EXPONENTIAL TIMES IN THE ONE-DIMENSIONAL GROSS–PETAEVSKII EQUATION WITH MULTIPLE WELL POTENTIAL

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Abstract. We consider the Gross-Petaevskii equation in 1 space dimension with a n-well trapping potential. We prove, in the semiclassical limit, that the finite dimensional eigenspace associated to the lowest n eigenvalues of the linear operator is slightly deformed by the nonlinear term into an almost invariant manifold $\mathcal{M}$. Precisely, one has that solutions starting on $\mathcal{M}$, or close to it, will remain close to $\mathcal{M}$ for times exponentially long with the inverse of the size of the nonlinearity. As heuristically expected the effective equation on $\mathcal{M}$ is a perturbation of a discrete nonlinear Schrödinger equation. We deduce that when the size of the nonlinearity is large enough then tunneling among the wells essentially disappears: that is for almost all solutions starting close to $\mathcal{M}$ their restriction to each of the wells has norm approximatively constant over the considered time scale. In the particular case of a double well potential we give a more precise result showing persistence or destruction of the beating motions over exponentially long times. The proof is based on canonical perturbation theory; surprisingly enough, due to the Gauge invariance of the system, no non-resonance condition is required.

1. Introduction

In this paper we study the dynamics of low energy states of the one-dimensional Gross-Petaevskii equation (hereafter also called nonlinear Schrödinger equation, NLS)

$$\left\{ \begin{array}{l} i\hbar\dot{\psi}^t = H_0\psi^t + \epsilon \left|\psi^t\right|^{2\sigma} \psi^t, \ \dot{\psi}^t = \frac{\partial \psi^t}{\partial t}, \\ \psi^t(x)|_{t=0} = \psi^0(x) \in L^2(\mathbb{R}), \ \|\psi^0\|_{L^2} = 1, \end{array} \right. \tag{1}$$

where σ is a positive integer number and

$$H_0 = -\hbar^2 \frac{d^2}{dx^2} + V, \ x \in \mathbb{R}, \tag{2}$$

is the linear Hamiltonian operator and $V(x)$ a n–well potential. By this we mean that V has n nondegenerate distinct minima $x_1, ..., x_n$ where the potential has essentially the same behavior (e.g. one can assume that its first r derivatives are equal at all the minima, for some positive integer $r \geq 4$). We also assume that the potential is trapping, i.e. V tends to infinity as $|x| \to \infty$. The situation

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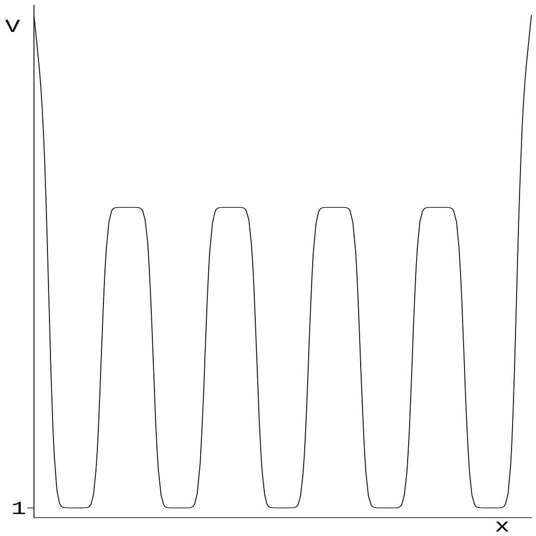

FIGURE 1. Plot of a trapping potential with n wells.

we have in mind is that of a Bose Einstein condensate trapped by an unbounded potential and also subjected to a periodic-like force field (see Figure 1); in such a case the parameter ϵ can be thought as a measure of the number of particles in the condensate (see, e.g. [23]).

Consider first the linearized problem. The fundamental state of H_0 is approximatively degenerate in the sense that, denoting by

$$\lambda_1 < \lambda_2 < ... < \lambda_n < ...$$

the eigenvalues of H_0, one has

$$\lambda_n - \lambda_1 \ll \lambda_{n+1} - \lambda_n$$

in the semiclassical limit, i.e. $\hbar \ll 1$. Then the most interesting situation occurs when the normalized eigenfunctions $\varphi_1, ..., \varphi_n$, corresponding to $\lambda_1, ..., \lambda_n$, are delocalized among the wells. Indeed, in such a case a solution in $\Phi_0 :=\text{span}(\varphi_1, ..., \varphi_n)$ performs a quasiperiodic motion and the probability of finding the particle in any fixed well undergoes great changes over a time scale of the order of $T = \pi\hbar/\omega$ with $\omega = (\lambda_n - \lambda_1)/2$. In the case of double well potential such a phenomenon is usually known as beating motion and the beating period is given by $T := \pi\hbar/\omega$, with $\omega = (\lambda_2 - \lambda_1)/2$.

The main question is the behavior of the system when the nonlinearity is restored. In the case of a double well potential the problem was tackled in a series of papers [1, 7, 10, 11, 17, 20, 21, 24, 25, 27]; in particular, it was shown that, up to times of order T, the dynamics is well described by an Hamiltonian integrable system with two degrees of freedom obtained by restricting the Hamiltonian, i.e. the energy of the system, to Φ_0. In particular, this result has been used in order to show that the beating motion is generic for values of the nonlinearity strength ϵ below a certain threshold value, while new localized states appear for larger nonlinearity strength (i.e. as the number of particles of a Bose-Einstein condensate increase) and for even larger values of the nonlinearity strength the beating motion disappears.

In the case of a multiple well potential the situation was studied e.g. in the paper [23] where the authors deduced (formally) the discrete nonlinear Schrödinger as an effective equation for the dynamics in Φ_0 and used it in order to study some of the features of the model. We are not aware of rigorous results in the case of a multiple well potential.

In the present paper we study the nonlinear dynamics using the methods of Hamiltonian perturbation theory for PDEs [3, 4, 5, 13] and we prove that the manifold Φ_0, which is invariant for the linear dynamics, is only slightly deformed by the nonlinearity into a new manifold $\mathcal{M}$ which is *approximatively invariant* for the complete dynamics. By this statement we mean that solutions starting on $\mathcal{M}$, or close to it, will remain close to $\mathcal{M}$ for times which are exponentially long with T; this result improves the one given by [7, 20, 21] for double well potentials where the control of the approximate solution was given for times of order T. Moreover we show (see Lemma 1) that the dynamics on $\mathcal{M}$ is described at first order by a discrete nonlinear Schrödinger equation

$$i\dot{\psi}_j = \delta_j\psi_j + \Lambda_j\psi_{j+1} + \Lambda_{j-1}\psi_{j-1} + \eta\psi_j\left|\psi_j\right|^{2\sigma} \ \ , \ j = 1, ..., n, \tag{3}$$

where $\psi_0 = \psi_{n+1} := 0$, $\Lambda_j, \delta_j, \eta$ are suitable constants and where, having in mind the case of Bose-Einstein condensates, $|\psi_j|^2$ represents the fraction of particles in the j-th well for $j = 1, ..., n$ (see Sect. 2.4 for their precise definition). In particular, it is quite easy to study the discrete NLS (3) from the anticontinuum limit [14] obtaining that when η is large enough then solutions corresponding to almost all initial data have the property that $|\psi_j|^2$ is essentially a constant of motion. In the case of double well potential, we get that the dynamics on $\mathcal{M}$ is (up to an exponentially small error) that of an integrable Hamiltonian system with two degrees of freedom. This allows us to control also the trajectories of the solutions on $\mathcal{M}$ showing that for small η the beating phenomenon persists for exponentially long times, while for higher values of η only motions which are essentially localized in one of the two wells exist, at least for exponentially long times.

We emphasize that from the technical point of view the main result (Theorem 2) is quite surprising since the application of canonical perturbation theory is typically possible only when some non-resonance conditions are satisfied. On the contrary, here the result is valid for *any* multiple well potential, whose eigenvalues might fulfill arbitrary resonance conditions (i.e. the eigenvalues can be linearly dependent over the relative integers). This is possible since NLS is an infinite dimensional Gauge invariant Hamiltonian system. To explain how this property is exploited we recall that canonical perturbation theory allows us to remove from the Hamiltonian all non-resonant monomials. In particular, given an arbitrary monomial it can be eliminated if it is non-resonant. However, in NLS only Gauge invariant monomials appear, and we will show that, for a Gauge invariant monomial, the non-resonance condition is (almost) trivially fulfilled. Actually, in order to avoid any restriction on the potential we have to use a resonant construction which is not self evident a priori (see Subsection 3.2). We think that these ideas could be useful in the study of Hamiltonian systems with symmetry, and possibly also for the investigation of further dynamical properties of NLS. A further technical ingredient which is fundamental for the proof is the use of Sobolev like spaces constructed as the domains of the powers of H_0. To use such spaces one has to show that they form Banach algebras under the pointwise multiplication. Here we give a detailed proof of such a property that we think could be useful in further investigations of NLS.

The paper is organized as follows. In Section 2 we state our main results (Theorem 2, Theorem 3 and their corollaries). Section 2 is divided into 5 subsections: in Subsection 2.1 we review some known facts about the structure of the low lying eigenvalues of the linear Schrödinger equation with an n well potential; in Subsection 2.2 we introduce the Sobolev like spaces in which NLS equation will be studied and give their main properties; in Subsection 2.3 we will state the result on the approximate invariant manifold; in Subsection 2.4 we will give the effective equation on the approximatively invariant manifold and deduce the localization properties of the solutions; finally in Subsection 2.5 we will study the particular case of a double well potential. In Section 3 we prove our main results. This section is also divided into 6 subsections that correspond to the different parts of the proof. The proof of Theorem 1 (algebra property of Sobolev like spaces) and of some technical Lemmas are left to appendixes A and B respectively.

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2. Main results

2.1. Linear theory.

Hypothesis 1. *The potential $V(x) \in C^\infty(\mathbb{R})$ is a real valued function such that:*

i. *$V(x)$ admits n minima at $x_1 < x_2 < \ldots < x_n$ such that*

$$V(x) > V_{min} = V(x_j) = 1, \quad \forall x \in \mathbb{R},\ x \neq x_j,\ j = 1, \ldots, n; \tag{4}$$

ii. *There exists a constant $C > 1$ such that*

$$C^{-1} \langle x \rangle^2 \leq V(x), \ \langle x \rangle = \sqrt{1 + x^2};$$

iii. *There exists a positive $m \geq 2$ such that for any $k \in \mathbb{N}$*

$$\left| \frac{d^k V(x)}{dx^k} \right| \leq C_k \langle x \rangle^{m-k}$$

for some positive constant C_k;

iv. *The minima are nondegenerate and*

$$\frac{d^2 V(x_j)}{dx^2} = C > 0 \tag{5}$$

with C independent of j;

v. *The shape of the potential at the bottom of the minimum x_j is approximatively independent of j; precisely: there exists $r \geq 4$ such that*

$$\frac{d^k V}{dx^k}(x_j) = \frac{d^k V}{dx^k}(x_i), \quad \forall i, j = 1, 2, \ldots, n, \quad \forall k = 2, \ldots, r. \tag{6}$$

Hereafter, C will always denote a positive, typically large, constant whose value changes from line to line, and which is independent of $\hbar$, ϵ and t.

The operator H_0 formally defined by (2) admits a self-adjoint realization (still denoted by H_0) on $L^2(\mathbb{R})$ (Theorem III.1.1 in [9]) with purely discrete spectrum. Let λ_k, $k \in \mathbb{N}$, be the non degenerate eigenvalues of H_0

$$\lambda_1 < \lambda_2 < \lambda_3 < \lambda_4 < \ldots < \lambda_k < \ldots, \ \lambda_k \stackrel{k \uparrow \infty}{\to} \infty,$$

with associated normalized (in L^2) eigenvectors $\varphi_k(x)$; the set $\{\varphi_k(x)\}_{k=1}^\infty$ is an orthonormal base of L^2.

The lowest part of the spectrum can be studied in the semiclassical limit using the construction of [12], that we shortly recall.

Having fixed a positive constant $a > 1 = V_{min}$ we consider the set $V^{-1}((-\infty, a))$ and we assume that a is such that this set is the union of n disjoint open sets $\mathcal{U}_j$ with $x_j \in \mathcal{U}_j$. Having fixed j we consider the operator formally defined on L^2 as

$$H_j = -\hbar^2 \frac{d^2}{dx^2} + V_j$$

where V_j is a modified potential defined as

$$V_j(x) = \begin{cases} V(x) & \text{for } \ x \in \mathcal{U}_j \\ \max[a, V(x)] & \text{for } \ x \notin \mathcal{U}_j \end{cases} \tag{7}$$

Let $\hat{\lambda}_j$ be the lowest eigenvalue of H_j with associated normalized eigenvector $\hat{\varphi}_j$. Using the semiclassical construction of the eigenvalues close to the bottom of a well (see e.g. [6, 22]) one has that assumption Hyp. 1 v., implies that

$$\hat{\lambda}_j = 1 + O(\hbar), \ |\hat{\lambda}_j - \hat{\lambda}_i| \le C\hbar^{r/2}$$

and

$$\|\hat{\varphi}_j(x) - \hat{\varphi}_i(x + x_i - x_j)\|_{L^2} \le C\hbar^{r/2},$$

for any $i, j = 1, 2, \ldots, n$.

