Stability of Spectral Eigenspaces in Nonlinear Schrödinger Equations

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ABSTRACT. We consider the time-dependent non linear Schrödinger equations with a double well potential. We prove, in the semiclassical limit, that the finite dimensional eigenspace associated to the lowest two eigenvalues of the linear operator is almost invariant for any time.

CONTENTS

1. Introduction

Here we consider the time-dependent nonlinear Schrödinger equation (hereafter NLS)

$$(1) \qquad \begin{cases} i\hbar\dot\psi^t = H_0\psi^t + \epsilon W\psi^t, \quad \epsilon \in \mathbb{R}, \ \dot\psi^t = \frac{\partial \psi^t}{\partial t}, \\ \psi^t(x)|_{t=0} = \psi^0(x) \in L^2(\mathbb{R}^d), \ \|\psi^0\|_{L^2} = 1, \end{cases}$$

where

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

is the linear Hamiltonian operator with symmetric double-well potential $V(x)$, and where

$$(3) \qquad\qquad\qquad\qquad W = W(|\psi|^2) = |\psi|^{2\sigma}$$

is a nonlinear perturbation, here σ is a positive real number such that

$$(4) \qquad\qquad 0 < \sigma < \infty \ \ \text{if} \ \ d = 1, 2 \ \ \text{and} \ \ 0 < \sigma < \frac{2}{d-2} \ \ \text{if} \ \ d > 2.$$

We recall that a double well potential is a positive potential symmetric with respect to the reflection through a hyperplane, and having two nondegenerate distinct absolute minima. When the nonlinear term is absent, the linear Hamiltonian H_0 has the two eigenfunctions corresponding to the two lowest eigenvalues which have either even or odd-parity. Given an initial datum which is a linear combination of such lowest eigenfunctions, then the corresponding solution performs a *beating motion*, namely the probability density oscillates periodically from a state almost concentrated on one minimum to a state almost concentrated on the other one. The *beating period* usually plays the role of unit of time. When the nonlinear term is restored, a symmetry breaking phenomenon occurs: that is, if the strength ϵ of the nonlinear term is larger than a threshold value then new asymmetric stationary states appears [1], [4], [12]. Furthermore, for higher strength ϵ of the nonlinear term, the beating motion is generically forbidden [5], [7], [9]. These results can be heuristically obtained by reducing the NLS equation to a 2–dimensional dynamical system, namely the restriction of (1) to the space generated by the lowest two eigenvectors. Mathematically the difficulty consists in proving that the dynamics of the complete NLS is close to the dynamics of the 2–dimensional reduced system. In [8], making use of semiclassical estimates and refined existence results for NLS this stability result has been obtained for *times of the order of the beating period* in dimensions $d = 1, 2$ and any $\sigma \in \mathbb{R}^+$.

In the present paper we concentrate on the case of local nonlinearity (3) in any dimension d and for σ satisfying (4), in this framework we extend the previous result by [8] proving that, in the semiclassical limit, the 2-dimensional eigenspace is almost invariant *for any time* (Theorem 1). However, due to the possible presence of positive Lyapunof exponents, our result does not allow to show that the 2-dimensional system describes the dynamics over time scales larger than ϵ^{-1}.

Our result is obtained here making use of variational methods and by introducing the scale of Hilbert spaces $\mathcal{X}_s = \mathcal{D}(H_0^{s/2})$, $s \geq 0$, constituted by the domains of the powers of H_0, endowed by the graph norm; in fact, we make use of the energy space $\mathcal{X}_1$.

We close this section by introducing some notations:

   - The notation $y = O(e^{-\Gamma/\hbar})$ means that there exist $\hbar^\star > 0$ and a positive constant $C > 0$, independent of $\hbar$, such that

$$|y| \leq Ce^{-\Gamma/\hbar}, \ \ \forall \hbar \in (0, \hbar^\star)$$

- The notation $y = \tilde{O}(e^{-\Gamma/\hbar})$ means that for any Γ', $0 < \Gamma' < \Gamma$, then $y = O(e^{-\Gamma'/\hbar})$; that is, there exist $\hbar^\star > 0$ and a positive constant $C = C_{\Gamma'} > 0$, independent of $\hbar$, such that

$$|y| \leq Ce^{-\Gamma'/\hbar}, \quad \forall \hbar \in (0, \hbar^\star).$$

- As usual, $\|\cdot\|_{L^p}$ usually denotes the norm of the space $L^p(\mathbb{R}^d)$; $\|\cdot\|_s$ denotes the norm of the Hilbert spaces $\mathcal{X}_s$, in such a notation $\mathcal{X}_0 = L^2(\mathbb{R}^d)$ and $\|\cdot\|_0 = \|\cdot\|_{L^2}$.
- As usual, $\mathbb{R}$ denotes the set of real numbers, $\mathbb{R}^+$ denotes the set of positive real numbers, $\mathbb{N}$ denotes the set of positive integer numbers, C denotes any positive constant independent of $\hbar$ and t, and $\langle x \rangle = \sqrt{1 + |x|^2}$, $|x|^2 = \sum_{j=1}^{d} x_j^2$, where $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$.

