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Destruction of the Beating Effect for a Non-Linear Schrödinger Equation

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Abstract: We consider a non-linear perturbation of a symmetric double-well potential as a model for molecular localization. In the semiclassical limit, we prove the existence of a critical value of the perturbation parameter giving the destruction of the beating effect. This value is twice the one corresponding to the first bifurcation of the fundamental state. Here we make use of a particular projection operator introduced by G. Nenciu in order to extend to an infinite dimensional space some known results for a two-level system.

1. Introduction

As it is well known, quantum double-well problems exhibit some caracteristic features such as “splitting of the energy levels”, “delocalization” and “beating effect”. It is also known that certain molecules, e.g. the ammonia one NH_3, are such that one of the nuclei (the nitrogen nucleus N in the case of ammonia), in the Born–Oppenheimer approximation, moves according to a double-well effective potential. The beating effect for such molecules, related to the periodic motion of a state passing from localization at one of the wells to localization at the other one, appears as an “inversion line” on the spectrum.

For non-isolated molecules we have the “red shift” of the “inversion line”, and, if the ammonia gas is at a pressure large enough (about 2 atmospheres) the inversion line disappears, the N nucleus becomes localized: the well known pyramidal shape of the molecule (molecular structure) appears. Thus, we see classical behaviors of microscopical systems. The cause of this phenomenon should be the polarity of the pyramidal molecule which polarizes the environement, so that the reaction field stabilizes the molecular structure.

We consider a standard model for molecular structure: a symmetric double-well potential with a non-linear perturbation [5]. In previous research [6, 7] a critical value of the perturbation parameter has been found giving a bifurcation of the fundamental state and new asymmetrical states.

The present research shows that for such a value of the parameter the dynamics is not qualitatively changed with respect to the unperturbed case; in particular the beating effect is unchanged. On the other side, here we found another critical value of the parameter at which we have the destruction of the beating effect. In particular, beating motion exists for any value of the parameter smaller than the critical one, at the limit of the critical value, the period of this motion diverges, and for larger values of the parameter the beating effect is absent (see Theorem 2 and Corollary 1). Curiously enough, this second critical value of the parameter is nearly (exactly in the limit considered) twice the previous one. The factor 2 between the critical values of the parameter is explained by the similar role played by two different “energy” invariants belonging to the original problem and to the linearized one respectively.

Our work is based on the reduction of the problem to a bi-dimensional space in the semiclassical limit and it makes use of the known results about the dynamics of the reduced two level problem [13, 17]. The paper is organized in the following way. In Sect. 2 we describe the model and we give the main results. In Sect. 3 we prove the theorems. In particular in Sect. 3.2 the reduction of the time-dependent problem into a bi-dimensional space in the semiclassical limit is given. In Sect. 3.3 we recall some known results about the bi-dimensional problem, concerning the trajectories and the frequencies of the motion for different values of the parameter. Finally, in Sect. 3.4 we prove the stability result and the existence of the critical parameter in the full problem.

2. Description of the Model and Main Results

We consider here the time-dependent non-linear Schrödinger equation

$$\begin{cases} i\hbar \frac{\partial \psi}{\partial t} = H_0\psi + f(x,\psi)\psi, \quad H_0\psi = -\frac{\hbar^2}{2m}\Delta\psi + V(x)\psi, \\ \psi(t,x)|_{t=0} = \psi^0(x) \end{cases} \tag{1}$$

where $V(x)$, $x \in \mathrm{R}^n$, is a double-well symmetric potential:

$$V(x', -x_n) = V(x), \quad x = (x', x_n) \in \mathrm{R}^n, \quad x' = (x_1, \dots, x_{n-1}),$$

and

$$f(x,\psi) = \epsilon \langle \psi, W\psi \rangle W(x), \tag{2}$$

where ϵ is a real parameter and $W \in C(\mathrm{R}^n)$ is a given real-valued, bounded, odd function:

$$W(x', -x_n) = -W(x), \quad x = (x', x_n). \tag{3}$$

In such a case W locally represents the position operator x_n and Eq. (1) would describe the effect of the spontaneous symmetry breaking for a symmetric molecule [4–7, 12].

It is well known [2] that when the nonlinear term has a form given by (2) then we have the conservation of the *energy* defined below:

$$\mathcal{H} = \langle H_0\psi, \psi \rangle + \frac{1}{2}\epsilon \langle \psi, W\psi \rangle^2 = \langle H_0\psi^0, \psi^0 \rangle + \frac{1}{2}\epsilon \langle \psi^0, W\psi^0 \rangle^2.$$

Hereafter, $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$ respectively denote the scalar product and the norm in the Hilbert space $L^2(\mathrm{R}^n)$.

Remark 1. If we consider the locally linear problem defined as

$$i\hbar \frac{\partial \psi}{\partial t} = H^{\mathrm{lin}}\psi,$$

where

$$H^{\mathrm{lin}}\psi = H_0\psi + f(x,\psi^0)\psi, \quad f(x,\psi^0) = \epsilon\langle\psi^0, W\psi^0\rangle W,$$

then we have the conservation of the energy defined as

$$\mathcal{E} = \langle\psi^0, H^{\mathrm{lin}}\psi^0\rangle = \langle H_0\psi^0, \psi^0\rangle + \epsilon\langle\psi^0, W\psi^0\rangle^2.$$

Let $\sigma(H_0)$ be the spectrum of the self-adjoint realization of H_0 on the Hilbert space $L^2(\mathbb{R}^n, dx)$. We assume that the discrete spectrum of H_0 is not empty and let $E_+ < E_-$ be the two lowest eigenvalues of H_0, with associated normalized eigenvectors φ_+ and φ_-. It is well known [8,14,15] that, under very general conditions on V, the splitting between the first two eigenvalues, defined as

$$\omega = E_- - E_+,$$

satisfies to the following asymptotic behavior:

$$\omega \sim e^{-C/\hbar}, \quad \text{as} \quad \hbar \to 0, \tag{4}$$

for some positive constant C (hereafter C denotes any generic positive constant). In the same limit we also have

$$\varphi_\pm(x) \sim \frac{1}{\sqrt{2}}\left[\varphi_0(x) \pm \varphi_0(-x)\right], \quad \text{as} \quad \hbar \to 0,$$

where $\varphi_0(x)$ is a function localized within one well, for instance the right-hand one corresponding to positive values of x_n. We also assume that

$$\operatorname{dist}\left[\{E_+, E_-\}, \sigma(H_0) \setminus \{E_+, E_-\}\right] \sim C\hbar, \quad \text{as} \quad \hbar \to 0, \tag{5}$$

for some positive C.