Let

$$\Gamma_j = \int_{x_j}^{x_{j+1}} \sqrt{V(x) - 1} dx, \ j = 1, 2, \ldots, n-1,$$

be the Agmon distance among the two minima x_j and x_{j+1}. Let Γ any fixed positive real number such that $\Gamma < \min_j \Gamma_j$. Then, from the theory of [12] there exist some constants c_{ij} such that for any i and j

$$\left\| \varphi_j - \sum_{k=1}^n c_{kj} \hat{\varphi}_k \right\|_{L^2} \le C e^{-\Gamma/\hbar}, \tag{8}$$

$$\|\hat{\varphi}_j \hat{\varphi}_i\|_{L^\infty} \le C e^{-\Gamma/\hbar}, \ i \ne j, \tag{9}$$

$$|\lambda_{i_j} - \hat{\lambda}_j| \le C e^{-\Gamma/\hbar} \ \text{ for some } \ i_j \in \{1, ..., n\}\,. \tag{10}$$

Moreover, the projector $\hat{\Pi}$ on $\hat{\Phi}_0$:=span$(\hat{\varphi}_j)$ is a bijection among Φ_0 :=span(φ_j) and $\hat{\Phi}_0$ itself. Remark also that one can choose the functions $\hat{\varphi}_j$ to be real valued.

Hence, the lowest n eigenvalues of H_0 fulfill

$$C^{-1}\hbar < \lambda_j - 1 < C\hbar \ , \quad j = 1, ..., n,$$

for some $C > 1$ and

$$\omega = \frac{1}{2}(\lambda_n - \lambda_1) \le C\hbar^{r/2} \tag{11}$$

Furthermore, making use of the same arguments, it follows also that

$$\inf_{j=1,\ldots,n} \ \inf_{\lambda \in \sigma(H_0) - \{\lambda_1, \ldots, \lambda_n\}} [\lambda - \lambda_j] \ge C^{-1}\hbar \tag{12}$$

We also use the following projectors

$$\Pi = \sum_{j=1}^n \langle \varphi_j, \cdot \rangle \varphi_j \quad \text{and} \quad \Pi_c = \mathbb{I} - \Pi \quad \text{and} \quad \Phi_0 = \Pi L^2;$$

Remark 1. *As already emphasized in the introduction the most interesting situation occurs when the true eigenfunctions φ_j are delocalized between the wells, a property that occurs if the potential is exactly periodic in some region or more generally if the order of magnitude of some the off diagonal elements of the matrix formed by the constants c_{ij} is of the same order of magnitude as the difference between the approximate eigenvalues $\hat{\lambda}_j$, a property that is quite difficult to ensure in a general situation. For this reason, essentially in order to fix ideas, we decided to state our assumptions in the form (i-v) above.*

2.2. **The nonlinear system: Analytic framework and well posedness.**

Definition 1. *For any integer $s \geq 0$ define the Hilbert space $\mathcal{X}^s := D(H_0^{s/2})$ endowed by the graph norm; more precisely in $\mathcal{X}^s$ we will use the following norm equivalent to the graph norm*

$$\|\phi\|_s^2 := \left\| H_0^{s/2}\phi \right\|_{L^2}^2 \equiv \langle H_0^s \phi, \phi\rangle_{L^2} = \int_{\mathbb{R}} \bar{\phi} H_0^s \phi \mathrm{d}x, \ \phi \in \mathcal{X}^s. \tag{13}$$

The main step for the proof that the spaces $\mathcal{X}^s$ form a Banach algebra under the pointwise multiplication is the following Theorem.

Theorem 1. *Let s be any positive integer number. For small enough $\hbar$ the two norms*

$$\|\phi\|_s^2 \quad \text{and} \quad \|(-\hbar^2\Delta)^{s/2}\phi\|_{L^2}^2 + \|V^{s/2}\phi\|_{L^2}^2 \tag{14}$$

are equivalent with an $\hbar$ independent constant.

The proof, which is a semiclassical variant of the proof of Lemma 7.2 of [26], is deferred to Appendix A.

Remark 2. *In particular one has that a function ϕ is in $\mathcal{X}^s$ if and only if it belongs to the Sobolev space H^s and it decays at infinity so fast that $|\phi|^2 V^s$ is integrable.*

In the spaces $\mathcal{X}^s$ with $s \geq 1$ the system (1) is semilinear, since, using (14) and Gagliardo-Niremberg inequality one has

Corollary 1. *For any integer $s \geq 1$ there exists a positive constant C_s independent of $\hbar$, such that*

$$\|\phi_1\phi_2\|_s \leq C_s \hbar^{-1/2} \|\phi_1\|_s \|\phi_2\|_s, \quad \forall \phi_1, \phi_2 \in \mathcal{X}^s, \ \hbar \ll 1. \tag{15}$$

Moreover, the map

$$\mathcal{X}^s \times \mathcal{X}^s \ni (\phi, \bar{\phi}) \mapsto |\phi|^{2\sigma}\phi \in \mathcal{X}^s$$

is entire analytic map for any $\hbar > 0$ and fulfills

$$\left\| |\phi|^{2\sigma}\phi \right\|_s \leq C_s \hbar^{-\sigma} \|\phi\|_s^{2\sigma+1}. \tag{16}$$

Remark 3. *In dimension $d > 1$ this result remains valid provided $s > d/2$.*

Then by standard Segal theory (see e.g. [16]) the system (1) is locally well posed in all the spaces $\mathcal{X}^s$ with $s \geq 1$. Actually $s > d/2$ is enough, but our proof only applies to integer values of s; in [26] a Strichartz inequality argument was used to show that it is also locally well posed (LWP) in $\mathcal{X}^s$ with some s smaller than $d/2$.

From now on we assume that the index s of the space is a fixed positive integer number and fulfills the condition $s \geq 1$. In the following, in order to fix ideas, one can just think of the case $s = 1$. We will denote by $d(.;.)$ the distance in the norm of $\mathcal{X}^s$.

2.3. **The nonlinear system: Approximatively invariant manifold.** In order to state our main result we assume that the size of the nonlinearity is small enough, i.e. $|\epsilon| \ll \hbar^\sigma$, and we introduce the small parameter.

$$\mu := \omega + \frac{|\epsilon|}{\hbar^\sigma} \ll 1, \tag{17}$$

where ω was defined in (11).

Theorem 2. *Consider the system* (1) *and fix a positive* $s \geq 1$. *There exists a positive* μ_* *such that, if* $\mu < \mu_* \hbar^{3/2}$, *then there exists a manifold* $\mathcal{M}$ *(dependent on all the parameters of the system) with the following properties:*

i. $\mathcal{M}$ *is close to* Φ_0, *i.e.*

$$d(\Phi_0, \mathcal{M}) \leq C\frac{\mu}{\hbar^{3/2}}, \tag{18}$$

where

$$d(\Phi_0, \mathcal{M}) = \sup_{\psi \in \Phi_0} \inf_{\varphi \in \mathcal{M}} \|\psi - \varphi\|_s,$$

and where $\|\varphi\|_s$ *is the norm* (13).

ii. *Let*

$$d_0 = d(\psi^0, \mathcal{M}) = \inf_{\varphi \in \mathcal{M}} \|\psi^0 - \varphi\|_s$$

be the initial distance from $\mathcal{M}$ *and let*

$$\delta = \max\left\{ d_0, \exp\left[-\frac{\mu_* \hbar^{3/2}}{2\mu} \right] \right\} \tag{19}$$

Then for all times t *fulfilling*

$$|t| \leq \frac{1}{C\hbar\mu\delta} \tag{20}$$

one has

$$d(\psi^t, \mathcal{M}) \leq C\delta \tag{21}$$

$$\left\|\Pi_c \psi^t\right\|_s \leq C\frac{\mu}{\hbar^{3/2}} \tag{22}$$

Such a manifold $\mathcal{M}$ *is called an* approximatively invariant manifold.

Remark 4. *The most interesting cases are when*

$$\delta = \exp\left[-\frac{\mu_* \hbar^{3/2}}{2\mu} \right] \quad or \quad \delta = C\frac{\mu}{\hbar^{3/2}}.$$

Indeed in the first case the time of validity of all the estimates is exponentially long, while in the second case it is easy to obtain the following Corollary.

Corollary 2. *Assume that* $\left\|\Pi_c \psi^0\right\|_s \leq C\mu\hbar^{3/2}$ *then, up to the times*

$$|t| \leq \frac{\hbar^{3/2}}{C\mu^2} \tag{23}$$

the estimate (22) *holds.*

Remark 5. *This Corollary is a direct extension of the results of* [11, 20, 21] *in which the estimate* (22) *has been proved (for the double well potential) for a time scale of order*

$$T = \frac{\pi\hbar}{\omega} \leq C\frac{\hbar}{\mu} \ll \mu^{-2}\hbar^{3/2}.$$

The improvment is due to the fact that our construction implies that $\mathcal{M}$ is linearly stable up to an exponentially small error.

2.4. **The nonlinear system: discrete NLS and suppression of tunneling.** To start with we remark that NLS is a Hamiltonian system (see Subsection 3.1 for a precise description) with Hamiltonian function given by

$$\mathcal{E}(\psi,\bar\psi) := \mathcal{E}_0(\psi,\bar\psi) + \epsilon\mathcal{P}_0(\psi,\bar\psi) \tag{24}$$

where

$$\mathcal{E}_0(\psi,\bar\psi) := \int_{\mathbb{R}} \bar\psi(x) H_0 \psi(x) dx$$

and

$$\mathcal{P}_0(\psi,\bar\psi) := \frac{1}{\sigma+1}\|\psi^{\sigma+1}\|^2_{L^2} := \frac{1}{\sigma+1}\int_{\mathbb{R}} \bar\psi^{\sigma+1}\psi^{\sigma+1} dx$$

The general idea is that for initial data close to Φ_0 the system should be well described by the Hamiltonian system obtained by restricting $\mathcal{E}$ to $\hat\Phi_0$ which is close to Φ_0. Denote

$$\psi = \sum_{j=1}^n \psi_j \hat\varphi_j \in \hat\Phi_0$$

then we have the following

Lemma 1. *The restriction of* (24) *to $\hat\Phi_0$ takes the form*

$$\begin{aligned}\mathcal{E}|_{\hat\Phi_0} \;=\; & \sum_{j=1}^n (\Omega+\nu_j)|\psi_j|^2 + \epsilon c\sum_{j=1}^n |\psi_j|^{2\sigma+2} + \sum_{j=2}^n c_j\left[\bar\psi_j\psi_{j-1} + \psi_j\bar\psi_{j-1}\right] + \\ & + O(e^{-2\Gamma/\hbar}) + \epsilon O(e^{-\Gamma/\hbar})\end{aligned}$$

where Γ was introduced before equation (8) *and*

$$\Omega = \frac{1}{n}\sum_{j=1}^n \lambda_j \ , \ \nu_j := \int_{\mathbb{R}} \bar{\hat\varphi}_j H_0 \hat\varphi_j dx - \Omega = O(\hbar^{r/2})$$

and

$$c = c(\hbar) := \frac{1}{\sigma+1}\frac{1}{n}\sum_{j=1}^n \|\hat\varphi_j\|^{2\sigma+2}_{L^{2\sigma+2}} = O\left(\hbar^{-\sigma/2}\right)$$

and

$$c_j := \int_{\mathbb{R}} \bar{\hat\varphi}_j H_0 \hat\varphi_{j-1} dx = O(e^{-\Gamma/\hbar})$$

Proof. Indeed, we have that

$$\mathcal{E}|_{\hat{\Phi}_0} = \mathcal{E}_0|_{\hat{\Phi}_0} + \epsilon\, \mathcal{P}_0|_{\hat{\Phi}_0} .$$

The first term takes the form

$$\mathcal{E}_0|_{\hat{\Phi}_0} = \sum_{j=1}^n |\psi_j|^2 d_{jj} + \sum_{|i-j|=1} \bar{\psi}_i \psi_j d_{ij} + \sum_{|i-j|\geq 1} \bar{\psi}_i \psi_j d_{ij}$$

with

$$d_{ij} = \int_{\mathbb{R}} \bar{\hat{\varphi}}_i H_0 \hat{\varphi}_j dx$$

and where (see, e.g., [12, 21]) $d_{i,j} = O(e^{-\Gamma/\hbar})$ when $|i-j| = 1$ and $d_{i,j} = O(e^{-2\Gamma/\hbar})$ when $|i-j| > 1$. For what concerns the second term, following [21] and making use of (9), we have that

$$\mathcal{P}_0|_{\hat{\Phi}_0} = \frac{1}{\sigma+1} \sum_{j=1}^n \|\hat{\varphi}_j\|^{2\sigma+2}_{L^{2\sigma+2}} |\psi_j|^{2\sigma+2} + O(e^{-\Gamma/\hbar})$$

where $\|\hat{\varphi}_j\|^{2\sigma+2}_{L^{2\sigma+2}} = O\left(\hbar^{-\sigma/2}\right)$ is approximatively independent of j. Remark also that, since the functions $\hat{\varphi}_j$ are real valued, the quantities c_j turn out to be real. □

Hence, up to higher order terms, to the Gauge transformation $\psi \to e^{i\Omega t/\hbar}\psi$ and to a rescaling of time $t \to \omega t/\hbar$ the restriction of (24) to $\hat{\Phi}_0$ is given by

$$\mathcal{K}_0 := \sum_{j=1}^n \delta_j |\psi_j|^2 + \eta \sum_{j=1}^n |\psi_j|^{2\sigma+2} + \sum_{j=1}^{n+1} \Lambda_j (\bar{\psi}_j \psi_{j-1} + \psi_j \bar{\psi}_{j-1}), \tag{25}$$

where

$$\eta = \frac{\epsilon c}{\omega} = O\left(\frac{|\epsilon|}{\omega \hbar^{\sigma/2}}\right) \ , \ \delta_j := \frac{\nu_j}{\omega} = O(1) \ , \ \Lambda_j := \frac{c_j}{\omega} = O\left(\frac{e^{-\Gamma/\hbar}}{\omega}\right)$$

and the equation of motion of (25) are given by

$$\dot{\psi}_j = -i \frac{\partial \mathcal{K}_0}{\partial \bar{\psi}_j}, \quad \text{with} \quad j = 1, ..., n.$$

The system (25) has an integral of motion (the restriction of the square of the L^2 norm to $\hat{\Phi}_0$) given by

$$\mathcal{I} := \sum_{j=1}^n |\psi_j|^2 \tag{26}$$

We analyze now the consequences of our Theorem for the dynamics. From the proof of Theorem 2 we will be able to exactly describe the restriction of the system to $\mathcal{M}$. Actually, we can state the following Theorem 3, which is a result of Theorem 6 stated below.