2. The model: preliminary assumptions and main result

2.1. Double well potentials.

HYPOTHESIS 1. *The double-well potential $V(x) \in C^\infty(\mathbb{R}^d)$ is a symmetric real valued function such that:*

i. *$V(x)$ admits two minima at $x = x_\pm$, $x_- \neq x_+$, such that*

$$V(x) > V_{min} = V(x_\pm), \quad \forall x \in \mathbb{R}^d, \ x \neq x_\pm;$$

for the sake of definitess let us assume

$$V_{min} = 1.$$

ii. *There exists $0 < m \leq 2$ such that, for large $|x|$ one has*

$$C\langle x \rangle^m \leq V(x) \leq C^{-1}\langle x \rangle^m$$

for some constant $0 < C < 1$;

iii. *For any multi-index $\alpha \in \mathbb{N}^d$ there exists a positive constant C_α such that*

$$\left| \partial_{x_1}^{\alpha_1} \partial_{x_2}^{\alpha_2} \cdots \partial_{x_d}^{\alpha_d} V(x) \right| \leq C_\alpha \langle x \rangle^{m-|\alpha|}$$

REMARK 1. *For the sake of definiteness, we assume that the symmetric potential is such that*

$$V(-x_1, x_2, \ldots, x_d) = V(x_1, x_2, \ldots, x_d) \ .$$

Furthermore, for the sake of simplicity we assume also that

$$\nabla V(x_\pm) = 0 \quad and \quad Hess\, V(x_\pm) > 0;$$

the case of degenerate minima, that is $det[HessV(x_\pm)] = 0$, could be treated in a similar way; however, we don't develop here the details.

REMARK 2. *As an example one can consider the following double-well potential*

$$V(x) = 1 + \sum_{j=1}^{d} \omega_j^2 x_j^2 + V_1(x)$$

where $V_1 \in L^\infty(\mathbb{R}^d)$ is a symmetric function

$$V_1(-x_1, x_2, \ldots, x_d) = V_1(x_1, x_2, \ldots, x_d).$$

2.2. Well-posedness of the Cauchy problem. Under Hyp. 1 the Cauchy problem (1)–(3) is locally well posed.

In fact, in the quadratic (i.e. $m = 2$) and sub-quadratic (i.e. $m < 2$) cases if $\psi^0 \in H^1$ is such that

$$\int_{\mathbb{R}^d} V(x)|\psi^0(x)|^2 \mathrm{d}^d x < \infty$$

then (see [11] and §9.2 in [3]) the Cauchy problem admits a unique bounded local solution $\psi^t \in H^1$ such that

$$\int_{\mathbb{R}^d} V(x)|\psi^t(x)|^2 \mathrm{d}^d x < \infty$$

for any $t \in [0, \delta)$, for some $\delta > 0$.

Moreover, ψ^t satisfies the following conservation norm

(5) $$\mathcal{N}(\psi^t) = \mathcal{N}(\psi^0) \ ,$$

where

$$\mathcal{N}(\psi) = \|\psi\|_{L^2} = \left[\int_{\mathbb{R}^d} |\psi^0(x)|^2 \mathrm{d}^d x \right]^{\frac{1}{2}}$$

and

$$\mathcal{E}_\epsilon(\psi^t) = \mathcal{E}_\epsilon(\psi^0)$$

where the *energy* functional is defined as

(6) $$\mathcal{E}_\epsilon(\psi) = \mathcal{E}_0(\psi) + \epsilon P(\psi) \ ,$$

where

$$\mathcal{E}_0(\psi) = \langle \psi, H_0 \psi \rangle_{L^2} \ \text{ and } \ P(\psi) = \frac{1}{1+\sigma}\|\psi^{\sigma+1}\|_{L^2}^2.$$

Furthermore, the solution ψ^t continuously depends on t and on the initial condition ψ^0.