Now, let

$$\varphi_R = \frac{1}{\sqrt{2}}(\varphi_+ + \varphi_-) \quad \text{and} \quad \varphi_L = \frac{1}{\sqrt{2}}(\varphi_+ - \varphi_-),$$

they are normalized functions such that

$$\varphi_R(x) \sim \varphi_0(x) \quad \text{and} \quad \varphi_L(x) \sim \varphi_0(-x), \quad \text{as}\ \hbar \to 0. \tag{6}$$

That is φ_R, the so-called *right-hand well wave-function*, is localized within the right-hand well and φ_L, the so-called *left-hand well wave-function*, is localized within the other well.

The solution of Eq. (1) can be written in the form

$$\psi(t,x) = a_R(t)\varphi_R(x) + a_L(t)\varphi_L(x) + \psi_c(t,x), \quad a_{R,L}(t) \in \mathbb{C}, \tag{7}$$

where $\psi_c = \Pi_c\psi$ is the projection of ψ on the eigenspace orthogonal to the two-dimensional space spanned by φ_R and φ_L; that is:

$$\Pi_c = \mathbb{I} - \langle\cdot, \varphi_R\rangle\varphi_R - \langle\cdot, \varphi_L\rangle\varphi_L.$$

It is well known that when the perturbation term f is absent in Eq. (1) then a state, initially prepared on the two lowest states, that is $\psi_c^0 \equiv 0$, generically makes experience of a beating motion between the two wells with period $4\pi\hbar/\omega$ and the expectation value

$$\langle W\rangle^t = \langle \psi(t,\cdot), W(\cdot)\psi(t,\cdot)\rangle$$

has an oscillating behavior within the interval $[-|w|, |w|]$, $w = \langle \varphi_R, W\varphi_R\rangle$.

Now, we are going to consider the effect of the perturbation f on these beating motions in the semiclassical limit.

In the following we assume that the perturbation strength is of the same order of the splitting and we introduce the non-linearity parameter defined as

$$\mu = \frac{c\epsilon}{\omega} = \mathcal{O}(1), \quad \text{as } \hbar \to 0, \tag{8}$$

where

$$c = 2w^2 = 2\rho_0^2, \quad w = \langle \varphi_R, W\varphi_R\rangle = \langle \varphi_+, W\varphi_-\rangle = \rho_0,$$

the choice of $\varphi_\pm$ can be made such that $\rho_0 \in \mathrm{R} - \{0\}$.

We state our main results:

Theorem 1. *For any $\psi^0 \in H^2(\mathrm{R}^n)$, Eq. (1) admits a unique solution $\psi \in C^1\left(\mathrm{R}_t; L^2(\mathrm{R}^n)\right) \cap C^0\left(\mathrm{R}_t; H^2(\mathrm{R}^n)\right)$ such that $\psi(0,x) = \psi^0(x)$. Moreover, for all $t \in \mathrm{R}$ we have that*

$$\|\psi(t,\cdot)\| = \|\psi^0(\cdot)\|. \tag{9}$$

Theorem 2. *If $\psi_c^0 = \Pi_c\psi^0 \equiv 0$ and if*

$$\left|\frac{2|\mathcal{H}-\Omega|}{\omega} - 1\right| > \delta, \quad \Omega = \frac{1}{2}(E_+ + E_-),$$

for some $\delta > 0$ fixed and any $\hbar$ small enough; then there exists τ_B and a positive constant C independent of $\hbar$ and ϵ such that for any $\alpha < 1$

$$\left\|\psi\left(t + \frac{2\tau_B}{\tilde{\omega}}, \cdot\right) - \psi(t,\cdot)\right\| = \mathcal{O}(\tilde{\omega}^\alpha), \quad \forall t \in [0, t^\star],$$

for $\hbar$ small enough, where

$$t^\star = \frac{\tau^\star}{\tilde{\omega}} \ln\left(\frac{1}{\tilde{\omega}}\right) \text{ and } \tau^\star = (\alpha - 1)/C.$$

In particular, the expectation value $\langle W\rangle^t$ is, up to an error of order $\mathcal{O}(\tilde{\omega}^\alpha)$, a periodic function with pseudo-period $T = 2\tau_B/\tilde{\omega}$ and:

(i) *if*

$$\frac{2|\mathcal{H}-\Omega|}{\omega} < 1 - \delta \tag{10}$$

for some $\delta > 0$ and any $\hbar$ small enough, then there exists $t_0 > 0$ such that for any $K \in \mathrm{N}$ and $\eta > 0$ fixed then

$$\langle W\rangle^t > 0, \quad t_0 + \eta + kT < t < t_0 + (k + 1/2)\,T - \eta,$$

and

$$\langle W\rangle^t < 0, \quad t_0 + (k+1/2)\,T + \eta < t < t_0 + (k+1)T - \eta$$

for any $k = 0, 1, \ldots, K$ *and* $\hbar$ *small enough;*

(ii) *in contrast, if*

$$\frac{2|\mathcal{H} - \Omega|}{\omega} > 1 + \delta \tag{11}$$

for some $\delta > 0$ *and any* $\hbar$ *small enough, then*

$$\langle W\rangle^t \neq 0, \quad \forall t \in [0, t^\star].$$

Remark 2. Condition (10) implies that $\mathcal{H} \in (E_+, E_-)$ and condition (11) implies that $\mathcal{H} \notin [E_+, E_-]$.

Remark 3. For an expression of the pseudo-period we refer to Sect. 3.3; in particular, τ_B is given by Eq. (45) in the case (10) and τ_B is given by Eq. (46) in the case (11).