Theorem 3. *Under the same assumptions of Theorem 2 there exists an analytic canonical transformation $\mathcal{T} : \mathcal{U} \to \mathcal{X}^s$, with $\mathcal{U}$ an open neighborhood of Φ_0 with size independent of μ and $\hbar$, such that*

$$\mathcal{E} \circ \mathcal{T} = \Omega \mathcal{I} + \omega \mathcal{K} + \tilde{\mathcal{R}}$$

where

i. $\mathcal{K} \circ \hat{\Pi} = \mathcal{K}$, *i.e.* $\mathcal{K}$ *depends only on the variables* $\psi_1, ..., \psi_n$,
ii. $\{\mathcal{I}, \mathcal{K}\} \equiv 0$ *i.e.* $\mathcal{I}$ *is an integral of motion for the system with Hamiltonian* $\mathcal{K}$
iii. $\mathcal{K} = \mathcal{K}_0 + O(\mu/\hbar^{3/2})$
iv. $\tilde{\mathcal{R}} = O\left[\exp -\left(\frac{\mu_* \hbar^{3/2}}{2\mu}\right)\right] + O\left(\|\Pi_c \psi\|_s^2\right)$ *and similar estimates hold for its vector field.*
v. $\mathcal{T} = \mathbb{I} + O(\mu/\hbar^{3/2})$ *i.e. the transformation is close to identity.*

Remark 6. *In this framework the manifold* $\mathcal{M}$ *turns out to simply be* $\mathcal{M} = \mathcal{T}(\Phi_0)$.

In particular it follows that the dynamics on $\mathcal{M}$ is, up to a small error, the same of a Hamiltonian system with Hamiltonian function close to $\mathcal{K}_0$ with an integral of motion given by $\mathcal{I}$. Thus, it is possible to deduce the following Corollary of Theorem 7 below, which is particularly relevant in the double well case.

Corollary 3. *Under the same assumptions of Theorem 2 one also has*

$$|\mathcal{I}(t) - \mathcal{I}(0)| \leq C \frac{\mu}{\hbar^{3/2}} \ , \quad |\mathcal{K}_0(t) - \mathcal{K}_0(0)| \leq C \frac{\mu}{\hbar^{3/2}} \tag{27}$$

up to the times (20).

We focus now on the exponentially long time scale, thus we assume that the quantity δ of Theorem 2 is given by

$$\delta = \exp\left[-\frac{\mu_* \hbar^{3/2}}{2\mu}\right]$$

and from (20) it follows that up to times of order $e^{\frac{\mu_* \hbar^{3/2}}{2\mu}}$ the vector field $X_{\tilde{\mathcal{R}}}$ of $\tilde{\mathcal{R}}$ fulfills the a priori estimate

$$\|X_{\tilde{\mathcal{R}}}\|_s \leq C \exp\left[-\frac{\mu_* \hbar^{3/2}}{\mu}\right]$$

Thus, up to an exponentially small drift, a Gauge transformation and a rescaling of time the dynamics on $\mathcal{M} \equiv \mathcal{T}(\Phi_0)$ is that of the n–dimensional Hamiltonian system $\mathcal{K}$, which is a perturbation of $\mathcal{K}_0$, i.e. of the discrete NLS (25).

It is worth mentioning that when $\eta = 0$ the dynamics of $\mathcal{K}_0$ is that of n decoupled harmonic oscillators corresponding to the normal modes of the linearized system. If $\Lambda_j \ll \delta_i$, for any i and j, then the normal modes are localized, i.e. each normal mode essentially involves only one of the ψ_j; on the contrary, in the much more interesting case where the δ_j are of the same order of magnitude of the Λ_j, typically the normal modes are collective motions of the system and, correspondingly, in typical solutions the term $|\psi_j(t)|^2$ undergoes great changes for each j.

In the opposite limit $\eta \to \infty$ (anticontinuum limit, see [14]), $\mathcal{K}_0$ becomes a system of decoupled anharmonic oscillators. Correspondingly $|\psi_j(t)|^2$ is a constant of motion. One can use KAM or Nekhoroshev theory in order to study the dynamics of $\mathcal{K}$ when $1 \ll \eta < \infty$ and to deduce results on the dynamics of the complete NLS equation.

Here we will state a result that can be obtained in this way. To this end, for any $\rho > 0$ fixed, we will denote

$$\mathcal{S}_\rho^n := \left\{ (\psi_1, ..., \psi_n) \in \mathbb{C}^n \ : \ \sum_{j=1}^n |\psi_j|^2 = 1 \text{ and } |\psi_j| > \rho \ , \ \forall j \right\}$$

and we will denote by $\left|\mathcal{S}_\rho^n\right|$ its Lebesgue measure.

Theorem 4. *(KAM theorem $\mathcal{K}$) Consider the Hamiltonian system $\mathcal{K}$, then there exists a constant $\eta_\star$, such that, for any $|\eta| > \eta_\star$ there exists a set $\mathcal{S}_\eta \subset \mathcal{S}_\rho^n$ with Lebesgue measure estimated by*

$$|\mathcal{S}_\eta| \geq \left|\mathcal{S}_\rho^n\right| - C\eta^{-1/2} \tag{28}$$

with the property that, if the initial datum is in $\mathcal{S}_\eta$ then the solution of the Hamiltonian system with Hamiltonian function $\mathcal{K}$ is quasiperiodic and fulfills

$$\left| |\psi_j(t)|^2 - |\psi_j(0)|^2 \right| < C\eta^{-1/2} \tag{29}$$

for any t.

To state a corresponding result for the NLS equation, consider the set $\mathcal{L}$ of the $\psi \in \mathcal{X}_s$ having L^2 norm equal to 1 and fulfilling

$$d(\psi, \mathcal{M}) \leq C \exp\left[-\frac{\mu_* \hbar^{3/2}}{2\mu}\right].$$

For $\psi \in \mathcal{L}$, denote $\sum_{j=1}^n \tilde{\psi}_j \hat{\varphi}_j = \hat{\Pi}\psi$ and

$$\tilde{\mathcal{S}}_\rho^n := \left\{ \psi \in \mathcal{L} \ : \ |\tilde{\psi}_j| > \rho \ , \ \forall j \right\}. \tag{30}$$

Corollary 4. *Consider the NLS equation* (1)*, under the same assumptions of theorem 2 assume also η large enough; then there exists a set $\tilde{\mathcal{S}}_\eta \subset \tilde{\mathcal{S}}_\rho^n$ whose "measure" is estimated by*

$$\left|\hat{\Pi}\tilde{\mathcal{S}}_\eta\right| \geq \left|\hat{\Pi}\tilde{\mathcal{S}}_\rho^n\right| - C\eta^{-1/2} \tag{31}$$

such that, if $\psi^0 \in \tilde{\mathcal{S}}_\eta$ then along the corresponding solution one has

$$\left| \left|\tilde{\psi}_j(t)\right|^2 - \left|\tilde{\psi}_j(0)\right|^2 \right| < C\eta^{-1/2} \tag{32}$$

for all the times t fulfilling (20)*.*

Remark 7. *All the constants in the above Theorem 4 depend on n, in* [2, 8] *one can find some n independent statements.*

2.5. **The double well potential.** In the particular case of a double well potential one can get much more precise results, both for the linear and for the nonlinear system.

By a double well potential we will mean here a potential $V(x) \in C^\infty(\mathbb{R})$ fulfilling assumptions (i-v) of Section 2.1 (with $n = 2$) and which moreover is symmetric with respect to spacial reflection $V(-x) = V(x)$. It is well known that the splitting ω between the two lowest eigenvalues fulfills the asymptotic estimate

$$\omega = \frac{1}{2}(\lambda_2 - \lambda_1) \leq Ce^{-\Gamma/\hbar}, \tag{33}$$

for any $\Gamma < \Gamma_1$ where Γ_1 is the Agmon distance between the two wells and C is a positive constant (depending on Γ), and moreover 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, thus, defining the *single well states*

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

they essentially coincide with the functions $\hat{\varphi}_j$ used in the multiple well case. In particular they fulfill

$$\|\varphi_R \varphi_L\|_{L^\infty} \leq C e^{-\Gamma/\hbar} \ , \quad \Gamma > 0. \tag{34}$$

Thus, for $\psi \in \Phi_0$, in this section *we will write*

$$\psi = \psi_1 \varphi_L + \psi_2 \varphi_R \tag{35}$$

Here the tunneling gives rise to the so called phenomenon of beating: for almost any initial datum $\psi^0 \in \Phi_0$ the expectation value of the position

$$\langle x \rangle^t = \int_{\mathbb{R}} x \left| \psi^t(x) \right|^2 dx \tag{36}$$

periodically oscillates between positive and negative values with a period given by $T := \pi\hbar/\omega$.

In this case the restricted approximate Hamiltonian $\mathcal{K}_0$ takes the form [21]

$$\mathcal{K}_0 := \bar{\psi}_2 \psi_1 + \psi_2 \bar{\psi}_1 + \eta \left(|\psi_1|^{2\sigma+2} + |\psi_2|^{2\sigma+2} \right) \tag{37}$$

with the same definition of η as in the previous subsections. Then Theorems 2 and 3 hold together with their corollaries. The main improvement that one can obtain in the double well case are due to the fact that since the system $\mathcal{K}$ is now a system with two degrees of freedom with an integral of motion independent of the Hamiltonian (namely $\mathcal{I}$), then it is integrable. This allows us to describe in a very precise way the trajectories of the system $\mathcal{K}$ which are just the intersection of the level surfaces of the functions $\mathcal{K}$ and $\mathcal{I}$. This is possible since $\mathcal{K}$ is close to $\mathcal{K}_0$.

To be definite, from now on, we will restrict to the case $\sigma = 2$.

The system $\mathcal{K}_0$, cf. (37), has been already studied in [11] (see also [17, 24, 25]) obtaining that, for $|\eta| < 2$ almost all solutions perform beating motions, while at $\eta = \pm 2$ a bifurcation occurs and new equilibria, localized close to the minima of the Hamiltonian function, appear. As η increase the domain of stability of such solutions increase its size, so that, for η large enough essentially only localize motions exist. Concerning the complete system we can state that if η is not at a bifurcation point, then non-homoclinic trajectories associated to the Hamiltonian $\mathcal{K}_0$ approximate the solution ψ^t for times of the order (20).

Corollary 5. *Under the same assumptions as in Theorem 2, assume also* $\eta \neq \pm 2$*; consider an initial datum such that* $\psi_1(0), \psi_2(0) \neq 0$*, and*

$$\mathcal{K}_0(0) \neq \frac{\eta}{2} - 1 \ \textit{if} \quad \eta > 0$$
$$\mathcal{K}_0(0) \neq 1 - \frac{\eta}{2} \ \textit{if} \quad \eta < 0$$

and also such that $\delta \leq C\mu\hbar^{3/2}$*; then, there exists a positive constant* $\mu_\sharp$*, depending only on how much the above quantities differ from the considered values, such that, provided* $\mu < \mu_\sharp \hbar^{3/2}$*, there exists a solution of the Hamiltonian system* (25) *with trajectory* γ *such that*

$$d(\psi^t, \gamma) \leq C \frac{\mu}{\hbar^{3/2}} \tag{38}$$

for the times (23).

Remark 8. *Homoclinic trajectories are absent when* $|\eta| \leq 2$*; initial conditions such that* $\mathcal{K}_0(0) = \frac{\eta}{2} - 1$*, for* $\eta > 2$*, and* $\mathcal{K}(0) = 1 - \frac{\eta}{2}$*, for* $\eta < -2$ *corresponds to an homoclinic trajectory.*

Remark 9. *The topology of the trajectory γ is determined by the condition*

$$d(\psi^0, \gamma) \leq C \frac{\mu}{\hbar^{3/2}} \tag{39}$$

in the sense that all curves fulfilling this condition have the same topology if the assumptions of the Corollary are fulfilled.

Remark 10. *Thus one has that also for the true system beats are present for $|\eta| < 2$ while their importance decreases as $|\eta|$ increase above 2. In particular for large values of η only motions localized close to one well are present* [25] *at least for the time scales controlled by our theorems.*

3. Proof of the main results

In order to simplify the notations all the proofs will be carried out in the case of a potential with only 2 wells.

3.1. **Hamiltonian Formalism.** First consider the real Hilbert space

$$\mathcal{X}^s_{\mathbb{R}} := D((H_{0,\mathbb{R}})^s)$$

where $H_{0,\mathbb{R}}$ is the operator H_0 restricted to real valued functions.