REMARK 3. *Notice that when $\epsilon > 0$ then the conservation of the energy implies that $\|\nabla \psi\| \leq C$ for any time, hence the solution is global, i.e. $\delta = +\infty$. For $\epsilon < 0$, in the sub-critical case $d\sigma < 2$ then the conservation of the energy still give the same estimate on $\|\nabla \psi\|$ and the global existence of the solution. In fact, for $\epsilon < 0$ small enough, by energy conservation and bootstrap arguments (see [8]) any solution is global in the critical $d\sigma = 2$ and super-critical $d\sigma > 2$ cases too.*

REMARK 4. *In fact, it could be also possible to consider the case of super-quadratic potentials where $m > 2$. Indeed, in such a case the Cauchy problem admits an unique solution ψ^t for any $t \in [0, \delta)$ when $\psi^0 \in \mathcal{X}_s$ (see Theorem 1.5 in [10]), where δ continously depends on $\|\psi^0\|_s$. However, it is not clear whether the conservation and the continuity of the energy hold; thus, we don't dwell here of the case of super-quadratic potentials.*

REMARK 5. *The choice $m > 0$ was done only in order to simplify the notations. Indeed our result holds also in the case $m = 0$, but, due to the appearence of continuous spectrum, in order to deal explicitely with such a case all the notations should be modifyed.*

2.3. Linear beats. The operator H_0 formally defined by (2) admits a self-adjoint realization (still denoted by H_0) on $L^2(\mathbb{R}^d)$ (Theorem III.1.1 in [**2**]) with purely discrete spectrum $\sigma(H_0) = \sigma_d(H_0)$, where $\sigma_d(H_0)$ denotes the discrete spectrum. Let λ_k, $k \in \mathbb{N}$, be the eigenvalues of H_0

$$\lambda_1 < \lambda_2 < \lambda_3 \leq \lambda_4 \leq \ldots \leq \lambda_k \leq \ldots$$

with associated normalized (in L^2) eigenvectors $\varphi_k(x)$. In particular, the lowest two eigenvalues of H_0 are non-degenerate and there exists $0 < C < 1$, independent of $\hbar$, such that

$$1 + C\hbar < \lambda_{1,2} < 1 + C^{-1}\hbar \quad \text{and} \quad \inf_{\lambda \in \sigma(H_0) - \{\lambda_1, \ \lambda_2\}}[\lambda - \lambda_{1,2}] \geq C\hbar$$

and

$$(7) \qquad\qquad \lambda - \lambda_2 \geq C\lambda\hbar, \ \forall \lambda \in \sigma(H_0) - \{\lambda_1, \ \lambda_2\} \ .$$

It is well known that the *splitting* between the two lowest eigenvalues

$$(8) \qquad\qquad \omega = \frac{1}{2}(\lambda_2 - \lambda_1)$$

vanishes as $\hbar$ goes to zero. In order to give a precise estimate of the splitting ω let

$$\Gamma = \inf_\gamma \int_\gamma \sqrt{V(x) - V_{min}}dx > 0$$

be the Agmon distance between the two wells; where γ is any path connecting the two wells, that is $\gamma \in AC([0,1], \mathbb{R}^d)$ such that $\gamma(0) = x_-$ and $\gamma(1) = x_+$. From standard WKB arguments (see [**6**]) it follows that the splitting is *exponentially small*, precisely that

$$(9) \qquad\qquad \omega = \tilde{O}(e^{-\Gamma/\hbar}).$$

The normalized eigenvectors $\varphi_{1,2}$ associated to $\lambda_{1,2}$ can be chosen to be real-valued functions such that φ_1 and φ_2 are respectively of even and odd-parity:

$$\varphi_j(-x_1, x_2, \ldots, x_d) = (-1)^{j+1}\varphi_j(x_1, x_2, \ldots, x_d), \quad j = 1, 2;$$

We define now the *single well states*

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

such that

$$\varphi_R(-x_1, x_2, \ldots, x_d) = \varphi_L(x_1, x_2, \ldots, x_d)$$

They are *localized on one well* in the sense that for any $r > 0$ there exists $C_r > 0$ such that

$$\int_{D_r(x_+)} |\varphi_R(x)|^2 dx = 1 + O(e^{-C_r/\hbar})$$

and

$$\int_{D_r(x_-)} |\varphi_L(x)|^2 dx = 1 + O(e^{-C_r/\hbar})$$

where $D_r(x_\pm)$ is the ball with center $x_\pm$ and radius r. For such a reason we call them *single-well* (normalized) states. In particular

$$\|\varphi_R\varphi_L\|_{L^\infty} = \tilde{O}(e^{-\Gamma/\hbar})$$

Let

$$\Pi = \langle \varphi_1, \cdot \rangle_{L^2} \varphi_1 + \langle \varphi_2, \cdot \rangle_{L^2} \varphi_2 \quad \text{and} \quad \Pi_c = \mathbb{I} - \Pi$$

be the projection operator onto the eigenspace orthogonal to the bi-dimensional space associated to the doublet $\{\lambda_{1,2}\}$. We will study the dynamics of equation (1) with initial data almost exactly concentrated on $\Phi_0 := \text{Span}(\varphi_1, \varphi_2)$.