For what concerns the dynamics of a state initially prepared on one well, e.g. the right-hand one, we have that:

Corollary 1 (Beating Destruction: The critical parameter). *Let* $\psi^0 = \psi_R$ *and* $\mu_\infty \neq \pm 2$*, where* $\mu = \mu_\infty + o(1)$*, as* $\hbar \to 0$*. Then the state returns near to the initial condition after a pseudo-period* T *of order* $1/\tilde{\omega}$*; that is for any* $\alpha < 1$ *and any* $K \in \mathrm{N}$ *fixed then:*

$$\|\psi(kT, \cdot) - \psi_R(\cdot)\| = \mathcal{O}(\tilde{\omega}^\alpha), \quad \text{for any } k = 1, 2, \ldots, K.$$

Moreover, if:

(i) $|\mu_\infty| < 2$*, then*

$$\|\psi\left((k+1/2)T, \cdot\right) - \psi_L(\cdot)\| = \mathcal{O}(\tilde{\omega}^\alpha), \quad k = 1, 2, \ldots, K,$$

and we have the beating motion between the two wells as in the unperturbed case;

(ii) $|\mu_\infty| > 2$*, then*

$$\langle W\rangle^t > 0, \quad \forall t \in [0, t^\star],$$

that is the state ψ *is localized within the right-hand well.*

3. Proof of the Theorems

3.1. Proof of Theorem 1. We denote

$$\tilde{\psi} = e^{itH_0/\hbar}\psi \quad \text{and} \quad \tilde{W} = e^{itH_0/\hbar} W e^{-itH_0/\hbar}.$$

Then Eq. (1) is equivalent to:

$$i\hbar\frac{\partial\tilde{\psi}}{\partial t} = F(\tilde{\psi}), \tag{12}$$

where

$$F(\tilde{\psi}) = \epsilon\langle\tilde{\psi}, \tilde{W}\tilde{\psi}\rangle\tilde{W}\tilde{\psi}$$

satisfies to the following Lipschitz-type estimate: for any $\tilde{\psi}_1, \tilde{\psi}_2 \in L^2(\mathrm{R}^n)$ we have that

$$\|F(\tilde{\psi}_1) - F(\tilde{\psi}_2)\| \leq C\epsilon \left(\|\tilde{\psi}_1\|^2 + \|\tilde{\psi}_2\|^2 \right) \|\tilde{\psi}_1 - \tilde{\psi}_2\| \tag{13}$$

for some positive constant C. Therefore, for ϵ small enough, a local existence and unicity result follows from Cauchy's theorem. Moreover, for any solution $\tilde{\psi}$ of (12) we have that

$$\frac{\partial \|\tilde{\psi}\|^2}{\partial t} = 2\Re \left\langle \frac{\partial \tilde{\psi}}{\partial t}, \tilde{\psi} \right\rangle = 2\hbar^{-1} \Im \langle F(\tilde{\psi}), \tilde{\psi} \rangle = 0;$$

hence, $\|\tilde{\psi}\|$ is constant with respect to t. As a consequence, $\left\| \frac{\partial \tilde{\psi}}{\partial t} \right\|$ remains uniformly bounded on any open interval of time where it is defined and thus the global existence in time follows from standard arguments. Finally, if $\psi^0 \in H^2(\mathrm{R}^n)$ one also has that $\tilde{\psi} \in C^\infty(\mathrm{R}_t; H^2(\mathrm{R}^n))$ and thus $\psi \in C^1\left(\mathrm{R}_t; L^2(\mathrm{R}^n)\right) \cap C^0\left(\mathrm{R}_t; H^2(\mathrm{R}^n)\right)$.

3.2. Reduction to a two-level system. Here, we prove a stability result which allows us to reduce the analysis of Eq. (1) to a bi-dimensional space. To this purpose we make use of some ideas contained in [10, 11] and [16]. Now, let

$$\tilde{\omega} = \frac{\omega}{\hbar} \quad \text{and} \quad H_1 = \frac{1}{\hbar} H_0, \tag{14}$$

where $\frac{\epsilon}{\tilde{\omega}\hbar} = \mathcal{O}(1)$ as $\hbar \to 0$. We treat $\tilde{\omega}$ as a new semiclassical parameter. We have that:

Theorem 3. *Let*

$$\psi(t,x) = a_R(t)\varphi_R(x) + a_L(t)\varphi_L(x) + \psi_c(t,x), \quad a_{R,L}(t) \in \mathrm{C}, \quad \psi_c = \Pi_c \psi,$$

be the solution of Eq. (1) satisfying the initial condition $\psi_c^0 \equiv 0$. Then there exists a positive constant C such that

$$\|H_0 \psi_c\| \leq C\tilde{\omega} e^{C\tilde{\omega}t}, \quad \|\psi_c\| \leq C\tilde{\omega} e^{C\tilde{\omega}t} \tag{15}$$

and

$$\left| a_{R,L}(t) - e^{-i(E_+ + E_-)t/2\hbar} A_{R,L}(t\omega/2\hbar) \right| \leq C\tilde{\omega} e^{C\tilde{\omega}t} \tag{16}$$

for $\hbar$ small enough and any $t \in \mathrm{R}^+$, where $A_{R,L}(\tau)$ are the solutions of the non-linear system

$$\begin{cases} iA_R' = -A_L + 2\nu_0\rho_0 A_R \\ iA_L' = -A_R - 2\nu_0\rho_0 A_L \end{cases}, \quad \begin{array}{l} A_{R,L}(0) = a_{R,L}(0) \\ |A_R(\tau)|^2 + |A_L(\tau)|^2 = 1 \end{array}, \tag{17}$$

where $'$ means the derivative with respect to τ and

$$\nu_0 = \nu_0(\tau) = \frac{\epsilon}{\hbar\tilde{\omega}} \rho_0 (|A_R(\tau)|^2 - |A_L(\tau)|^2), \quad \rho_0 = \langle \varphi_+, W\varphi_- \rangle.$$

In particular, for any $\alpha \in (0,1)$, then

$$\|H_0 \psi_c\| \leq C\tilde{\omega}^\alpha, \quad \|\psi_c\| \leq C\tilde{\omega}^\alpha \tag{18}$$

and

$$\left| a_{R,L}(t) - e^{-i(E_+ + E_-)t/2\hbar} A_{R,L}(t\omega/2\hbar) \right| \leq C\tilde{\omega}^\alpha$$

for any $t \in [0, t^\star]$, $t^\star = (\tau^\star/\tilde{\omega}) \ln(1/\tilde{\omega})$, $\tau^\star = (\alpha - 1)/C$.