We make $\mathcal{X}^s_{\mathbb{R}} \oplus \mathcal{X}^s_{\mathbb{R}}$ a symplectic space by introducing the *semiclassical* symplectic form

$$\alpha\left((p,q);(p',q')\right) := \hbar \int_{\mathbb{R}} \left[p'(x)q(x) - p(x)q'(x)\right] \mathrm{d}x.$$

Given a smooth real valued function $\mathcal{H}(p,q)$, then we define its Hamiltonian vector field $X_{\mathcal{H}} \in \mathcal{X}^s_{\mathbb{R}} \oplus \mathcal{X}^s_{\mathbb{R}}$ by the property

$$\alpha(X_{\mathcal{H}}, h) = \mathrm{d}\mathcal{H} h \tag{40}$$

for any $h = (h_p, h_q) \in \mathcal{X}^s_{\mathbb{R}} \oplus \mathcal{X}^s_{\mathbb{R}}$, where $\mathrm{d}\mathcal{H}$ denotes the differential of $\mathcal{H}$. It is well known that $X_{\mathcal{H}}$ is in general defined only on a subset of $\mathcal{X}^s_{\mathbb{R}} \oplus \mathcal{X}^s_{\mathbb{R}}$. Define also the L^2 gradient $\nabla_p \mathcal{H}$ of $\mathcal{H}$ with respect to p by

$$\langle \nabla_p \mathcal{H}, h_p \rangle_{L^2} := \int_{\mathbb{R}} \nabla_p \mathcal{H}(x) h_p(x) dx = \mathrm{d}_p \mathcal{H} h_p, \quad \forall h_p \in \mathcal{X}^s_{\mathbb{R}}, \tag{41}$$

and similarly we introduce the quantity $\nabla_q \mathcal{H}$. Then

$$X_{\mathcal{H}} = \hbar^{-1}(-\nabla_q \mathcal{H}, \nabla_p \mathcal{H}),$$

and thus the Hamilton equations of $\mathcal{H}$ are given by

$$\frac{d}{dt}(p,q) = X_{\mathcal{H}}(p,q) \iff \left(\dot{p} = -\frac{1}{\hbar}\nabla_q \mathcal{H}\ ,\ \dot{q} = \frac{1}{\hbar}\nabla_p \mathcal{H}\right). \tag{42}$$

The Poisson brackets between two functions $\mathcal{H}$ and $\mathcal{K}$ is defined as

$$\{\mathcal{H}, \mathcal{K}\} := \alpha(X_{\mathcal{H}}, X_{\mathcal{K}}) = -\frac{1}{\hbar} \int_{\mathbb{R}} \left[\nabla_p \mathcal{H} \nabla_q \mathcal{K} - \nabla_q \mathcal{H} \nabla_p \mathcal{K}\right] \mathrm{d}x \tag{43}$$

which in general is only defined on a subdomain of $\mathcal{X}^s_{\mathbb{R}} \oplus \mathcal{X}^s_{\mathbb{R}}$.

We shall use complex coordinates in $\mathcal{X}^s_{\mathbb{R}} \oplus \mathcal{X}^s_{\mathbb{R}}$ identifying this space with $\mathcal{X}^s$, through

$$(p,q) \mapsto \psi = \frac{1}{\sqrt{2}}(q + ip).$$

Therefore, we set

$$\nabla_{\psi} = \frac{1}{\sqrt{2}}(\nabla_q - i\nabla_p) \quad \text{and} \quad \nabla_{\bar{\psi}} = \frac{1}{\sqrt{2}}(\nabla_q + i\nabla_p) \tag{44}$$

so that, if $\mathcal{H} = \mathcal{H}(\psi, \bar{\psi})$ is a smooth real valued function, we have the identification

$$X_{\mathcal{H}}(\psi, \bar{\psi}) = -\frac{i}{\hbar}\nabla_{\bar{\psi}}\mathcal{H}(\psi, \bar{\psi}) \ . \tag{45}$$

and in complex coordinates the Poisson brackets are computed by

$$\{\mathcal{H}, \mathcal{K}\} := \frac{i}{\hbar}\int_{\mathbb{R}} \left[\nabla_{\psi}\mathcal{H}\nabla_{\bar{\psi}}\mathcal{K} - \nabla_{\bar{\psi}}\mathcal{H}\nabla_{\psi}\mathcal{K}\right] \mathrm{d}x \tag{46}$$

With such a notation then the NLS (1) can be written in the form of a Hamiltonian system, the corresponding Hamiltonian function being the energy eq. (24).

Remark 11. *Such a Hamiltonian is invariant under the action of the Gauge group*

$$\psi(x) \to \psi(x)e^{-i\beta}, \tag{47}$$

for any β independent of x. The corresponding conserved quantity is the L^2 norm

$$\mathcal{N}(\psi, \bar{\psi}) = \int_{\mathbb{R}} |\psi(x)|^2 \mathrm{d}x. \tag{48}$$

Equivalently one has

$$\{\mathcal{E}, \mathcal{N}\} \equiv 0. \tag{49}$$

Let $\{\lambda_k\}_{k=1}^{\infty}$ and $\{\varphi_k(x)\}_{k=1}^{\infty}$ be the eigenvalues and the normalized eigenvectors of H_0, let

$$\psi(x) = \sum_{k=1}^{\infty} \zeta_k \varphi_k(x) \ , \tag{50}$$

and define the Hilbert spaces ℓ^2_s of the complex sequences such that

$$\|\zeta\|_s^2 := \sum_{k\geq 1} \lambda_k^s |\zeta_k|^2 < \infty \tag{51}$$

In such a way we have defined the correspondence

$$\psi \in \mathcal{X}^s \leftrightarrow \mathcal{U}(\psi) := \zeta \equiv (\zeta_1, \zeta_2 ... \zeta_j, ...) \in \ell^2_s$$

which is a unitary isomorphism. In particular, if $\mathcal{E}$ is the Hamiltonian (24), then $\mathcal{E} \circ \mathcal{U}^{-1}$ (still denoted by $\mathcal{E}$) is the Hamiltonian of the same system written in terms of the new variables ζ. In terms of these variables the quadratic part $\mathcal{E}_0$ of the Hamiltonian is given by

$$\mathcal{E}_0 = \sum_{j\geq 1} \lambda_j \left|\zeta_j\right|^2 \tag{52}$$

and the Poisson brackets can be written as

$$\{\mathcal{H}, \mathcal{K}\} = \frac{i}{\hbar}\sum_{k=1}^{\infty}\left[\frac{\partial \mathcal{H}}{\partial \zeta_k}\frac{\partial \mathcal{K}}{\partial \bar{\zeta}_k} - \frac{\partial \mathcal{H}}{\partial \bar{\zeta}_k}\frac{\partial \mathcal{K}}{\partial \zeta_k}\right]$$

Remark 12. *From now on we will work in the space ℓ^2_s and moreover, in order to simplify,* **we rescale time by the transformation** $t \mapsto t/\hbar$*, thus the Poisson brackets take the form*

$$\{\mathcal{H}, \mathcal{K}\} = i \sum_{k=1}^{\infty} \left[\frac{\partial \mathcal{H}}{\partial \zeta_k} \frac{\partial \mathcal{K}}{\partial \bar{\zeta}_k} - \frac{\partial \mathcal{H}}{\partial \bar{\zeta}_k} \frac{\partial \mathcal{K}}{\partial \zeta_k} \right] \tag{53}$$

3.2. **Non coupling monomial.** It is useful to introduce also a different notation for the first two variables (here we recall that we are working in the double well case) and for the remaining ones, thus let us denote

$$u_1 := \zeta_1 \ , \quad u_2 := \zeta_2 \ , \quad z_j := \zeta_j \ , \quad j \geq 3. \tag{54}$$

Consider now a monomial of the form

$$\zeta^K \bar{\zeta}^L = u^k \bar{u}^l z^m \bar{z}^n \tag{55}$$

where we used the notations

$$\begin{array}{l} K = (k, m), \ L = (l, n) \\ k = (k_1, k_2), \ m = (m_3, m_4, m_5, ...), \ l = (l_1, l_2), \ n = (n_3, n_4, n_5, ...) \\ u^k \equiv u_1^{k_1} u_2^{k_2}, \ z^m \equiv z_3^{m_3} z_4^{m_4} \ldots z_q^{m_q} \ldots \end{array} \tag{56}$$

Remark 13. *A monomial of the form* (55) *is Gauge invariant, i.e. invariant under the transformation*

$$\psi \mapsto e^{i\beta} \psi \quad \textit{that is} \quad \zeta_k \mapsto e^{i\beta} \zeta_k$$

if and only if $|K| = |L|$*, where*

$$|K| = \sum_j |K_j|.$$

In fact (55) *is Gauge invariant if, and only if,*

$$0 = \left\{ \mathcal{N}(\zeta, \bar{\zeta}), \zeta^K \bar{\zeta}^L \right\} = i \left(\sum_j (K_j - L_j) \right) \zeta^K \bar{\zeta}^L \tag{57}$$

where $\mathcal{N}(\zeta, \bar{\zeta}) = \sum_{j \geq 1} |\zeta_j|^2$ *is the* L^2 *norm; that is* $|K| = |L|$ *again.*

Due to our assumption Hyp.1 on the potential one has

Lemma 2. *Let* $\sigma(H_0)$ *be the spectrum of the linear operator* H_0 *and let* $\hbar$ *be small enough. There exists a sequence of (not necessarily continuous with respect to* $\hbar$*) functions* $\{E_\gamma(\hbar)\}_{\gamma \in \mathbb{N}}$*,* $0 < E_0 < 1$ *and there exists a positive constant* $C > 1$*, independent of* $\hbar$ *and* γ*, such that:*

i. $[E_\gamma - C^{-1}\hbar, E_\gamma + C^{-1}\hbar] \cap \sigma(H_0) = \emptyset$*;*
ii. $1 < E_\gamma - E_{\gamma-1} < 3$ *for all* $\hbar$ *and all* $\gamma \geq 1$*;*
iii. *For any* $\hbar$ *fixed, we consider the sets of indexes*

$$J_\gamma(\hbar) = J_\gamma := \{ j \in \mathbb{N} \ : \ E_{\gamma-1} < \lambda_j < E_\gamma \} ,$$

then the cardinality of these sets is estimated as

$$\# J_\gamma(\hbar) \leq \frac{C}{\hbar}.$$

Proof. The proof is an immediate consequence of the following result (see Theorem (V-11) in [18], see also Theorem (XIII-81) in [19]):

$$N_{[\alpha,\beta]} = \frac{1}{2\pi\hbar}\left[\left|\left\{(x,p)\in\mathbb{R}^2 \ : \ \alpha \le p^2+V(x)\le\beta\right\}\right| + O(\hbar)\right]$$

where $N_{[\alpha,\beta]}$ is the number of eigenvalues of H_0 contained in the interval $[\alpha,\beta]$ and where $|.|$ denotes the Lebesgue measure of a set. Indeed, let us consider the intervals $[2\gamma, 2\gamma+1]$, $\gamma\in\mathbb{N}$, then the number of eigenvalues of H_0 belonging to these intervals is given by

$$\begin{aligned} N(\gamma) &:= N_{[2\gamma,2\gamma+1]} = \\ &= \frac{1}{2\pi\hbar}\left[\left|\left\{(x,p)\in\mathbb{R}^2 \ : \ 2\gamma \le p^2+V(x)\le 2\gamma+1\right\}\right| + O(\hbar)\right] \le \frac{C}{\hbar} \end{aligned}$$

since $V(x)\ge C\langle x\rangle^2$, for some positive constant C independent of $\hbar$ and γ. From this estimate it follows that there exists at least one value $E_\gamma\in(2\gamma,2\gamma+1)$ and $C>1$ satisfying i.. Furthermore, conditions ii. and iii. immediately follow since

$$1=(2\gamma)-[2(\gamma-1)+1]\le E_\gamma - E_{\gamma-1}\le(2\gamma+1)-2(\gamma-1)=3$$

and

$$\#J_\gamma \le N(\gamma)+N(\gamma-1)\le\frac{2C}{\hbar}.$$

□

We fix a sequence with such properties.

Hereafter, all the perturbative construction will involve only Gauge invariant monomial (hence $|K|=|L|$). Keeping this in mind we give the following

Definition 2. *A monomial of the form* (55) *will be called* coupling *if the indexes* (K,L) *fulfill the following conditions*

i. $|K|=|L|$
ii. $|m|+|n|=1,2$
iii. *if* $m_i=1$ *and* $n_j=1$ *then* $i\in J_\gamma$ *and* $j\in J_{\gamma'}$ *with* $\gamma\neq\gamma'$.

A monomial which is not coupling will be called non coupling. *A polynomial containing* **only** *coupling (reps. non coupling) monomial will be called coupling (reps. non coupling).*

Remark 14. *For Gauge invariant monomials the condition* i. *is always fulfilled. Furthermore, in terms of the indexes* k,l,m,n *condition* i. *reads*

$$|k|-|l|=|n|-|m| \tag{58}$$

Remark 15. *Any Gauge invariant analytic function can be uniquely decomposed into the sum of a coupling and a noncoupling part. We recall that, as in finite dimensional spaces, an analytic function is a function whose Taylor series is convergent (see e.g.* [15]*).*

We also define a new ($\hbar$ dependent) norm in the space $\mathcal{X}^s$ as follows

Definition 3. *Denote*

$$\mathcal{N}_E(z,\bar z) := \sum_\gamma E_\gamma^s \sum_{j\in J_\gamma, j\ge 3} |z_j|^2 \tag{59}$$

then the quantity

$$\|(u,z)\|_E^2 \equiv \|\zeta\|_E^2 := |u_1|^2 + |u_2|^2 + \mathcal{N}_E(z,\bar{z}) \tag{60}$$

will be called E-norm of ζ. *Denote* ℓ_E^2 *the space of sequences* $z = \{z_j\}_{j\geq 3}$ *equipped with the norm* $\mathcal{N}_E(z,\bar{z})$. *By abuse of notation sometime we will also write*

$$\|z\|_E^2 := \mathcal{N}_E(z,\bar{z}).$$

Remark 16. *The E-norm is equivalent to the standard norm of* $\mathcal{X}^s$ *with an* $\hbar$ *independent constant. The proof is a trivial computation and is left to the reader.*

Lemma 3. *Let* $\zeta^K\bar{\zeta}^L$ *be a non coupling Gauge invariant monomial of degree at most two in* $z,\bar{z}$ *(i.e.* $|n|+|m|\leq 2$*), then one has*

$$\left\{\mathcal{N}_E, \zeta^K\bar{\zeta}^L\right\} = 0 \quad \textit{and} \quad \left\{|u_1|^2+|u_2|^2, \zeta^K\bar{\zeta}^L\right\} = 0 \tag{61}$$