REMARK 6. *If one takes initial data ψ^0 in Φ_0, i.e. of the form*

$$\psi^0 = \zeta_1 \varphi_1 + \zeta_2 \varphi_2 = \zeta_R \varphi_R + \zeta_L \varphi_L, \quad \zeta_R = \frac{\zeta_1 + \zeta_2}{\sqrt{2}}, \quad \zeta_L = \frac{\zeta_1 - \zeta_2}{\sqrt{2}}$$

then the linear *Schrödinger equation*

$$\begin{cases} i\hbar \dot{\psi}^t = H_0 \psi^t, \\ \psi^t(x)|_{t=0} = \psi^0(x) \in L^2(\mathbb{R}^d), \ \Pi_c \psi^0 = 0, \end{cases}$$

has an explicit solution given by

$$\psi^t(x) = e^{-i\Omega t/\hbar} \left[(\zeta_R \varphi_R + \zeta_L \varphi_L) \cos(\omega t/\hbar) + i (\zeta_L \varphi_R + \zeta_R \varphi_L) \sin(\omega t/\hbar) \right]$$

where

(10) $$\Omega = \frac{\lambda_1 + \lambda_2}{2} \ , \quad \omega = \frac{\lambda_2 - \lambda_1}{2}$$

That is $\psi^t(x)$ performs a beating motion *with* beating period

$$T = \frac{2\pi\hbar}{\omega}$$

Such a period usually plays the role of unit of time.

2.4. The nonlinear system. To introduce the analytic framework in which we will work we first give the following

DEFINITION 1. *For any integer number $s \geq 0$ we define the Hilbert space $\mathcal{X}_s := D(H_0^{s/2})$ equipped with the norm*

$$\|\psi\|_s^2 := \|H_0^{s/2}\psi\|_{L^2}^2 \equiv \langle H_0^s \psi, \psi \rangle_{L^2}$$

REMARK 7. *Here we will use the energy space $\mathcal{X}_1$. In particular, the Gagliardo-Niremberg inequality yields the following*

$$\|\psi\|_{L^{2\sigma+2}} \leq \frac{C}{\hbar^{e_\sigma}} \|(-\hbar^2 \Delta)^{1/2} \psi\|_{L^2}^{e_\sigma} \cdot \|\psi\|_{L^2}^{1-e_\sigma}$$

where $\|\psi\|_{L^2} = 1$ and $e_\sigma = \sigma d/(2\sigma + 2)$. Hence, we can conclude that

$$\|\psi\|_{L^{2\sigma+2}} \leq \frac{C}{\hbar^{e_\sigma}} \|\psi\|_1^{e_\sigma}$$

since

$$\left\| \left(-\hbar^2 \Delta \right)^{\frac{1}{2}} \psi \right\|_{L^2}^2 = \langle \psi, -\hbar^2 \Delta \psi \rangle \leq \langle \psi, H_0 \psi \rangle = \|\psi\|_1^2.$$

3. Main Results

Let ω be the splitting (8) (which satisfies the asymptotic estimate (9)), and let ϵ be the strength of the non-linear term. The norm $\|\varphi_{1,2}^{\sigma+1}\|_{L^2}^2$ of the unperturbed eigenvectors $\varphi_{1,2}$ is of order $\hbar^{-d\sigma/2}$ [**8**].

HYPOTHESIS 2. *We assume that the non linear pertutbation is of the order of the splitting; that is we assume that the real-valued parameter ϵ depends on $\hbar$ in such a way*

$$(11) \qquad \frac{|\epsilon|\hbar^{-d\sigma/2}}{\omega} \leq C, \quad \forall \hbar \in (0, \hbar^\star)$$

for some positive constant C, independent of $\hbar$, and for some $\hbar^\star$.

REMARK 8. *The ratio*

$$\eta = \frac{\epsilon \hbar^{-d\sigma/2}}{\omega}$$

plays the role of effective nonlinearity parameter. The above assumption implies that $|\eta| \leq C$.