Proof. In order to prove the theorem we investigate the solution ψ of (1) with initial data:

$$\psi^0 = a_+^0 \varphi_+ + a_-^0 \varphi_-, \quad |a_+^0|^2 + |a_-^0|^2 = 1. \tag{19}$$

In order to do that, we make the change of time scale:

$$t \to \tau = \frac{\omega t}{2\hbar} = \frac{\tilde{\omega} t}{2}$$

which transform (1) into (for the sake of simplicity ψ still denotes the solution of the new equation):

$$\frac{i\tilde{\omega}}{2} \frac{\partial \psi}{\partial \tau} = H_1 \psi + \frac{\epsilon}{\hbar} \langle \psi, W\psi \rangle W\psi. \tag{20}$$

Our first aim is to construct an approximation of ψ as $\tilde{\omega} \to 0^+$. Let us define

$$\|\chi\|_0 = \|\chi\|, \ \chi \in L^2(\mathrm{R}^n), \quad \text{and} \quad \|\chi\|_1 = \|\tilde{H}_1 \chi\|, \ \chi \in D(\tilde{H}_1),$$

where

$$\tilde{H}_1 = H_1 + c_1 \mathrm{I}, \quad c_1 \ \text{is such that} \ \tilde{H}_1 \geq \mathrm{I}, \tag{21}$$

and therefore

$$\|\chi\|_0 \leq \|\chi\|_1 \quad \text{for any} \quad \chi \in D(\tilde{H}_1).$$

We start by proving the following lemma.

Lemma 1. *Let* ψ *be the solution of Eq. (20) with initial data (19). Let* $j = 0$ *or* $j = 1$, $\varphi \in C^1(\mathrm{R}_\tau; L^2(\mathrm{R}^n)) \cap C^0(\mathrm{R}_\tau; H^2(\mathrm{R}^n))$ *be such that* $\|\varphi(\tau, \cdot)\| \leq C$ *for some* $C > 0$ *and any* τ,

$$\|\varphi(0, \cdot) - \psi^0(\cdot)\|_j = \mathcal{O}(\tilde{\omega})$$

and

$$\phi = \left(-\frac{i\tilde{\omega}}{2} \frac{\partial}{\partial \tau} + H_1 + \frac{\epsilon}{\hbar} \langle \varphi, W\varphi \rangle W \right) \varphi \tag{22}$$

be such that

$$\|\phi(\tau, \cdot)\|_j = \mathcal{O}(\tilde{\omega}^2) \tag{23}$$

uniformly for $\tau \geq 0$ *and* $\tilde{\omega}$ *small enough. Then, there exists* $C > 0$ *such that:*

$$\|\varphi(\tau, \cdot) - \psi(\tau, \cdot)\|_j \leq C\tilde{\omega} e^{C\tau}, \ \forall \tau \geq 0. \tag{24}$$

Proof. In order to prove this lemma, first consider $j = 0$. Let us denote

$$\tilde{\varphi} = e^{2i\tau H_1/\tilde{\omega}}\varphi, \ \ \tilde{\psi} = e^{2i\tau H_1/\tilde{\omega}}\psi, \ \ \tilde{\phi} = e^{2i\tau H_1/\tilde{\omega}}\phi, \ \ u = \tilde{\varphi} - \tilde{\psi}$$

and

$$\tilde{W} = e^{2i\tau H_1/\tilde{\omega}} W e^{-2i\tau H_1/\tilde{\omega}}.$$

We have

$$\frac{i\tilde{\omega}}{2}u' = \frac{\epsilon}{\hbar}\left(\langle\varphi, W\varphi\rangle\tilde{W}\tilde{\varphi} - \langle\psi, W\psi\rangle\tilde{W}\tilde{\psi}\right) - \tilde{\phi}$$

and therefore

$$\begin{aligned}\left|\frac{\partial\|u\|^2}{\partial\tau}\right| &= 2|\Re\langle u', u\rangle| \\ &= 4\left|\Im\left\langle\frac{\epsilon}{\hbar\tilde{\omega}}\left(\langle\varphi, W\varphi\rangle\tilde{W}\tilde{\varphi} - \langle\psi, W\psi\rangle\tilde{W}\tilde{\psi}\right) - \frac{1}{2\tilde{\omega}}\tilde{\phi}, u\right\rangle\right| \\ &\le C\left(\|u\|^2 + \tilde{\omega}\|u\|\right) \le C\left(\|u\|^2 + \tilde{\omega}^2\right) \qquad (25)\end{aligned}$$

for any $\tau \ge 0$ and for some constant $C > 0$ since (8), (23) and $ab \le \frac{1}{2}a^2 + \frac{1}{2}b^2$ for any $a, b > 0$. As a result it follows that

$$\frac{\partial}{\partial\tau}\left(e^{-C\tau}\|u\|^2\right) \le Ce^{-C\tau}\tilde{\omega}^2,$$

and thus, since $u|_{\tau=0} = \mathcal{O}(\tilde{\omega})$:

$$e^{-C\tau}\|u\|^2 \le C\tilde{\omega}^2 \qquad (26)$$

for some $C > 0$. Then (24) immediately follows.