Proof. First remark that if $u^k\bar{u}^l z^n\bar{z}^m$ is noncoupling of degree at most two in $z,\bar{z}$ then one has $|k|=|l|$ and thus

$$\left\{u_1\bar{u}_1 + u_2\bar{u}_2, u^k\bar{u}^l z^n\bar{z}^m\right\} = i(|k|-|l|)u^k\bar{u}^l z^n\bar{z}^m = 0. \tag{62}$$

Furthermore, either it is of degree zero in $z,\bar{z}$ or there exists $\bar{\gamma}$ and $\bar{j},\tilde{j} \in J_{\bar{\gamma}}$ such that $n_{\bar{j}} = 1$ and $m_{\tilde{j}} = 1$. In the first case one has that

$$\left\{\mathcal{N}_E, \zeta^K\bar{\zeta}^L\right\} = \left\{\mathcal{N}_E(z,\bar{z}), u^k\bar{u}^l\right\} = 0$$

In the second case, then

$$\begin{aligned}\left\{\mathcal{N}_E(z,\bar{z}), u^k\bar{u}^l z^n\bar{z}^m\right\} &= u^k\bar{u}^l \sum_\gamma E_\gamma^s \sum_{j\in J_\gamma} \left\{z_j\bar{z}_j, u^k\bar{u}^l z^n\bar{z}^m\right\} \\ &= u^k\bar{u}^l z^n\bar{z}^m E_{\bar{\gamma}}^s \sum_{j\in J_{\bar{\gamma}}} i(n_j - m_j) = 0\end{aligned}$$

□

Thus the E–norm is invariant under the dynamics of a noncoupling Hamiltonian of degree at most 2 in $z,\bar{z}$. In the more general case one has

Corollary 6. *Let* $\mathcal{Z}$ *be a non coupling polynomial. Assume that it has a smooth vector field, then there exists* C *such that*

$$\left|\left\{\mathcal{N}_E, \mathcal{Z}\right\}(u,\bar{u},z,\bar{z})\right| \leq C\left[\mathcal{N}_E(z,\bar{z})\right]^{3/2} \tag{63}$$

3.3. **Normal form construction.** Let us rewrite $\mathcal{E}(\psi,\bar{\psi})$ as follows

$$\mathcal{E} = \mathcal{H}_0 + \epsilon\mathcal{P}_\epsilon$$

where

$$\mathcal{H}_0(\psi,\bar{\psi}) := \Omega(|\zeta_1|^2+|\zeta_2|^2) + \sum_{j\geq 3}\lambda_j\left|\zeta_j\right|^2, \quad \Omega := \frac{\lambda_1+\lambda_2}{2}, \tag{64}$$

and

$$\mathcal{P}_\epsilon(\psi,\bar{\psi}) := \frac{\omega}{\epsilon}(|\zeta_2|^2 - |\zeta_1|^2) + \mathcal{P}_0(\psi,\bar{\psi}). \tag{65}$$

We are going to prove that there exists a canonical transformation $\mathcal{T}_\epsilon$ which gives the Hamiltonian the form

$$\mathcal{E}\circ\mathcal{T}_\epsilon = \mathcal{H}_0 + \epsilon\mathcal{Z}_\epsilon + \mathcal{R} \tag{66}$$

where $\mathcal{Z}_\epsilon$ is a non coupling polynomial and $\mathcal{R}$ has a smooth vector which is exponentially small with ϵ^{-1}.

The construction will be recursive. To this end we assume one has been able to construct a canonical transformation $\mathcal{T}_r$ putting the Hamiltonian in the form

$$\mathcal{E} \circ \mathcal{T}_r \equiv \mathcal{E}^{(r)} = \mathcal{H}_0 + \epsilon \mathcal{Z}^{(r)}(\epsilon) + \epsilon^{r+1} \mathcal{R}^{(r)}(\epsilon) \tag{67}$$

with $\mathcal{Z}^{(r)}$ being a noncoupling polynomial and where $\mathcal{R}^{(r)}(\epsilon)$ has a vector field which is bounded, uniformly with respect to ϵ ($\mathcal{Z}^{(0)} = 0$ and $\mathcal{R}^{(0)} = \mathcal{P}_\epsilon$). We look for an auxiliary Hamiltonian $\mathcal{G}_{r+1}$ such that considering the corresponding Hamilton equations

$$\dot{\zeta} = X_{\mathcal{G}_{r+1}}(\zeta)$$

and the corresponding flow ϕ^t_{r+1} one has that $\mathcal{E}^{(r)} \circ \phi^{\epsilon^{r+1}}_{r+1}$ is in the form (67) with $r+1$ in place of r.

Explicitly one has

$$\begin{aligned} \mathcal{E}^{(r)} \circ \phi^{\epsilon^{r+1}}_{r+1} &= \mathcal{H}_0 + \epsilon \mathcal{Z}^{(r)} && (68) \\ &+ \epsilon^{r+1} \left(\mathcal{R}^{(r)} + \{\mathcal{H}_0, \mathcal{G}_{r+1}\} \right) && (69) \\ &+ \mathcal{H}_0 \circ \phi^{\epsilon^{r+1}}_{r+1} - \mathcal{H}_0 - \epsilon^{r+1} \{\mathcal{H}_0, \mathcal{G}_{r+1}\} && (70) \\ &+ \epsilon \left(\mathcal{Z}^{(r)} \circ \phi^{\epsilon^{r+1}}_{r+1} - \mathcal{Z}^{(r)} \right) && (71) \\ &+ \epsilon^{r+1} \left(\mathcal{R}^{(r)} \circ \phi^{\epsilon^{r+1}}_{r+1} - \mathcal{R}^{(r)} \right) && (72) \end{aligned}$$

Now, it is quite easy to understand that (70–72) are higher order terms (they will be estimated later), while (69) is the term of order ϵ^{r+1}. Thus, if one is able to choose $\mathcal{G}_{r+1}$ so that

$$\mathcal{R}^{(r)} + \{\mathcal{H}_0, \mathcal{G}_{r+1}\} \tag{73}$$

is non coupling, then the coupling terms are pushed to order $r+2$, and

$$\mathcal{Z}^{r+1} = \mathcal{Z}^r + \epsilon^r \left[\mathcal{R}^{(r)} + \{\mathcal{H}_0, \mathcal{G}_{r+1}\} \right]$$

is non coupling.

The main step of the proof is the construction and the estimate of such a function $\mathcal{G}$ fulfilling the homological equation associated to (73).

3.4. **Framework and notations.** Before proceeding to the construction and the estimation of such a $\mathcal{G}$ it is useful to extend the setting in which we will work. Indeed, since we are working with analytic functions it is useful to work in the *complexification* of our space. More precisely, *we consider now a phase space in which the variables $v := \bar{u}$ and $w := \bar{z}$ are independent of u, z.* Actually this is equivalent to complexify the space in which vary the variables p, q of section 3.1. With such an extension the Poisson bracket will take the form

$$\{\mathcal{H}, \mathcal{K}\} = i \sum_{k=1}^{2} \left[\frac{\partial \mathcal{H}}{\partial u_k} \frac{\partial \mathcal{K}}{\partial v_k} - \frac{\partial \mathcal{K}}{\partial u_k} \frac{\partial \mathcal{H}}{\partial v_k} \right] + i \sum_{j=3}^{\infty} \left[\frac{\partial \mathcal{H}}{\partial z_j} \frac{\partial \mathcal{K}}{\partial w_j} - \frac{\partial \mathcal{K}}{\partial z_j} \frac{\partial \mathcal{H}}{\partial w_j} \right]$$

Such a phase space will be denoted by $\mathcal{X}^s_{\mathbb{C}}$. In $\mathcal{X}^s_{\mathbb{C}}$ we will use the norm

$$\lceil (u, v, z, w) \rceil := \max \left\{ \|(u, v)\|_{\mathbb{C}^2}, \|(z, w)\|_E \right\} \tag{74}$$

with $\|(z,w)\|_E$ defined by

$$\|(z,w)\|_E^2 := \|z\|_E^2 + \|w\|_E^2\,, \quad \text{where} \quad \|\cdot\|_E^2 = \mathcal{N}_E(\cdot,\bar{\cdot}). \tag{75}$$

Sometimes it is also useful to use more compact notations for the phase space variables, thus we will also write $\zeta := (u,z)$, $\eta := (v,w)$, $\xi := (\zeta,\eta)$.

Moreover, given $R>0$ we will denote by B_R the ball of radius R and center 0 in the phase space:

$$B_R = \{\xi \in \mathcal{X}^s_{\mathbb{C}} \ : \ \lceil \xi \rceil \le R\}\,.$$

Given an analytic function $\mathcal{H}$ with Hamiltonian vector $X_{\mathcal{H}}$ analytic as a map from B_R to $\mathcal{X}^s_{\mathbb{C}}$ we will denote

$$|X_{\mathcal{H}}|_R := \sup_{\xi\in B_R} \lceil X_{\mathcal{H}}(\xi) \rceil \quad \text{and} \quad |\mathcal{H}|_R := \sup_{\xi\in B_R} |\mathcal{H}(\xi)|\,, \tag{76}$$

with norm defined by (74).

Remark 17. *By Corollary 1, our initial perturbation* $\mathcal{P}_\epsilon$*, defined by* (65)*, is such that*

$$|X_{\mathcal{P}_\epsilon}|_R \le \frac{\omega}{\epsilon} R + \frac{C}{\hbar^\sigma} R^{2\sigma+1} \tag{77}$$

3.5. **Solution of the Homological equation.** In this section we will construct and estimate the solution of the Homological equation associated to (73); that is we look for $\mathcal{G}_{r+1}$ such that (73) is non coupling.

Precisely, consider the Gauge invariant Hamiltonian function $\mathcal{H}$ and decompose it (Remark (15)) as $\mathcal{H} = \mathcal{F} + \mathcal{Z}$ with $\mathcal{Z}$ non coupling and $\mathcal{F}$ coupling, and consider the equation

$$\{\mathcal{H}_0, \mathcal{G}\} = \mathcal{F}, \quad \mathcal{F} = \text{ coupling part of } \mathcal{H} \tag{78}$$

then we are going to prove the following.

Theorem 5. *If* $\mathcal{H}$ *has a Hamiltonian vector* $X_{\mathcal{H}}$ *analytic as a map from* B_R *to* $\mathcal{X}^s_{\mathbb{C}}$*, then there exists a solution* $\mathcal{G}$ *of* (78) *which is coupling and has a vector field* $X_{\mathcal{G}}$ *with the same analyticity properties; moreover there exists a positive* $\alpha = \alpha(\hbar)$ *such that the following inequality holds*

$$|X_{\mathcal{G}}|_R \le \frac{1}{\alpha} |X_{\mathcal{H}}|_R \tag{79}$$

moreover $\alpha(\hbar) \ge C^{-1}\hbar^{3/2}$

Before starting the proof we need some preparation. Since $\mathcal{F}$ is coupling then it is of degree at most 2 with respect to z and w. Therefore, we can decompose $\mathcal{F}$ as follows

$$\mathcal{F} := \mathcal{F}^{10} + \mathcal{F}^{01} + \mathcal{F}^{20} + \mathcal{F}^{11} + \mathcal{F}^{02} \tag{80}$$

with

$$\mathcal{F}^{10} = \left\langle F^{10}(u,v); z \right\rangle, \quad \mathcal{F}^{01} = \left\langle F^{01}(u,v); w \right\rangle \tag{81}$$

$$\mathcal{F}^{20} = \left\langle F^{20}(u,v) z; z \right\rangle, \quad \mathcal{F}^{02} = \left\langle F^{02}(u,v) w; w \right\rangle \tag{82}$$

$$\mathcal{F}^{11} = \left\langle F^{11}(u,v) z; w \right\rangle \tag{83}$$

and $\langle .;. \rangle$ be the scalar product of the real Hilbert space ℓ^2 defined by

$$\left\langle z^{(1)}; z^{(2)} \right\rangle := \sum_{j\geq 3} z_j^{(1)} z_j^{(2)} \tag{84}$$

and F^{01}, F^{10} which are $\mathcal{X}^s_{\mathbb{C}}$ valued functions of (u,v) and F^{20}, F^{02}, F^{11} functions taking values in suitable spaces of linear operators. We will denote by $F^{01}_j(u,v)$ the components of F^{01}; we will denote by $F^{02}_{ij}(u,v)$ the matrix elements of $F^{02}(u,v)$, and similarly for the other quantities.

Lemma 4. *The Homological equation* (78) *has a formal solution $\mathcal{G}$ with the same structure as $\mathcal{F}$ (cf.* (80)-(83)*), but with the quantities G's defined by*

$$G^{10}_j(u,v) := \frac{F^{10}_j(u,v)}{i(\lambda_j - \Omega)}, \quad G^{01}_j(u,v) := \frac{F^{01}_j(u,v)}{-i(\lambda_j - \Omega)} \tag{85}$$

$$G^{20}_{jl}(u,v) := \frac{F^{20}_{jl}(u,v)}{i(\lambda_j + \lambda_l - 2\Omega)}, \quad G^{02}_{jl}(u,v) := \frac{F^{02}_{jl}(u,v)}{-i(\lambda_j + \lambda_l - 2\Omega)} \tag{86}$$

$$G^{11}_{jl}(u,v) := \frac{F^{11}_{jl}(u,v)}{i(\lambda_j - \lambda_l)} \tag{87}$$

Remark 18. *In* (87) *one always has $j \neq l$ since terms of the form $F^{11}_{jj}(u,v)$ are always noncoupling; furthermore, one has that j and l cannot belong to the same set J_γ. The solution $\mathcal{G}$ is* coupling.