The main result of this section is the following

THEOREM 1. *Assume Hypotheses 1,2, and consider the Cauchy problem (1)–(3). Then there exist positive constants $0 < C < 1$ and γ such that, if $\hbar$ is small enough and the initial datum ψ^0 fulfills*

$$(12) \qquad \|\Pi_c \psi^0\|_1 \leq C|\epsilon|^{1/2} ,$$

then one has

$$(13) \qquad \|\Pi_c \psi^t\|_1 \leq \frac{|\epsilon|^{1/2}}{C\hbar^\gamma}, \quad \forall t \in \mathbb{R} .$$

Hence the 2-dimensional space $\Phi_0 := \Pi\left[L^2(\mathbb{R}^d)\right]$ is almost invariant. Thus one expects that corresponding to initial data satisfying (12) the dynamics is well described by the restriction of the equations of motion to Φ_0. Actually such a restricted dynamical system coincides, up to (formal) order ϵ^2, with the 2-dimensional dynamical systems

$$(14) \qquad \begin{cases} i\hbar\dot{c}_R = -\omega c_L + \Omega c_R + \epsilon C_\sigma |c_R|^{2\sigma} c_R \\ i\hbar\dot{c}_L = \Omega c_L - \omega c_R + \epsilon C_\sigma |c_L|^{2\sigma} c_L \end{cases},$$

where

$$C_\sigma = \|\varphi_R\|_{L^{2\sigma+2}}^{2\sigma+2} = \|\varphi_L\|_{L^{2\sigma+2}}^{2\sigma+2} = O(\hbar^{-d\sigma/2}),$$

which has the integral of motion

$$\mathcal{I}(c_R, c_L) = \Omega(|c_R|^2 + |c_L|^2) - \omega(\bar{c}_R c_L + \bar{c}_L c_R) + C_\sigma \frac{\epsilon}{\sigma + 1}\left(|c_R|^{2(\sigma+1)} + |c_L|^{2(\sigma+1)}\right) .$$

Moreover, such an Hamiltonian system has an independent integral of motion (the quadratic part of the Hamiltonian), and thus it is integrable. The 2–dimensional system was studied in detail in [**5**] obtaining that when the nonlinearity parameter $\eta = \frac{\hbar^{-d\sigma/2}\epsilon}{\omega}$ is large enough almost all its solution do not posses the beating property, i.e. the probability density remains concentrated in one well.

Concerning the relation between the solution of the two dimensional system and the solution of the complete system we have the following

COROLLARY 1. *Let $\varphi^a(t) = C_R\varphi_R + C_L\varphi_L$, where C_R and C_L are the solution of the 2–dimensional system (14) with initial datum $\varphi^a(0)$ with of norm 1, i.e. $|c_R|^2 + |c_L|^2 = 1$. Denote $\varphi(t) := \Pi\psi(t)$, where $\psi(t)$ is the solution of the complete system (1) with the same initial datum. Then there exist a positive C and a positive α such that the following estimate holds:*

$$\|\varphi^a(t) - \varphi(t)\|_{L^2} \le C\frac{\epsilon^{3/2}}{\hbar^\alpha}|t| \ .$$

4. Proof of the main results

Let

$$\psi^t(x) = \sum_{k=1}^\infty \zeta_k(t)\varphi_k(x),$$

and define the Hilbert spaces ℓ_s^2 of the complex sequences $\zeta = \{\zeta_k\}_{k\in\mathbb{N}}$ such that

$$\|\zeta\|_s^2 := \sum_{k\ge 1} \lambda_k^s |\zeta_k|^2 < \infty$$

and remark that in such a way we have defined the correspondence

$$\psi \in \mathcal{X}_s \leftrightarrow \zeta = \mathcal{U}(\psi) \in \ell_s^2$$

which is a unitary isomorphism.

In terms of these variables the norm and quadratic part $\mathcal{E}_0$ of the Hamiltonian are given by

$$\mathcal{N} = \sum_{k\ge 1} |\zeta_k|^2 = \|\zeta\|_0^2 \quad \text{and} \quad \mathcal{E}_0 = \sum_{k\ge 1} \lambda_k |\zeta_k|^2 = \|\zeta\|_1^2.$$

REMARK 9. *In order to simplify the notations,* **we rescale time by the transformation** $t \mapsto t/\hbar$. *With such a notation the beating period is now given by*

$$T = \frac{2\pi}{\omega}$$

4.1. Variational results. We recall that we work here in the energy space $\mathcal{X}_1$. Thus, in this section, norms and distances will always be in this space.

To exploit the fact that both $\mathcal{E}_\epsilon$ and $\mathcal{N}$ are conserved along the flow we have to introduce a few geometrical lemmas.