Moreover, we have that (24) is still true when we replace the usual norm $\|\chi\|$ by $\|\chi\|_1 = \|\tilde{H}_1\chi\|$, $\chi \in D(H_1)$, where $\tilde{H}_1 = H_1 + c_1 \mathrm{I} \ge \mathrm{I}$ for some c_1. Indeed, let $\tilde{\varphi}$, $\tilde{\psi}$, $\tilde{W}$ and $\tilde{\phi}$ as above and let now

$$u_1 = \tilde{H}_1(\tilde{\varphi} - \tilde{\psi}).$$

Then

$$\frac{i\tilde{\omega}}{2}u_1' = \frac{\epsilon}{\hbar}\left(\langle\varphi, W\varphi\rangle\tilde{H}_1\tilde{W}\tilde{\varphi} - \langle\psi, W\psi\rangle\tilde{H}_1\tilde{W}\tilde{\psi}\right) - \tilde{H}_1\tilde{\phi}$$

and

$$\begin{aligned}\left|\frac{\partial\|u_1\|^2}{\partial\tau}\right| &= 4\left|\Im\left\langle\frac{\epsilon}{\hbar\tilde{\omega}}\left(\langle\varphi, W\varphi\rangle\tilde{H}_1\tilde{W}\tilde{\varphi} - \langle\psi, W\psi\rangle\tilde{H}_1\tilde{W}\tilde{\psi}\right) - \frac{1}{2\tilde{\omega}}\tilde{H}_1\tilde{\phi}, u_1\right\rangle\right| \\ &\le C\left(\|u_1\|^2 + \tilde{\omega}\|u_1\|\right) \le C\left(\|u_1\|^2 + \tilde{\omega}^2\right)\end{aligned}$$

for some constant $C > 0$ since (8), (23) and $\tilde{H}_1 W \tilde{H}_1^{-1}$ and $\tilde{H}_1^{-1}$ are bounded operators, uniformly with respect to $\tilde{\omega}$. As above, it follows that (26) is true, from which (24) follows. □

Now, in order to prove Theorem 3 we explicitly construct a solution φ satisfying the assumptions of Lemma 1. We re-write Eq. (22) as:

$$\left(-\frac{i\tilde{\omega}}{2}\frac{\partial}{\partial\tau}+H_1+\tilde{\omega}\nu W\right)\varphi=\phi, \tag{27}$$

where

$$\nu=\nu(\tau)=\frac{\epsilon}{\hbar\tilde{\omega}}\langle\varphi, W\varphi\rangle, \quad \frac{\epsilon}{\hbar\tilde{\omega}}=\mathcal{O}(1), \quad \text{as } \hbar\to 0,$$

and where φ and ϕ must satisfy the conditions

$$\begin{cases} \|\varphi(0,\cdot)-\psi^0(\cdot)\|_1 \le C\tilde{\omega}, \\ \|\varphi(\tau,\cdot)\| \le C, \ \forall\tau\ge 0, \\ \|\phi(\tau,\cdot)\|_1 \le C\tilde{\omega}^2, \ \forall\tau\ge 0, \end{cases} \tag{28}$$

for some $C>0$, ψ^0 is given by (19).

We denote by $\Pi_0=\mathbb{I}-\Pi_c$ the orthogonal projection onto $\mathbb{C}\varphi_+\oplus\mathbb{C}\varphi_-$, that is:

$$\Pi_0=\frac{1}{2\pi i}\oint_\gamma (\zeta-H_1)^{-1}\,d\zeta,$$

where γ is a simple complex loop encircling $\left\{\frac{1}{\hbar}E_+, \frac{1}{\hbar}E_-\right\}$, leaving the rest of $\sigma(H_1)$ in its exterior and such that (see (5))

$$\operatorname{dist}(\gamma,\sigma(H_1))\ge C,$$

for some constant $C>0$. We also set:

$$\Pi_1=\frac{1}{2\pi i}\oint_\gamma (\zeta-H_1)^{-1}\,W\,(\zeta-H_1)^{-1}\,d\zeta \tag{29}$$

and, for any $\nu\in C^1(\mathbb{R})$,

$$\Pi_{\nu(\tau)}=\Pi_0+\tilde{\omega}\nu(\tau)\Pi_1. \tag{30}$$

From the definition, from (5) and (21) and since

$$H_1\Pi_1=-W\Pi_0+\frac{1}{2\pi i}\oint_\gamma \zeta(\zeta-H_1)^{-1}W(\zeta-H_1)^{-1}d\zeta,$$

then it follows that

$$\|\Pi_1\chi\|_1\le C\|\chi\|_1, \tag{31}$$

for any $\chi\in D(H_1)$.

We look for a solution φ of the linear equation (27) of the form

$$\varphi(\tau)=\Pi_{\nu(\tau)}\left[b_+(\tau)\varphi_++b_-(\tau)\varphi_-\right]. \tag{32}$$

For such a choice of φ and from the definition of ν we have

$$\nu(\tau)=\frac{\epsilon}{\hbar\tilde{\omega}}\langle\varphi, W\varphi\rangle=\frac{\epsilon}{\hbar\tilde{\omega}}\left\{\nu_0+\tilde{\omega}\alpha(\tau)\nu(\tau)+\tilde{\omega}^2\beta(\tau)\nu^2(\tau)\right\}, \tag{33}$$

where

$$\nu_0 = \sum_{\ell,\ \ell'=1}^{2} \bar{b}_{s(\ell)} b_{s(\ell')} \langle \varphi_{s(\ell')}, W\varphi_{s(\ell)} \rangle = 2\Re \left(b_+ \bar{b}_- \rho_0 \right),$$

$s(1) = +$ and $s(2) = -$, since (3), and $\alpha(\tau)$ and $\beta(\tau)$ are functions independent of $\tilde{\omega}$ given by:

$$\alpha = \sum_{\ell,\ \ell'=1}^{2} b_{s(\ell')} \bar{b}_{s(\ell)} \alpha_{s(\ell'),s(\ell)}, \quad \beta = \sum_{\ell,\ \ell'=1}^{2} b_{s(\ell')} \bar{b}_{s(\ell)} \beta_{s(\ell'),s(\ell)},$$

where

$$\alpha_{\pm,\pm} = \left[\langle \varphi_\pm, W\Pi_1 \varphi_\pm \rangle + \langle \Pi_1 \varphi_\pm, W\varphi_\pm \rangle \right], \quad \beta_{\pm,\pm} = \langle \Pi_1 \varphi_\pm, W\Pi_1 \varphi_\pm \rangle.$$

From this fact and since $\frac{\epsilon}{\hbar\tilde{\omega}} = \mathcal{O}(1)$, it follows that $\|\varphi(\tau,\cdot)\| \le C$ and ν satisfies the following behavior:

$$\nu,\ \nu' = \mathcal{O}(1), \quad \text{uniformly w.r. to } \tilde{\omega} > 0 \text{ small enough and } \tau \ge 0, \tag{34}$$

provided that the unknown functions $b_\pm$ and their first derivative are bounded uniformly with respect to τ and $\tilde{\omega}$.

