \rangle^t = c[|a_R(t)|^2 - |a_L(t)|^2] + r, \quad c = \langle X \varphi_R, \varphi_R \rangle,
\]
where the remainder term \( r \) satisfies the uniform estimate
\[
|r| = 2 |\Re [a_R \bar{a}_L (X \varphi_R, \varphi_L) + \langle X \psi, \psi_c \rangle]| \leq 2 \|[\varphi_R \varphi_L]_{\infty} + \|X\|_{\infty} \|\psi\|_{\infty} \|\psi_c\|_{\infty} \|
\leq Ce^{-Ch^{-1}}, \quad \forall t \in [0, h\tau'/\omega].
\]
If we denote by \( z(t) \) the imbalance function defined in (30) then it follows that
\[
|a_R(t)|^2 - |a_L(t)|^2 = z(t) + Ce^{-Ch^{-1}}, \quad \forall t \in [0, h\tau'/\omega],
\]
hence

\[ \langle X \rangle^t = cz(t) + Ce^{-Ch^{-1}}, \quad \forall t \in [0, \hbar \tau'/\omega]. \]

Then, we have that:

**Theorem 4.** Let Hyp. 1 and 2 be satisfied. Let \( k^2 \) be defined as in (31), it depends on the initial wavefunction \( \psi^0 \). Let \( \tau' > 0 \) fixed, \( \langle X \rangle^t \) is, up to a remainder term, a periodic function for any \( t \in [0, \hbar \tau'/\omega] \). In particular, if:

i) \( k^2 < 1 \) then \( \langle X \rangle^t \) periodically assumes positive and negative values (i.e. the beating motion still persists);

ii) \( k^2 > 1 \) then \( \langle X \rangle^t \) has a definite sign (i.e. the beating motion is forbidden).

**Remark 7.** Let us close by underlining that when the wavefunction is initially prepared on just one well, e.g. \( \psi^0 = \varphi_R \), then

\[ I = -\frac{1}{4} \eta \quad \text{and} \quad k^2 = \frac{1}{16} \eta^2. \]

Therefore, from the theorem above it follows that for \( |\eta| \) larger than the critical value 4 the beating motion is forbidden. In such a way, we put on a full rigorous basis the results obtained by [16] in the two-level approximation.

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