Denote

$$\mathcal{H}_0(\psi) := \Omega(|\zeta_1|^2 + |\zeta_2|^2) + \sum_{k\ge 3} \lambda_k |\zeta_k|^2 = \sum_{k\ge 1} \nu_k |\zeta_k|^2$$

and

$$\mathcal{P}_\epsilon(\psi) := \omega(|\zeta_2|^2 - |\zeta_1|^2) + \epsilon P(\psi) \ ,$$

where $\nu_1 = \nu_2 = \Omega$, $\nu_k = \lambda_k$ for $k \ge 3$ and Ω and ω are defined in (10), so that $\mathcal{E}_\epsilon = \mathcal{H}_0 + \mathcal{P}_\epsilon$.

In this section we will almost always use real coordinates p_j, q_j defined by

$$\zeta_j = \frac{q_j + ip_j}{\sqrt{2}} \ ,$$

so all the functions will be considered as functions of ψ, (p, q), or ζ_j according to convenience.

Define the (smooth) surface

$$\mathcal{S} := \{\psi \in \mathcal{X}_1 \ : \ \mathcal{N}(\psi) = 1\} \ ,$$

and consider the function $h_0 := \mathcal{H}_0\big|_{\mathcal{S}}$.

LEMMA 1. *The manifold*

$$N := \mathcal{S} \cap \Pi\left(L^2(\mathbb{R}^d)\right) =$$

$$= \left\{\psi \in \mathcal{X}_1 \ : \ \psi = \zeta_1\varphi_1 + \zeta_2\varphi_2 \ , \quad |\zeta_1|^2 + |\zeta_2|^2 = \frac{p_1^2 + q_1^2 + p_2^2 + q_2^2}{2} = 1\right\}$$

is an absolute minimum of h_0. Furthermore, for any point $\psi \in N$ decompose the tangent space $T_\psi\mathcal{S}$ as

$$T_\psi\mathcal{S} = T_\psi N \oplus (T_\psi N)^\perp.$$

Then, the second differential $\mathrm{d}_\psi^2 h_0$ of h_0 at a point $\psi \in N$ is such that

$$(15) \qquad \mathrm{d}_\psi^2 h_0(X, X) \geq C\hbar\|X\|_1^2 \ , \quad \forall X \in (T_\psi N)^\perp$$

REMARK 10. *Since the function h_0 is smooth one also has*

$$(16) \qquad \mathrm{d}_\psi^2 h_0(X, X) \leq C\|X\|_1^2 \ , \quad \forall X \in (T_\psi N)^\perp$$

with a suitable C.

PROOF. It is a trivial application of the method of the Lagrange multipliers. Consider $\mathcal{H}_0 + \lambda\mathcal{N}$; the critical points of h_0 are obtained by finding the zeros (on $\mathcal{S}$) of the equations

$$(17) \qquad \frac{\partial(\mathcal{H}_0 + \lambda\mathcal{N})}{\partial p_j} = \frac{1}{2}(\nu_j + \lambda)p_j \ ,$$

where $\nu_j = \Omega$ for $j = 1, 2$ and $\nu_j = \lambda_j$ for $j \geq 3$, and of the analogous equation for q_j. Thus a solution of (17) is given by $\lambda = -\Omega$ and $\psi \in N$. It follows that N is constituted by critical points of h_0. It follows that the second differential of h_0 at such points is well defined. Moreover, we recall that, given a vector

$$Y = \sum_{j \geq 1}(Q_j + iP_j)\varphi_j \in T_\psi\mathcal{S},$$

one has

$$\mathrm{d}_\psi^2 h_0(Y, Y)$$
$$= \sum_{j,l}\left(P_j P_l \frac{\partial^2(\mathcal{H}_0 + \lambda\mathcal{N})}{\partial P_j \partial P_l} + 2P_j Q_l \frac{\partial^2(\mathcal{H}_0 + \lambda\mathcal{N})}{\partial P_j \partial Q_l} + Q_j Q_l \frac{\partial^2(\mathcal{H}_0 + \lambda\mathcal{N})}{\partial Q_j \partial Q_l}\right)$$
$$= \sum_{j \geq 1}(\nu_j + \lambda)\left(P_j^2 + Q_j^2\right)$$

where $\lambda = -\Omega$ is the Lagrange multiplier determined from the criticality condition. By the condition $Y \in (T_\psi N)^\perp$ one has $P_j = Q_j = 0$ for $j = 1, 2$ and thus one has

$$\mathrm{d}_\psi^2 h_0(Y, Y) \geq \sum_{j \geq 3} C\hbar\left(P_j^2 + Q_j^2\right) = C\hbar\|Y\|_1^2 \ , \quad \forall Y \in (T_\psi N)^\perp$$

since (7), and therefore the claim on the second differential follows. In particular N is a minimum of h_0. In a similar way one can show that all the other critical points of h_0 are saddle points. $\qquad\square$