Now, observing that:

$$\left[-\frac{i\tilde{\omega}}{2} \frac{\partial}{\partial \tau} + H_1 + \tilde{\omega}\nu W, \Pi_\nu \right] = K,$$

where

$$K = -\frac{i\tilde{\omega}^2}{2} \nu' \Pi_1 + \tilde{\omega}\nu \left([H_1, \Pi_1] + [W, \Pi_0] \right) + \tilde{\omega}^2 \nu^2 [W, \Pi_1]$$

is such that

$$\|K\chi\|_1 \le C\tilde{\omega}^2 \|\chi\|_1$$

since (34),

$$[H_1, \Pi_1] + [W, \Pi_0] = 0,$$

by definition of Π_1, and since $\tilde{H}_1 W \tilde{H}_1^{-1}$ is a bounded operator. By inserting (32) into (27) we obtain that $b_+(\tau)$ and $b_-(\tau)$ must satisfy to the following equation:

$$\Pi_{\nu(\tau)} \{ c_+ \varphi_+ + c_- \varphi_- \} = \phi, \quad c_\pm = -\frac{i\tilde{\omega}}{2} b_\pm' + \left(\frac{E_\pm}{\hbar} + \tilde{\omega}\nu W \right) b_\pm, \tag{35}$$

where

$$\begin{cases} b_\pm(0) = a_\pm + \mathcal{O}(\omega), \\ \phi = -K(b_+\varphi_+ + b_-\varphi_-), \quad \|\phi(\tau,\cdot)\|_1 \le C\tilde{\omega}^2, \ \forall \tau \ge 0, \end{cases}$$

and $\nu = \frac{\epsilon}{\hbar\tilde{\omega}} \langle \varphi, W\varphi \rangle = \nu_0 + \mathcal{O}(\tilde{\omega})$ has to satisfy (34).

Now, we have that

$$\Pi_{\nu(\tau)}\left(W\varphi_\pm\right) = \Pi_0 W\varphi_\pm + \tilde{\omega}\nu(\tau)\Pi_1 W\varphi_\pm,$$

where

$$\Pi_0 W\varphi_\pm = \langle\varphi_+, W\varphi_\pm\rangle\varphi_+ + \langle\varphi_-, W\varphi_\pm\rangle\varphi_-$$

and

$$\|\tilde{\omega}\nu(\tau)\Pi_1 W\varphi_\pm\|_1 \le C\tilde{\omega}\|W\varphi_\pm\|_1 \le C\tilde{\omega},$$

since (31). Moreover, let

$$\begin{aligned}&(\zeta - H_1)^{-1} K_1 \\ &\quad = (\zeta - H_1 - \tilde{\omega}\nu W)^{-1} - (\zeta - H_1)^{-1} - (\zeta - H_1)^{-1}\tilde{\omega}\nu W(\zeta - H_1)^{-1}\end{aligned}$$

where

$$\begin{aligned}K_1 &= \left[\mathrm{I} - \tilde{\omega}\nu W(\zeta - H_1)^{-1}\right]^{-1} - \mathrm{I} - \tilde{\omega}\nu W(\zeta - H_1)^{-1} \\ &= \tilde{\omega}^2\nu^2(\zeta - H_1)^{-1} W(\zeta - H_1)^{-1} W\left[\mathrm{I} - \tilde{\omega}\nu W(\zeta - H_1)^{-1}\right]^{-1}\end{aligned}$$

is such that for any $\zeta \in \gamma$ then

$$\|K_1\chi\|_1 \le C\tilde{\omega}^2\|\chi\|_1.$$

From this it follows that

$$\Pi_{\nu(\tau)} = \frac{1}{2\pi i}\oint_\gamma (\zeta - H_1 - \tilde{\omega}\nu W)^{-1} d\zeta + K_2,$$

where $\|K_2\chi\|_1 \le C\tilde{\omega}^2\|\chi\|_1$; hence we can write that:

$$\Pi^2_{\nu(\tau)} = \Pi_{\nu(\tau)} + K_3, \quad \|K_3\chi\|_1 \le C\tilde{\omega}^2\|\chi\|_1.$$

Therefore:

$$\begin{aligned}\Pi_{\nu(\tau)}c_+\varphi_+ &= \Pi_{\nu(\tau)}\left[-\frac{i\tilde{\omega}}{2}b'_+ + \left(\frac{E_+}{\hbar} + \tilde{\omega}\nu W\right)b_+\right]\varphi_+ \\ &= \Pi^2_{\nu(\tau)}\left[-\frac{i\tilde{\omega}}{2}b'_+ + \left(\frac{E_+}{\hbar} + \tilde{\omega}\nu W\right)b_+\right]\varphi_+ + \phi_1 \\ &= \Pi_{\nu(\tau)}\left[\left(-\frac{i\tilde{\omega}}{2}b'_+ + \frac{1}{\hbar}E_+b_+\right)\varphi_+ + \tilde{\omega}\nu b_+\langle\varphi_-, W\varphi_+\rangle\varphi_-\right] + \phi_2,\end{aligned}$$

where $\|\phi_\ell\|_1 \le C\tilde{\omega}^2$, $\ell = 1, 2$, and $\langle\varphi_+, W\varphi_+\rangle = 0$. Therefore, (35) can be re-written as:

$$\Pi_{\nu(\tau)}\{d_+\varphi_+ + d_-\varphi_-\} = \phi_3, \quad d_\pm = -\frac{i\tilde{\omega}}{2}b'_\pm + \frac{1}{\hbar}E_\pm b_\pm + \tilde{\omega}\nu\rho_0 b_\mp,$$

where

$$b_\pm(0) = a^0_\pm + \mathcal{O}(\tilde{\omega}), \quad \|\phi_3(\tau,\cdot)\|_1 = \mathcal{O}(\tilde{\omega}^2), \quad \forall\tau \ge 0,$$

with $\rho_0 = \langle \varphi_+, W\varphi_- \rangle \in \mathbb{R}$. As a result it is enough to find $b_\pm$, bounded together with their first derivative for any τ, such that

$$\begin{cases} -\frac{i\tilde{\omega}}{2} b_+' + \frac{1}{\hbar} E_+ b_+ + \tilde{\omega}\nu_0\rho_0 b_- = 0 \\ -\frac{i\tilde{\omega}}{2} b_-' + \frac{1}{\hbar} E_- b_- + \tilde{\omega}\nu_0\rho_0 b_+ = 0 \\ b_\pm(0) = a_\pm^0, \quad \nu_0 = 2\frac{\epsilon}{\hbar\tilde{\omega}} \Re(b_+ \bar{b}_- \rho_0) \end{cases} . \tag{36}$$

Setting:

$$a_R = \frac{1}{\sqrt{2}}(b_+ + b_-) \quad \text{and} \quad a_L = \frac{1}{\sqrt{2}}(b_+ - b_-)$$

the system (36) becomes

$$\begin{cases} -\frac{i\tilde{\omega}}{2} a_R' = -\frac{E_- + E_+}{2\hbar} a_R + \frac{1}{2}\tilde{\omega} a_L - \tilde{\omega}\nu_0\rho_0 a_R \\ -\frac{i\tilde{\omega}}{2} a_L' = -\frac{E_- + E_+}{2\hbar} a_L + \frac{1}{2}\tilde{\omega} a_R + \tilde{\omega}\nu_0\rho_0 a_L \\ \nu_0 = \frac{\epsilon}{\hbar\tilde{\omega}} \rho_0 (|a_R|^2 - |a_L|^2) \\ a_R(0) = \frac{1}{\sqrt{2}}(a_+^0 + a_-^0) \quad \text{and} \quad a_L(0) = \frac{1}{\sqrt{2}}(a_+^0 - a_-^0) \end{cases} , \tag{37}$$

and we look for a solution of the form:

$$a_R(\tau) = A_R(\tau) e^{-i(E_+ + E_-)\tau/\hbar\tilde{\omega}}, \quad a_L(\tau) = A_L(\tau) e^{-i(E_+ + E_-)\tau/\hbar\tilde{\omega}}$$

with A_R and A_L independent of ω. Then (37) is transformed into the correspondent system:

$$\begin{cases} iA_R' = -A_L + 2\nu_0\rho_0 A_R \\ iA_L' = -A_R - 2\nu_0\rho_0 A_L \end{cases}, \tag{38}$$

where

$$\nu_0 = \frac{\epsilon}{\hbar\tilde{\omega}} \rho_0 (|A_R|^2 - |A_L|^2), \quad A_{R,L}(0) = a_{R,L}(0).$$

It easy to verify that $|A_L(\tau)|^2 + |A_R(\tau)|^2 = 1$ since $\rho_0 \in \mathbb{R}$; hence, the solutions $A_{R,L}(\tau)$ exist for any τ and they are bounded, together with their first derivative, uniformly with respect to τ and $\tilde{\omega}$ small enough since $\frac{\epsilon}{\hbar\tilde{\omega}} = \mathcal{O}(1)$. Then (34) will be satisfied uniformly with respect to $\tilde{\omega}$ (actually (38) is independent of $\tilde{\omega}$). From these facts and by (30), (32) and Lemma 1 then the solution of (19)–(20) satisfies the estimates (15) and (16). Theorem 3 is proved. $\square$

3.3. Dynamics of the two-level system. In order to study the system of Eqs. (17) we re-write it in the form

$$\begin{cases} iA_R' = -A_L + 2\mu|A_R|^2 A_R \\ iA_L' = -A_R + 2\mu|A_L|^2 A_L \end{cases}, \quad \begin{matrix} A_{R,L}(0) = a_{R,L}(0) \\ |A_R(\tau)|^2 + |A_L(\tau)|^2 = 1 \end{matrix}, \tag{39}$$

where $'$ denotes the derivative with respect to τ, $c = 2\rho_0^2$, $\mu = \frac{c\epsilon}{\omega}$ plays the role of the parameter of non-linearity and we re-define $A_{R,L}(\tau)$ up to a phase factor, i.e. $A_{R,L}(\tau) \to A_{R,L}(\tau)e^{i2c\tau}$.

Remark 4 (Gross–Pitaevskii equation). If the perturbation term has the form

$$f(x,\psi)=\epsilon|\psi(x)|^2W(x), \tag{40}$$

where $W(x)$ is a given real-valued even function: $W(x',-x_n)=W(x)$, then Eq. (1) takes the form of the Gross–Pitaevskii equation [1] and we have the conservation of the *energy* defined below:

$$\mathcal{H}=\langle H_0\psi,\psi\rangle+\frac{1}{2}\epsilon\langle\psi^2,W\psi^2\rangle.$$

In particular, the same arguments given above prove that the two-level system for the Gross–Pitaevskii equation takes the form (39), where $c=\langle\varphi_R,W|\varphi_R|^2\varphi_R\rangle$ and where the function W is such that this scalar product is defined.