Proof. We consider explicitly only the term $\mathcal{G}^{01}$, since all the other terms can be studied exactly in the same way. First define

$$\mathcal{H}^{(1)}(u,v) := \Omega(u_1 v_1 + u_2 v_2) \ , \quad \mathcal{H}^{(\infty)}(z,w) := \sum_{j\geq 3} \lambda_j z_j w_j,$$

so that $\mathcal{H}_0 = \mathcal{H}^{(1)} + \mathcal{H}^{(\infty)}$. Now one has

$$\begin{aligned} \left\{\mathcal{H}_0, \mathcal{G}^{01}\right\} &= \left\{\mathcal{H}^{(1)}, \mathcal{G}^{01}\right\} + \left\{\mathcal{H}^{(\infty)}, \mathcal{G}^{01}\right\} \\ &= \sum_j \left[\left\{\mathcal{H}^{(1)}, G^{01}_j\right\} - i\lambda_j G^{01}_j\right] w_j \end{aligned} \tag{88}$$

where we simply computed explicitly $\left\{\mathcal{H}^{(\infty)}, \mathcal{G}^{01}\right\}$. Thus to ask

$$\left\{\mathcal{H}_0, \mathcal{G}^{01}\right\} = \mathcal{F}^{01} \tag{89}$$

is equivalent to ask

$$\left\{\mathcal{H}^{(1)}, G^{01}_j\right\} - i\lambda_j G^{01}_j = F^{01}_j \tag{90}$$

We compute now the above Poisson Bracket. To this end decompose G^{01}_j in Taylor series, one has

$$G^{01}_j(u,v) = \sum_{kl} G^{01}_{j,kl} u^k v^l \ , \tag{91}$$

from which

$$\left\{\mathcal{H}^{(1)}, G^{01}_j\right\} = \sum_{kl} G^{01}_{j,kl} i\Omega(|l| - |k|) u^k v^l \tag{92}$$

but, assuming that $\mathcal{G}^{01}$ is coupling (which will be verified in a while), due to the limitation (58), one has $|k|-|l|=|m|-|n|=-1$ (due to the fact that $\mathcal{G}^{01}$ is linear in w), and therefore

$$\left\{\mathcal{H}^{(1)}, G_j^{01}\right\} = i\Omega G_j^{01} \ . \tag{93}$$

Inserting this expression in (90) one gets

$$i\Omega G_j^{01} - i\lambda_j G_j^{01} = F_j^{01}$$

which shows that the function $\mathcal{G}^{01}$ of (85) actually fulfills the equation (89) and is coupling. All the other terms can be studied in the same way; a detailed proof is omitted. □

End of the Proof of Theorem 5. We will explicitly prove only the estimate of the norms of the vector fields of $X_{\mathcal{G}^{01}}$ and $X_{\mathcal{G}^{11}}$, the other being similar and simpler. We start with $X_{\mathcal{G}^{01}}$. Consider first the vector field of $\mathcal{F}^{01}$, whose components have the form

$$X^{u_l}_{\mathcal{F}^{01}} = i\left\langle \frac{\partial F^{01}}{\partial v_l}; w\right\rangle \tag{94}$$

$$X^{z}_{\mathcal{F}^{01}} = iF^{01} \tag{95}$$

Since $\mathcal{F}$ is the coupling part of $\mathcal{H}$ then

$$X^{u}_{\mathcal{F}^{01}} = d_w X^u_{\mathcal{H}}(u,v,0,0)w \tag{96}$$

and therefore, adding also the v components, Cauchy inequality implies that

$$\left\| \frac{\partial F^{01}}{\partial(u,v)}(u,v)\right\|_{\mathcal{L}(\mathcal{X}^s_{\mathbb{C}},\mathbb{C}^4)} \leq \frac{1}{R}\sup_{B_R}\lceil X^{(u,v)}_{\mathcal{H}}(u,v,z,w)\rceil = \frac{1}{R}\left|X^{(u,v)}_{\mathcal{H}}\right|_R \tag{97}$$

where the norm at l.h.s. is the norm as a linear operator from $\mathcal{X}^s_{\mathbb{C}}$ to $\mathbb{C}^4$. Using this inequality and making use of (85) it is very easy to estimate $X^{(u,v)}_{\mathcal{G}^{01}}$: to this end define $\tilde{w}_j := w_j/i(\lambda_j-\Omega)$ and let $C>1$ be such that

$$C^{-1}\hbar := \inf_{j\geq 3}|\lambda_j-\Omega|. \tag{98}$$

Then one has

$$\|\tilde{w}\|_E \leq C\|w\|_E/\hbar$$

and, using the definition of $\mathcal{G}^{01}$, cf. (85), one has

$$X^u_{\mathcal{G}^{01}} = i\left\langle\frac{\partial F^{01}}{\partial v};\tilde{w}\right\rangle \tag{99}$$

and similarly for the v components, and thus

$$\left|X^{(u,v)}_{\mathcal{G}^{01}}\right|_R \leq \frac{C}{\hbar}\left|X^{(u,v)}_{\mathcal{H}}\right|_R \tag{100}$$

for some $C>1$. The estimate of the z components of the vector field is simpler (due to the simpler form of the z component) and collecting the two one gets

$$|X_{\mathcal{G}^{01}}|_R \leq \frac{C}{\hbar}|X_{\mathcal{H}}|_R \tag{101}$$

We come now to the estimate of the vector field of $\mathcal{G}^{11}$. Preliminary to this estimate we remark that the components of the vector field of $\mathcal{F}^{11}$ are given by

$$X^{(u,v)}_{\mathcal{F}^{11}} = d^2_{zw} X^{(u,v)}_{\mathcal{H}}(u,v,0,0)[z,w] \tag{102}$$

$$X^{w}_{\mathcal{F}^{11}} = d_z X^{w}_{\mathcal{H}}(u,v,0,0)z = F^{11}z \tag{103}$$

thus in particular, by Cauchy inequality,

$$\sup_{B_R} \left\| F^{11}(u,v) \right\|_{\mathcal{L}(\ell^2_E,\ell^2_E)} \leq \frac{1}{R} \left| X^w_{\mathcal{H}} \right|_R \tag{104}$$

where the norm at l.h.s. is the norm as a linear operator from ℓ^2_E to ℓ^2_E.

In order to estimate $X^z_{\mathcal{G}^{11}}$ we have just to estimate the norm of the operator (from ℓ^2_E to itself) whose matrix is defined in (87). To this end remark that the boundedness of G^{11} as an operator from ℓ^2_E to itself (or to its dual) is equivalent to the boundedness of the operator with matrix elements $t_l G^{11}_{jl} s_j$ as an operator from ℓ^2 to itself, where t_l, s_j are suitable positive numbers (in fact, ℓ^2 and ℓ^2_E are spaces with not equivalent norms). Thus Lemma 8 of the appendix ensures that

$$\sup_{B_R} \left\| G^{11}(u,v) \right\|_{\mathcal{L}(\ell^2_E,\ell^2_E)} \leq \frac{1}{\alpha} \left| X^w_{\mathcal{H}} \right|_R , \quad \alpha \geq C^{-1} \hbar^{3/2}, \tag{105}$$

for some $C > 1$, since $|\lambda_j - \lambda_l| \geq C^{-1}\hbar$ if j and l belong to different sets J_γ. Working in a similar way for the other components and the other parts of the vector field of the function $\mathcal{G}$ one gets the result. □

From the proof (especially (96), (102) and (103)) also the following useful Lemma follows

Lemma 5. *The following estimates hold*

$$|X_{\mathcal{F}}|_R \leq 5\,|X_{\mathcal{H}}|_R \ , \quad |X_{\mathcal{Z}}|_R \leq 6\,|X_{\mathcal{H}}|_R \ , \quad |\mathcal{Z}|_R \leq 6\,|\mathcal{H}|_R \tag{106}$$

3.6. **Quantitative estimates.** First we fix a positive R in such a way that $X_{\mathcal{P}_\epsilon}$ is analytic on B_R, and choose constants P, P^* (that depend on $\hbar$ and on all the other parameters) such that

$$|X_{\mathcal{P}_\epsilon}|_R \leq P \ , \quad |\mathcal{P}_\epsilon|_R \leq P^* . \tag{107}$$

All along this section we fix a small value of $\hbar$, and will make explicit estimates so that at the end it will be possible to insert the dependence on $\hbar$ of the final estimate.

Lemma 6. *(Iterative Lemma) Consider a Gauge invariant Hamiltonian of the form*

$$\mathcal{E}^{(r)} = \mathcal{H}_0 + \epsilon \mathcal{Z}^{(r)} + \epsilon^{r+1} \mathcal{R}^{(r)}, \tag{108}$$

with $\mathcal{Z}^{(r)}$ non coupling and where $\mathcal{R}^{(0)} = \mathcal{P}_\epsilon$ and $\mathcal{Z}^{(0)} = 0$. Fix $\delta < R/(r+1)$, assume that the Hamiltonian vector fields of $\mathcal{Z}^{(r)}$ and of $\mathcal{R}^{(r)}$ are analytic on $B_{R-r\delta}$, *and that*

$$\left|X_{\mathcal{Z}^{(r)}}\right|_{R-r\delta} \leq \begin{cases} 0 & \text{if} \quad r=0 \\ 6P\sum_{i=0}^{r-1}\left(\frac{\epsilon}{\epsilon_0}\right)^i & \text{if} \quad r\geq 1 \end{cases}, \tag{109}$$

$$\left|\mathcal{Z}^{(r)}\right|_{R-r\delta} \leq \begin{cases} 0 & \text{if} \quad r=0 \\ 6P^*\sum_{i=0}^{r-1}\left(\frac{\epsilon}{\epsilon_0}\right)^i & \text{if} \quad r\geq 1 \end{cases} \tag{110}$$

$$\left|X_{\mathcal{R}^{(r)}}\right|_{R-r\delta} \leq \frac{P}{\epsilon_0^r}, \quad \left|\mathcal{R}^{(r)}\right|_{R-r\delta} \leq \frac{P^*}{\epsilon_0^r}, \tag{111}$$

with

$$\epsilon_0 := \frac{\alpha\delta}{75P}, \quad \textit{where} \quad \alpha=\alpha(\hbar)\geq C^{-1}\hbar^{3/2}, \tag{112}$$

then, if $\left(\frac{\epsilon}{\epsilon_0}\right) < 1/2$ *there exists a Hamiltonian function* $\mathcal{G}_{r+1}$ *analytic on* $B_{R-\delta r}$ *generating the canonical transformation* $\phi_{r+1}^{\epsilon^{r+1}}$ *such that* $\mathcal{E}^{(r)}\circ\phi_{r+1}^{\epsilon^{r+1}}$ *has the form* (108) *and satisfies the estimates* (109)-(111) *with* $r+1$ *in place of* r*, moreover the new Hamiltonian is Gauge invariant and the canonical transformation fulfills*

$$\sup_{\lceil\xi\rceil\leq R-(r+1)\delta}\left\lceil \xi-\phi^{\epsilon^{r+1}}(\xi)\right\rceil \leq \epsilon\left(\frac{\epsilon}{\epsilon_0}\right)^r\frac{P}{\alpha} \tag{113}$$

Proof. Decompose $\mathcal{R}^{(r)}$ into its coupling part $\mathcal{F}_r$ and its noncoupling part $\mathcal{Z}_r$. Define $\mathcal{Z}^{(r+1)} := \mathcal{Z}^{(r)}+\epsilon^r\mathcal{Z}_r$ and use Lemma 5 to estimate $\left|X_{\mathcal{Z}^{(r+1)}}\right|_{R-\delta(r+1)}$. Use Theorem 2 to construct $\mathcal{G}_{r+1}$ as the solution of

$$\{\mathcal{H}_0;\mathcal{G}_{r+1}\} = -\mathcal{F}_r$$

then

$$\left|X_{\mathcal{G}_{r+1}}\right|_{R-r\delta} \leq \frac{1}{\alpha}\left|X_{\mathcal{R}^{(r)}}\right|_{R-r\delta} \leq \frac{P}{\alpha\epsilon_0^r} \tag{114}$$

The Hamiltonian $\mathcal{E}^{(r)}\circ\phi^{\epsilon^{r+1}}$ was computed in subsection 3.2 and is given by equations (68)–(72), which has the form (108) provided one defines

$$\mathcal{R}^{(r+1)} = \mathcal{R}_a^{(r+1)}+\mathcal{R}_b^{(r+1)}+\mathcal{R}_c^{(r+1)}$$

where

$$\mathcal{R}_a^{(r+1)} = \epsilon^{-(r+2)}(70),\ \mathcal{R}_b^{(r+1)} = \epsilon^{-(r+2)}(71) \ \text{ and } \ \mathcal{R}_c^{(r+1)} = \epsilon^{-(r+2)}(72).$$

Then, from Lemma 11, with $\mu=\epsilon^{(r+1)}$, it follows that

$$\begin{aligned}
\left|X_{\mathcal{R}_b^{(r+1)}}\right|_{(R-r\delta)-\delta} &\leq \frac{5}{\delta\epsilon^{r+1}}\mu\left|X_{\mathcal{Z}^{(r)}}\right|_{R-r\delta}\left|X_{\mathcal{G}_{(r+1)}}\right|_{R-r\delta} \\
&\leq \frac{5}{\delta}\left[6P\sum_{i=0}^{r-1}\left(\frac{\epsilon}{\epsilon_0}\right)^i\right]\left(\frac{P}{\alpha\epsilon_0^r}\right) \\
&\leq \frac{60P^2}{\alpha\delta\epsilon_0^r}
\end{aligned}$$

since $\epsilon \le \frac{1}{2}\epsilon_0$. Similarly

$$
\begin{aligned}
\left|X_{\mathcal{R}_c^{(r+1)}}\right|_{(R-r\delta)-\delta} &\le \frac{5}{\delta\epsilon}\mu \left|X_{\mathcal{R}^{(r)}}\right|_{R-r\delta}\left|X_{\mathcal{G}_{(r+1)}}\right|_{R-r\delta} \\
&\le \frac{5\epsilon^r}{\delta}\left(\frac{P}{\epsilon_0^r}\right)\left(\frac{P}{\alpha\epsilon_0^r}\right) \le \frac{5P^2}{\alpha\delta\epsilon_0^r}\left(\frac{\epsilon}{\epsilon_0}\right)^r \\
&\le \frac{5P^2}{2^r\alpha\delta\epsilon_0^r}
\end{aligned}
$$