REMARK 11. *By definition it follows that*

$$h_0|_N \equiv \Omega.$$

LEMMA 2. *There exists a positive C such that, provided*

$$(18) \qquad h_0(\psi) - \Omega < \frac{1}{C}\hbar^\beta, \quad \text{for some } \beta > 3,$$

then one has

$$(19) \qquad \frac{\hbar}{C}\left[d(\psi, N)\right]^2 \le h_0(\psi) - \Omega \le C\left[d(\psi, N)\right]^2 .$$

PROOF. This is a standard result in differential geometry; we give here its simple proof for the sake of completeness. Actually it is based on the use of the exponential coordinates (see appendix A for their construction), which are coordinates

$$\psi \to (n, w) \in N \times (T_{(n,0)}N)^\perp$$

in which the intersection of N with the domain of definition of the coordinates coincides with $w = 0$; moreover for any $\psi = (n, w)$ one has

$$d(\psi, N) := d\left((n, w); N\right) = \|w\|_1 .$$

where the distance is as usual defined as the length of the shortest geodesic from ψ to N. Using these coordinates, consider the Taylor expansion in w, at a point of N, of the function

$$(20) \qquad h_0(n, w) - h_0(n, 0) = \mathrm{d}^2_{(n,0)}h_0(w, w) + O(\|w\|_1^3) ,$$

where $h_0(n, w) = h_0(\psi)$ and $h_0(n, 0) \equiv \Omega \equiv h_0|_N$. From this fact and from (15) and (18) then the left hand side inequality (19) follows. The right hand side inequality of (19) follow from (16) and (20). $\qquad\square$

COROLLARY 2. *Let $\psi \in \mathcal{S}$ such that $\|\Pi_c\psi\|_1 = \mu = O(\hbar^{\beta/2})$ for some $\beta > 3$, then*

$$(21) \qquad C\hbar^{\frac{1}{2}}\mu \le d(\psi, N) \le C\hbar^{-\frac{1}{2}}\mu$$

for some $C > 0$.

PROOF. Indeed, since

$$\begin{aligned} h_0(\psi) &= \Omega\left(|\zeta_1|^2 + |\zeta_2|^2\right) + \sum_{k\ge 3}\lambda_k|\zeta_k|^2 \\ &= \Omega\left(|\zeta_1|^2 + |\zeta_2|^2\right) + \|\Pi_c\psi\|_1^2 \\ &= \Omega - \Omega\|\Pi_c\psi\|_0^2 + \|\Pi_c\psi\|_1^2 \end{aligned}$$

then

$$h_0(\psi) - \Omega = \|\Pi_c\psi\|_1^2 - \Omega\|\Pi_c\psi\|_0^2 \le \|\Pi_c\psi\|_1^2 = \mu^2 .$$

From this fact and from Lemma 2 the right hand side inequality (21) follows. Similarly

$$h_0(\psi) - \Omega = \sum_{j\ge 3}(\lambda_j - \Omega)|\zeta_j|^2 \ge C\hbar\sum_{j\ge 3}\lambda_j|\zeta_j|^2 \ge C\hbar\|\Pi_c\psi\|_1^2$$

from which the left hand side inequality (21) follows.   □

Proof of theorem 1. First remark that $\psi^0 \in \mathcal{S}$ and $\|\Pi_c \psi^0\|_1 = \mu = O(\epsilon^{1/2})$ implies (see Corollary 2) $d(\psi^0, N) < C\hbar^{-1/2}\mu = \tilde{O}(\epsilon^{1/2})$. Then, remark that from (11) then

$$
\begin{aligned}
\mathcal{E}(\psi^0) &= \|\psi_0\|_1^2 + \frac{\epsilon}{1+\sigma}\|\psi_0^{\sigma+1}\|_{L^2}^2 \\
&= \|\Pi\psi_0\|_1^2 + O(\epsilon^{1/2}) = \Omega + O(\epsilon^{1/2})
\end{aligned}
$$

and that, by conservation of energy and Remark 7 one has $\|\psi(t)\|_1 \le 2\Omega$ for all times. From this fact and from Remark 7 one also has the following a priori estimate

$$
|\mathcal{P}_\epsilon(\psi(t))| \le C\frac{\epsilon}{\hbar^\beta}
$$

for some β; thus, using (19) one has the chain of inequalities

$$
\begin{aligned}
[d(\psi(t), N)]^2 &\le \frac{C}{\hbar}[h_0(\psi(t)) - \Omega] \\
&\le \frac{C}{\hbar}\left[\left(h_0(\psi^0) - \Omega\right) + \left(\mathcal{E}_\epsilon(\psi(t)) - \mathcal{E}_\epsilon(\psi^0)\right) + \left(\mathcal{P}_\epsilon(\psi^0) - \mathcal{P}_\epsilon(\psi(t))\right)\right] \\
&\le \frac{C}{\hbar}\left[\left(h_0(\psi^0) - \Omega\right) + \left(\mathcal{P}_\epsilon(\psi^0) - \mathcal{P}_\epsilon(\psi(t))\right)\right] \le \frac{C}{\hbar^{\beta+1}}\epsilon .
\end{aligned}
$$

From this fact and from (21) then the claim follows.   □

Finally, Corollary 1 immediately follows by comparing the two-level approximation (14) with (1) and by means of estimate (13) and standard Gronwall's Lemma arguments (see e.g. [**8**]).

Appendix A. Construction of exponential coordinates

Let M and N be Riemannian manifolds modeled on Hilbert spaces H and K, with norms $\|\cdot\|_H$ and $\|\cdot\|_K$; denote by g the metric of M; let $i : N \to M$ be a smooth isometric embedding. In the following, for the sake of simplicity, we will identify N and with $i(N)$, and similarly for related objects and spaces (as TN).

LEMMA 3. *Let x_0 be a point of N and let $W = (T_{(x_0)}N)^\perp$, then there exists a coordinate system of M defined in a neighborhood $\mathcal{U} \subset M$ of x_0 with the following properties:*

    i. $\mathcal{U} \ni x \mapsto (n, w) \in N \times W$;
    ii. *let $d(x, N)$ be the distance usually defined as the length of the shortest geodesic from $x \in N$ to N; then $d((n, w); N) = \|w\|_K$.*

PROOF. We proceed in some steps. To start with we choose a coordinate system (n, w_1) with origin $x_0 \in N$ such that, if $(n, w_1) \in \mathcal{V}_1 \subset N \times W$, where $\mathcal{V}_1$ is a neighborhood of x_0; then the intersection of N with the domain of definition of the coordinate system coincides with the set $(n, 0)$. Let

$$
\Pi_n : \mathcal{V}_1 \subset N \times W \to \left(T_{(n,0)}N\right)^\perp
$$

be the orthogonal projector with respect to the scalar product $g_{(n,0)}$. Define the map

$$
\mathcal{V}_1 \ni (n, w_1) \mapsto (n, \Pi_n w_1) \in \mathcal{V} .
$$

If $\mathcal{V}_1$ is small enough, then such a map is an isomorphism on its image, since its differential at the origin is invertible. Thus it defines a new coordinate system. Let $(n,0) \in V_1$, then in these coordinates one has

$$T_{(n,0)}N = \{(X_1, X_2) \in N \times W \ : \ X_2 = 0\}$$
$$(T_{(n,0)}N)^\perp = \{(X_1, X_2) \in N \times W \ : \ X_1 = 0\}$$

We use such a coordinate system in order to define the needed coordinate system. Take $(n,w) \in N \times W$ small enough, and consider the geodesic $\gamma_{(n,w)}(s)$ starting from $(n,0)$ with initial velocity w. Consider the (exponential) map

$$(n,w) \mapsto \gamma_{(n,w)}(1) \ ,$$

by implicit function theorem it is locally invertible (its differential at the origin is the identity), and thus any point x of a neighborhood $\mathcal{U}$ of x_0 can be represented uniquely by the points (n,w) such that $\gamma_{(n,w)}(1) = x_0$. Remark that moreover one has

$$(22) \qquad \ell(\gamma) := \int_0^1 \sqrt{g(\dot\gamma(s), \dot\gamma(s))} ds = \|w\|_K$$

since $\dot\gamma(0) = \|w\|_K$ and $g(\dot\gamma(s), \dot\gamma(s))$ is independent of s along geodesic lines.

In the coordinate system just introduced, let $x = (n,w)$ then its distance from N is the length of the shortest geodesic joining x to N. In turn such a geodesic is perpendicular to N. Thus $(n,0)$ is the point where it starts and w is the tangent vector at such a point. Then property ii. follows from (22). $\qquad\square$

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