Furthermore, from Lemma 12, with $\mathcal{H} = \mathcal{R}^{(r)}$ and $\mu = \epsilon^{(r+1)}$, it follows that

$$
\begin{aligned}
\left|X_{\mathcal{R}_a^{(r+1)}}\right|_{(R-r\delta)-\delta} &\le \frac{25}{\delta\epsilon^{r+2}}\mu^2 \left|X_{\mathcal{R}^{(r)}}\right|_{R-r\delta}\left|X_{\mathcal{G}_{(r+1)}}\right|_{R-r\delta} \\
&\le \frac{25\epsilon^r}{\delta}\left(\frac{P}{\epsilon_0^r}\right)\left(\frac{P}{\alpha\epsilon_0^r}\right) \le \frac{25P^2}{\alpha\delta\epsilon_0^r}\left(\frac{\epsilon}{\epsilon_0}\right)^r \\
&\le \frac{25P^2}{2^r\alpha\delta\epsilon_0^r}
\end{aligned}
$$

Hence

$$
\begin{aligned}
\left|X_{\mathcal{R}^{(r+1)}}\right|_{(R-r\delta)-\delta} &\le \frac{P}{\alpha\delta}\left[\frac{25P}{2^r\epsilon_0^r} + \frac{60P}{\epsilon_0^r} + \frac{5P}{2^r\epsilon_0^r}\right] \\
&\le \frac{P}{\alpha\delta}\left[\frac{P}{\epsilon_0^r}\left(60 + \frac{30}{2^r}\right)\right] \qquad (115)
\end{aligned}
$$

If $r = 0$ then the second term is not present and the square bracket in (115) is equal to $30P$; if $r \ge 1$, one has that the square bracket in (115) is less than $75P/\epsilon_0^r$ and thus the thesis on the vector fields follows. The estimates of the moduli are obtained in a similar way from Lemma 5. □

It is clear that the Hamiltonian (24) of the NLS fulfills the assumptions of the Lemma with $r = 0$ and thus the Lemma allows us to put our Hamiltonian in normal form up to any order r. To obtain the exponentially small estimate of the remainder take $\delta = R/2r$ in order to fix the domain of definition of the final Hamiltonian, and then choose an optimal value of r, this can be done by minimizing the estimate of the remainder or simply choosing

$$
r_* := \left[\frac{R\alpha}{150eP\epsilon}\right]
$$

(with [.] denoting the integer part). One thus obtains the following Theorem which is the main technical result of the paper, where $\mathcal{Z} = \epsilon\mathcal{Z}^{(r_*)}$ and $\mathcal{R} = \epsilon^{r_*+1}\mathcal{R}^{(r_*)}$.

Theorem 6. *Consider the Hamiltonian $\mathcal{E}$ (cfr. (24)), define*

$$
\epsilon_* := \frac{\alpha R}{150eP}, \qquad (116)
$$

assume $|\epsilon| < \epsilon_*/2$ then there exists an analytic canonical transformation $\mathcal{T}$ such that

$$
\mathcal{E}\circ\mathcal{T} = \mathcal{H}_0 + \mathcal{Z} + \mathcal{R}, \qquad (117)
$$

with $\mathcal{Z}$ non coupling; both $\mathcal{Z}$ and $\mathcal{R}$ have a vector field which is analytic in $B_{R/2}$ and fulfill the estimate

$$|X_{\mathcal{Z}}|_{R/2} \leq 12\epsilon P \ , \quad |X_{\mathcal{R}}|_{R/2} \leq \epsilon P \exp\left[-\left(\frac{\epsilon_*}{\epsilon}\right)\right] \tag{118}$$

$$|\mathcal{Z}|_{R/2} \leq 12\epsilon P^*, \quad |\mathcal{R}|_{R/2} \leq \epsilon P^* \exp\left[-\left(\frac{\epsilon_*}{\epsilon}\right)\right] \tag{119}$$

Moreover the transformed Hamiltonian is Gauge invariant and the canonical transformation fulfills

$$\sup_{\lceil\xi\rceil \leq R/2} \lceil \xi - \mathcal{T}(\xi) \rceil \leq 2\epsilon \frac{P}{\alpha} \tag{120}$$

It is also important to reformulate the Theorem computing P in terms of the original quantities $\omega, \epsilon, \hbar$ i.e. using (77), thus one easily gets the following

Corollary 7. *Fix a positive R, consider the Hamiltonian $\mathcal{E}$ (cfr. (24)), define the small parameter*

$$\mu := \omega + \frac{|\epsilon|}{\hbar^\sigma}, \tag{121}$$

then there exists $\mu_* > 0$ independent of $\hbar, \omega, \epsilon$, such that, if $\mu < \mu_* \hbar^{3/2}/2$ then there exists an analytic canonical transformation $\mathcal{T}$ which transform $\mathcal{E}$ into (117), where

$$|X_{\mathcal{Z}}|_{R/2} \leq C\mu \ , \quad |X_{\mathcal{R}}|_{R/2} \leq C\mu \exp\left[-\frac{\mu_* \hbar^{3/2}}{\mu}\right] \tag{122}$$

$$|\mathcal{Z}|_{R/2} \leq C\mu, \quad |\mathcal{R}|_{R/2} \leq C\mu \exp\left[-\frac{\mu_* \hbar^{3/2}}{\mu}\right] \tag{123}$$

Moreover the transformed Hamiltonian is Gauge invariant and the canonical transformation fulfills

$$\sup_{\lceil\xi\rceil \leq R/2} \lceil \xi - \mathcal{T}(\xi) \rceil \leq C \frac{\mu}{\hbar^{3/2}} \tag{124}$$

Theorem 3 is a direct corollary of Corollary 7.

The manifold $z = 0$ is approximately invariant for the dynamics of the system (117) and on such a manifold the dynamics is that of a Hamiltonian system with a Hamiltonian function which is an exponentially small perturbation of

$$\mathcal{K}(u, \bar{u}) := \mathcal{Z}(u, \bar{u}, 0, 0). \tag{125}$$

Such a system has the additional integral of motion

$$\mathcal{I}(u, \bar{u}) = \sum_j |u_j|^2 \ . \tag{126}$$

In the true nonlinear system one has

Theorem 7. *Assume $\mu < \mu_* \hbar^{3/2}$ and consider the Cauchy problem for the system (117) which is equivalent to NLS. Define*

$$\delta^2 = \max\left\{ \exp\left[-\frac{\mu_* \hbar^{3/2}}{\mu}\right], \|z_0\|_s^2 \right\}$$

(z_0 being the initial datum for z) then, one has

$$\|z(t)\|_s \leq C\delta \tag{127}$$

and

$$|\mathcal{I}(t)-\mathcal{I}(0)|\leq C\delta^2\ ,\quad |\mathcal{K}(t)-\mathcal{K}(0)|\leq C\mu\delta^2 \tag{128}$$

for all times t fulfilling

$$|t|\leq\frac{1}{C\mu\delta}. \tag{129}$$

Proof. First remark that due to the equivalence of the E norm and the s norm one has

$$\sqrt{\mathcal{N}_E(\zeta_0)}=\|z_0\|_E\leq C\delta. \tag{130}$$

Thus, by (63) and (123) one has

$$\frac{d\mathcal{N}_E}{dt}\leq C\mu(\mathcal{N}_E)^{3/2}+C\mu\exp\left[-\frac{\mu_*\hbar^{3/2}}{\mu}\right]\sqrt{\mathcal{N}_E}\leq C\mu(\mathcal{N}_E)^{3/2} \tag{131}$$

which can be solved giving the estimate

$$\mathcal{N}_E(t)\leq 2\delta^2 \tag{132}$$

for the times (129). The estimate of $\|z(t)\|_s$ follows from equivalence of the norms. To obtain the estimate of the diffusion of $\mathcal{I}$ simply remark that $\mathcal{N}=\mathcal{I}+\mathcal{N}_E$ is an exact integral of motion and use the estimate (132). Finally, to estimate the diffusion of $\mathcal{K}$ remark that the total Hamiltonian is an integral of motion, but one has

$$|\mathcal{E}\circ\mathcal{T}-\mathcal{H}_0+\mathcal{K}|\leq C\mu\left(\|z(t)\|_s^2+\exp\left[-\frac{\mu_*\hbar^{3/2}}{\mu}\right]\right) \tag{133}$$

which using the previous estimates implies the thesis. □

Proof of Theorem 2. Define first $\mathcal{M}:=\mathcal{T}(\Phi_0)$. In order to distinguish between the original coordinates of the NLS equation and the new coordinates introduced by the transformation $\mathcal{T}$ we will denote the new variables by adding a prime, i.e. we will write $\zeta=\mathcal{T}(\zeta')$. Remark that since $\mathcal{T}$ is Lipschitz together with its inverse, then for any couple of points $\zeta,\tilde{\zeta}$ one has

$$C^{-1}\left\|\zeta-\tilde{\zeta}\right\|_s\leq\left\|\zeta'-\tilde{\zeta}'\right\|_s\leq C\left\|\zeta-\tilde{\zeta}\right\|_s \tag{134}$$

and therefore

$$d(\psi^0,\mathcal{M})\leq\delta\Longrightarrow d(\zeta^{0\prime},\Phi_0)\leq C\delta\iff\|z_0'\|_s\leq C\delta \tag{135}$$

where by a slight abuse of notation we wrote $\psi^0=\mathcal{T}(\zeta')$. Thus eq. (127) implies (21) for the considered times. To get (22), just remark that (again with a slight abuse of notation)

$$\Pi_c\psi=z=z'+O\left(\frac{\mu}{\hbar^{3/2}}\right)$$

and thus (127) implies (22). □

The proof of Corollary 3 is also a direct consequence of eqs. (128) when one considers the deformation induced by the change of variables. A detailed proof is omitted.

Appendix A. Proof of Theorem 1

For possible future reference, in this section we will work in $\mathbb{R}^d$.

We start by recalling some notations and definitions from Robert [18] that will be used in the following

Definition 4. *A function $m:\mathbb{R}^{2d}\to[0,+\infty)$ is called a* tempered weight *if there exist $C_0, N_0>0$ such that*

$$m(X)\le C_0 m(X_1)(1+|X-X_1|)^{N_0}\ ,\quad \forall X,X_1\in\mathbb{R}^{2d} \tag{136}$$

Definition 5. *A function $a\in C^\infty(\mathbb{R}^{2d})$ is called a semiclassical symbol with weight (m,ρ), with $\rho\ge0$, if for any multi index α there exists a constant C_α such that*

$$|\partial^\alpha a(X)|\le C_\alpha\frac{m(X)}{(1+|X|)^{\rho|\alpha|}}\ ,\quad \forall X\in\mathbb{R}^{2d} \tag{137}$$

In this case we write $a\in\Sigma^m_\rho$.

In the following we will also need an extension to $\hbar$ dependent families of symbols.

Definition 6. *A smooth map $\hbar\mapsto a(\hbar)\in\Sigma^m_\rho$ is called an $\hbar$-admissible symbol of class (m,ρ), if for any integer N large enough one has*

$$a(\hbar)=a_0+\hbar a_1+\hbar^2a_2+...+\hbar^N a_N+r_{N+1} \tag{138}$$

with $a_j\in\Sigma^{m,-2j}_\rho$ and $r_{N+1}(\hbar)$ bounded in $\Sigma^{m,-2(N+1)}_\rho$. Here $\Sigma^{m,K}_\rho$ is the class of symbols with weight

$$\left(m\,(1+|X|)^{K\rho},\rho\right).$$

Given an $\hbar$-admissible symbol a of class (m,ρ), one defines the corresponding Weyl operator acting on L^2 by

$$Op^w(a)\psi(x):=\frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^{2d}}\mathrm{e}^{i\frac{(x-y,\xi)}{2}}a\left(\frac{x+y}{2},\xi,\hbar\right)\psi(y)\mathrm{d}^dy\mathrm{d}^d\xi \tag{139}$$

By the theory of [18] one has that, for any $\hbar>0$, such an operator is well defined on the Schwartz space. Under suitable conditions it extends to a selfadjoint operator on L^2.

Definition 7. *A strongly admissible operator of weight (m,ρ) is a C^∞ application*

$$A:(0,\hbar_*)\to\mathcal{L}(S(\mathbb{R}^d),L^2(\mathbb{R}^d))$$

such that there exists an admissible symbol $a\in\Sigma^m_\rho$ such that $A(\hbar)=Op^w(a(\hbar))$.

One of the most important properties of strongly admissible operators is the given by the following Theorem.

Theorem 8. *(Theorem II-32 of [18]) Let $A=Op^w(a)$ and $B=Op^w(b)$ be two strongly admissible operators of weights (m,ρ) and (n,ρ) respectively; then AB is a strongly admissible operator with symbol $c(\hbar)$ and weight (mn,ρ). Moreover, if $a\sim\sum_{j\ge0}\hbar^ja_j$ and $b\sim\sum_{j\ge0}\hbar^jb_j$ then $c\sim\sum_{j\ge0}\hbar^jc_j$ with*

$$c_j=\sum_{|\alpha|+|\beta|+k+l=j}\frac{1}{\alpha!\beta!}\left(\frac12\right)^{|\alpha|}\left(\frac12\right)^{|\beta|}(\partial^\alpha_\xi D^\beta_x a_k)(\partial^\beta_\xi D^\alpha_x b_l) \tag{140}$$

where $D_x = -i\partial_x$. Furthermore, for any $N \geq 0$, one has

$$c = \sum_{j=0}^{N} \hbar^j c_j + \hbar^{N+1}\delta_{N+1}, \tag{141}$$

and, for any α, β there exists a positive finite M such that the following estimate holds (for simplicity we restrict to the case $\rho = 0$)

$$\left|\partial_x^\alpha \partial_\xi^\beta \delta_{N+1}(x,\xi)\right| \leq Cm(x,\xi)n(x,\xi) \tag{142}$$

$$\times \left[\sum_{j=0}^{N} \left(p_{mM}(a_j)p_{nM}(r_{N+1}(b)) + p_{nM}(b_j)p_{mM}(r_{N+1}(a))\right)\right. \tag{143}$$

$$\left. + \sum_{N \leq j+k \leq 2N} p_{mM}(a_j)p_{qM}(b_k) + p_{mM}(r_{N+1}(a))p_{nM}(r_{N+1}(b))\right] \tag{144}$$

where we denoted by $r_{N+1}(a)$ the remainder of the asymptotic expansion of a truncated at order N and we denoted

$$p_{mM}(a) = \sup_{|\alpha|+|\beta|\leq M,\ (x,\xi)} \frac{|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)|}{m(x,\xi)}. \tag{145}$$

Fix a positive integer $s \geq 1$ denote $A = H_0^s$ (where H_0 is the operator (2)), from Theorem 8 it follows that $A = Op^w(a)$ with a suitable a having principal symbol $a_0 = (\xi^2 + V)^s$. Denote also $b := \xi^{2s} + V^s$ and $B = Op^w(b)$. Since $V(x) \geq 1$ then one has

$$\frac{1}{C} \leq \frac{1}{C} b(x,\xi) \leq a_0(x,\xi) \leq Cb(x,\xi),\ \forall (x,\xi) \in \mathbb{R}^{2d}. \tag{146}$$

Lemma 7. *One has*

$$\|A\psi\|_{L^2} \leq C\|B\psi\|_{L^2}, \quad \forall \psi \in D(B), \tag{147}$$

$$\|B\psi\|_{L^2} \leq C\|A\psi\|_{L^2}, \quad \forall \psi \in D(A). \tag{148}$$

Proof. Consider b^{-1}, then $b^{-1} \in \Sigma_0^{b^{-1}}$. Denote $\mathcal{B} := Op^w(b^{-1})$. By Theorem 8 one has

$$A\mathcal{B} = Op^w\left(\frac{a_0}{b}\right) + \hbar Op^w(\delta_1) \tag{149}$$

$$B\mathcal{B} = \mathbb{I} + \hbar Op^w(\delta_2) \tag{150}$$

with $\delta_{1,2}$ estimated by (142)-(144). Since $\frac{a_0}{b}$ is bounded together with its derivatives, it follows that $\Delta_1 := Op^w(\delta_1)$ is bounded. Similarly $\Delta_2 := Op^w(\delta_2)$ is bounded.

Thus, using Neumann formula one gets that the operator $\mathbb{I} + \hbar\Delta_2$ is invertible provided $\hbar$ is small enough. So, from (150) one has

$$(\mathbb{I} + \hbar\Delta_2)^{-1}B\mathcal{B} = \mathbb{I} \quad \Longleftrightarrow \quad \mathcal{B}^{-1} = (\mathbb{I} + \hbar\Delta_2)^{-1}B. \tag{151}$$

Finally one has

$$\begin{aligned} \|A\psi\|_{L^2} &= \left\|A\mathcal{B}\mathcal{B}^{-1}\psi\right\|_{L^2} \leq \|A\mathcal{B}\|_{\mathcal{L}(L^2,L^2)} \left\|\mathcal{B}^{-1}\psi\right\|_{L^2} \\ &\leq C\left\|(\mathbb{I} + \hbar\Delta_2)^{-1}B\psi\right\|_{L^2} \leq C\|B\psi\|_{L^2}. \end{aligned} \tag{152}$$

□

Appendix B. Technical Lemmas

We start by a Lemma which is needed for the estimate of the solution of the homological equation. In its statement we will denote by ℓ^2 the real Hilbert space of the sequences $(z_j)_{j\geq 3}$ endowed by the scalar product

$$\langle z; z'\rangle := \sum_{j\geq 3} z_j z_j' = \sum_{\gamma} \sum_{j\geq 3,\ j\in J_\gamma} z_j z_j'$$

Lemma 8. *Let $F:\ell^2\to\ell^2$ be a bounded linear operator, assume that the corresponding matrix elements F_{jl} are different from zero only if $j\in J_\gamma$ and $l\in J_{\gamma'}$ with $\gamma\neq\gamma'$. Define a new linear operator G with matrix*

$$G_{jl} := \frac{F_{jl}}{i(\lambda_l-\lambda_j)} \tag{153}$$

Then there exists a positive C such that the following estimate holds

$$\left\|G\right\|_{\mathcal{L}(\ell^2,\ell^2)} \leq \frac{C}{\hbar^{3/2}} \left\|F\right\|_{\mathcal{L}(\ell^2,\ell^2)}\ , \tag{154}$$

Proof. First we recall that $|\lambda_j-\lambda_l|\geq C^{-1}\hbar$ if $j\in J_\gamma$ and $l\in J_{\gamma'}$ for $\gamma\neq\gamma'$, and that $\#J_\gamma\leq C/\hbar$. Fix $l\in J_{\gamma'}$. First remark that

$$\sum_j |F_{jl}|^2 \leq \left\|F\right\|^2_{\mathcal{L}(\ell^2,\ell^2)} \tag{155}$$

then, by Schwartz inequality

$$\sum_j |G_{jl}| \leq \left(\sum_j |F_{jl}|^2\right)^{1/2} \left(\sum_{j\in J_\gamma,\gamma\neq\gamma'} \frac{1}{|\lambda_l-\lambda_j|^2}\right)^{1/2}$$

Fix $l\in J_{\gamma'}$ and estimate

$$\sum_j \frac{1}{|\lambda_l-\lambda_j|^2} = \sum_{\gamma\neq\gamma'}\sum_{j\in J_\gamma} \frac{1}{|\lambda_l-\lambda_j|^2} \tag{156}$$

$$= \left(\sum_{\gamma=\gamma'\pm1} + \sum_{\gamma=1}^{\gamma'-2} + \sum_{\gamma\geq\gamma'+2}\right)\left(\sum_{j\in J_\gamma}\frac{1}{|\lambda_l-\lambda_j|^2}\right) \tag{157}$$

but, due to the choice of the numbers E_γ one has

$$|\lambda_j-\lambda_l| \geq \begin{cases} C^{-1}\hbar & \text{if} \quad \gamma=\gamma'\pm1 \\ E_{\gamma'}-E_\gamma & \text{if} \quad \gamma\leq\gamma'-2 \\ E_{\gamma-1}-E_{\gamma'} & \text{if} \quad \gamma\geq\gamma'+2 \end{cases} \tag{158}$$

thus (156) is estimated by

$$\left(\sup_\gamma \#J_\gamma\right)\left(\frac{2C^2}{\hbar^2} + \sum_{\gamma=1}^{\gamma'-2}\frac{1}{(E_{\gamma'}-E_\gamma)^2} + \sum_{\gamma\geq\gamma'+2}\frac{1}{(E_{\gamma-1}-E_{\gamma'})^2}\right) \tag{159}$$

Since the sums in (159) are convergent due to our choice of the sequence E_γ on has

$$\sum_j \frac{1}{|\lambda_l-\lambda_j|^2} \leq \frac{C}{\hbar^3}$$

which gives

$$\sum_j |G_{jl}| \le \frac{C}{\hbar^{3/2}} \|F\|_{\mathcal{L}(\ell^2,\ell^2)} \tag{160}$$

¿From this one has

$$\begin{aligned}\|Gz\|^2_{\ell^2} &= \sum_j \left|\sum_l G_{jl} z_l\right|^2 \le \sum_j \left(\sum_l |G_{jl}|\right)\left(\sum_l |G_{jl}|\,|z_l|^2\right) \\ &= \left(\sum_l |G_{jl}|\right)\sum_j \left(\sum_l |G_{jl}|\,|z_l|^2\right) \le \frac{C\,\|F\|^2_{\mathcal{L}(\ell^2,\ell^2)}}{\hbar^3} \|z\|^2_{\ell^2}\end{aligned}$$

□

We report now some Lemmas from [3] which are needed for the proof of Lemma 6. Here μ will be small parameter (not the small parameter used in the main part of the text) that in applications will be replaced by ϵ^r with some r.

Lemma 9. *Let $\mathcal{G} : B_\rho \to \mathbb{C}$, $\rho > 0$ be a function whose Hamiltonian vector field is analytic as map from $B_\rho \to \mathcal{X}^s_{\mathbb{C}}$; fix a positive $\delta < \rho$. Assume $\mu \left|X_{\mathcal{G}}\right|_\rho < \delta$ and consider the flow ϕ^t of the corresponding Hamiltonian vector field. Then, for $|t| \le \mu$, one has*

$$|\phi^t - \mathbb{I}|_{\rho-\delta} \le \mu \left|X_{\mathcal{G}}\right|_\rho \ . \tag{161}$$

Proof. It is just an application of the equality

$$\xi(t) - \xi(0) = \int_0^t \frac{d\xi}{dt}(s)ds = \int_0^t X_{\mathcal{G}}(\xi(s))ds \ .$$

□

Lemma 10. *Consider $\mathcal{G}$ as above and let $\mathcal{H}$ be an analytic function with vector field analytic in B_ρ, fix $0 < \delta < \rho$ assume $\mu \left|X_{\mathcal{G}}\right|_\rho \le \delta/3$, then, for $|t| \le \mu$, one has*

$$\left|X_{\mathcal{H}\circ\phi^t}\right|_{\rho-\delta} \le \left(1 + \frac{3}{\delta}\mu \left|X_{\mathcal{G}}\right|_\rho\right) \left|X_{\mathcal{H}}\right|_\rho$$

Proof. First remark that, since ϕ^t is a canonical transformation one has

$$X_{\mathcal{H}\circ\phi^t}(\xi) = d\phi^{-t}(\phi^t(\xi)) X_{\mathcal{H}}(\phi^t(\xi)) \tag{162}$$

from which

$$X_{\mathcal{H}\circ\phi^t}(\xi) = \left(d\phi^{-t}(\phi^t(\xi)) - \mathbb{I}\right) X_{\mathcal{H}}(\phi^t(\xi)) + X_{\mathcal{H}}(\phi^t(\xi)).$$

To estimate the first term fix $\delta_1 := \delta/3$; we have

$$\begin{aligned}\sup_{\lceil\xi\rceil \le \rho-3\delta_1} \lceil d\phi^{-t}(\phi^t(\xi)) - \mathbb{I}\rceil &\le \sup_{\lceil\xi\rceil \le \rho-2\delta_1} \lceil d\phi^{-t}(\xi) - \mathbb{I}\rceil \\ &\le \frac{1}{\delta_1} \sup_{\lceil\xi\rceil \le \rho-\delta_1} \lceil \phi^{-t}(\xi) - \xi\rceil \le \frac{\mu}{\delta_1} \left|X_{\mathcal{G}}\right|_\rho .\end{aligned}$$

Going back to δ and adding the trivial estimate of the second term one has the thesis. □

Lemma 11. *Let $\mathcal{G}$ and $\mathcal{H}$ be as above, fix $0<\delta<\rho$, and assume $\mu\left|X_{\mathcal{G}}\right|_{\rho}<\delta/3$, then, for $|t|\leq\mu$ one has*

$$\left|X_{\mathcal{H}\circ\phi^t-\mathcal{H}}\right|_{\rho-\delta}\leq\frac{5}{\delta}\left|X_{\mathcal{H}}\right|_{\rho}\mu\left|X_{\mathcal{G}}\right|_{\rho}$$

Proof. One has

$$X_{\mathcal{H}\circ\phi^t}(\xi)-X_{\mathcal{H}}(\xi)=\left(d\phi^{-t}(\phi^t(\xi))-\mathbb{I}\right)X_{\mathcal{H}}(\phi^t(\xi))+\left[X_{\mathcal{H}}(\phi^t(\xi))-X_{\mathcal{H}}(\xi)\right]\ .$$

The norm of the square bracket is easily estimated using Lagrange Theorem and the Cauchy inequality in order to bound $dX_{\mathcal{H}}$. The other term was already estimated in Lemma 10, so we have the thesis. □

Although $\mathcal{H}_0$ has unbounded vector field the vector field of $\mathcal{H}_0\circ\phi^{\mu}-\mathcal{H}_0$ is bounded, more precisely we have

Lemma 12. *Let $\mathcal{H}$, $\mathcal{H}_0$, $\mathcal{F}$ and $\mathcal{G}$ as in §2.3; that is $\mathcal{G}$ is the solution of the Homological equation* (78)*; denote by ϕ^t the flow of the corresponding Hamiltonian vector field and*

$$\ell(\xi):=\mathcal{H}_0(\phi^{\mu}(\xi))-\mathcal{H}_0(\xi)-\mu\left\{\mathcal{H}_0,\mathcal{G}\right\},$$

then the vector field of ℓ is analytic and, for any $\delta<\rho$, satisfies

$$\left|X_{\ell}\right|_{\rho-\delta}\leq\mu^2\frac{25}{\delta}\left|X_{\mathcal{G}}\right|_{\rho}\left|X_{\mathcal{H}}\right|_{\rho}.$$

Proof. One has

$$\mathcal{H}_0(\phi^{\mu}(\xi))-\mathcal{H}_0(\xi)=\int_0^{\mu}\frac{d}{dt}\mathcal{H}_0(\phi^t(\xi))dt=-\int_0^{\mu}\mathcal{F}(\phi^t(\xi))dt,$$

where we used the homological equation (78) to calculate $\{\mathcal{H}_0,\mathcal{G}\}$. Then one has

$$\ell(\xi)=\int_0^{\mu}\left[\mathcal{F}(\phi^t(\xi))-\mathcal{F}(\xi)\right]dt;$$

Using Lemma 5 and Lemma 11 one gets the thesis. □

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