In discussing two-level systems we have characterized the states in terms of

$$A_R(\tau)=p(\tau)e^{i\alpha(\tau)}\quad\text{and}\quad A_L(\tau)=q(\tau)e^{i\beta(\tau)}, \tag{41}$$

where p, q, α and β are real-valued functions, $0\le p\le 1$ and $0\le q\le 1$. From the redundancy of the common phase factor we have that the state can be described now by means of a vector in an abstract Euclidean three-dimensional space with components $(p,q\cos(\beta-\alpha),q\sin(\beta-\alpha))$. In particular, from the normalization condition $p^2+q^2=1$, it belongs, in such an Euclidean space, to the surface of the sphere. Hence, in order to study the solution of the two-level system (39) we represent the surface of the sphere by means of a *Mercator*-type chart; that is by means of two real coordinates (P,z), where $P=p^2\in[0,1]$ is the square of the modulus of A_R and $z=\alpha-\beta\in\mathcal{T}=\mathrm{R}/2\pi\mathrm{Z}=[0,2\pi)$ belongs to the one-dimensional torus and represents the difference between the phases of A_R and A_L (see Ch. 13, [9]). We underline that this representation is singular at $P=0$ and $P=1$; in fact, for $P=0$ (respectively $P=1$) and any z we have localization on the left-hand (respectively right-hand) well.

If the non-linear term is absent in Eq. (39), then $P(\tau)$ is a periodic function with period π and, if initially $P(0)=0$ or $P(0)=1$, then $P(\tau)$ periodically assumes the values 0 and 1.

The system of equations (39) has been recently studied [13]. Here, we recall the most relevant results.

Lemma 2. *et $P(\tau)=p^2(\tau)$ and $z(\tau)=\alpha(\tau)-\beta(\tau)$; then $P(\tau)$ and $z(\tau)$ satisfy the following system of ordinary differential equations:*

$$\begin{cases} P'=2\sqrt{P}\sqrt{1-P}\sin z\\ z'\ =(1-2P)\left[2\mu+\frac{1}{\sqrt{P}\sqrt{1-P}}\cos z\right] \end{cases}. \tag{42}$$

Equations (42) have four stationary solutions

$$\begin{aligned}
&\text{(I)}\quad (P=1/2,z=0)\,,\\
&\text{(II)}\quad (P=1/2,z=\pi)\,,\\
&\text{(III)}\quad \left(P=\frac{1+\sqrt{1-1/\mu^2}}{2},z=\frac{\pi}{2}\left[1+\frac{|\mu|}{\mu}\right]\right),\quad \text{if } |\mu|\ge 1,\\
&\text{(IV)}\quad \left(P=\frac{1-\sqrt{1-1/\mu^2}}{2},z=\frac{\pi}{2}\left[1+\frac{|\mu|}{\mu}\right]\right),\quad \text{if } |\mu|\ge 1,
\end{aligned}$$

where, for $|\mu| < 1$, (I) and (II) are *center points* while, for $\mu > 1$ (respectively $\mu < -1$), the stationary solutions (I) (respectively (II)), (III) and (IV) are *center points* and the stationary solution (II) (respectively (I)) is a *saddle point*.

Moreover, the function

$$I = I(P, z, \mu) = \sqrt{P}\sqrt{1-P}\left[\mu\sqrt{P}\sqrt{1-P} + \cos z\right] \tag{43}$$

is an integral of motion and the dynamics of the two-level system, with initial condition (P_0, z_0), could be described by means of the integral path defined by the implicit equation $I(P, z, \mu) = I(P_0, z_0, \mu)$. In particular, we consider the following two behaviors:

[C1] $P(\tau)$ is a periodic continuous function, with given period τ_B, such that $P(\tau) = \frac{1}{2}$, for $\tau = \tilde{\tau}, \tilde{\tau} + \frac{1}{2}\tau_B$, for some $\tilde{\tau}$, and $P(\tau) < \frac{1}{2}$ and $P(\tau + \frac{1}{2}\tau_B) > \frac{1}{2}$ for any $\tau \in (\tilde{\tau}, \tilde{\tau} + \frac{1}{2}\tau_B)$.

[C2] $P(\tau)$ is a periodic continuous function such that $P(\tau) \neq \frac{1}{2}$ for any τ.

We have that:

Lemma 3. *Let* $(P_0, z_0) \in [0, 1] \times \mathcal{T}$ *be the initial state in the two-level representation. We have:*

(i) *if* $|\mu| \leq 1$, *then* $P(\tau)$ *has a time behavior of type* **C1** *for any initial condition* (P_0, z_0), *but the ones corresponding to the stationary solutions* (I) *and* (II) *(see Fig. 1);*

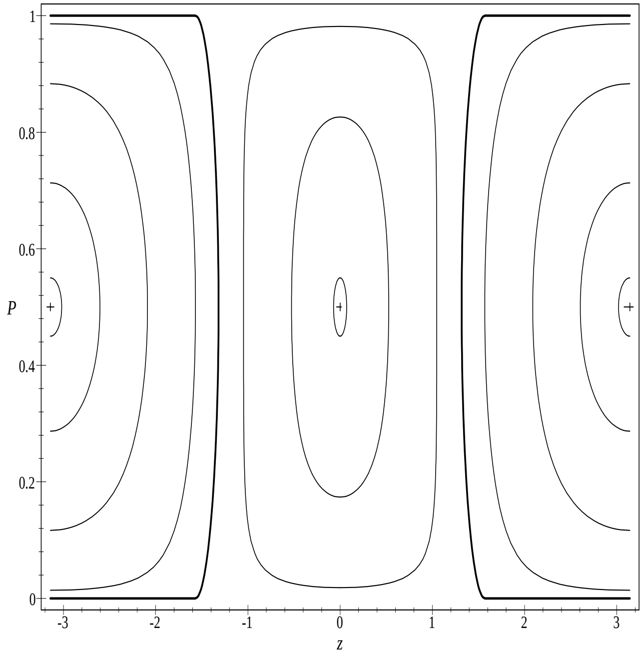

Fig. 1. Integral paths of the equation $I(P, z, \mu) = \tilde{I}$ for some values of $\tilde{I}$ and for $\mu = -\frac{1}{2}$ fixed. The bold line represents the integral path of the beating motion, that is the transition from localization on a well to localization on the other one. Localization on the right-hand (respectively left-hand) well occurs at $P = 1$ (respectively $P = 0$) for any z

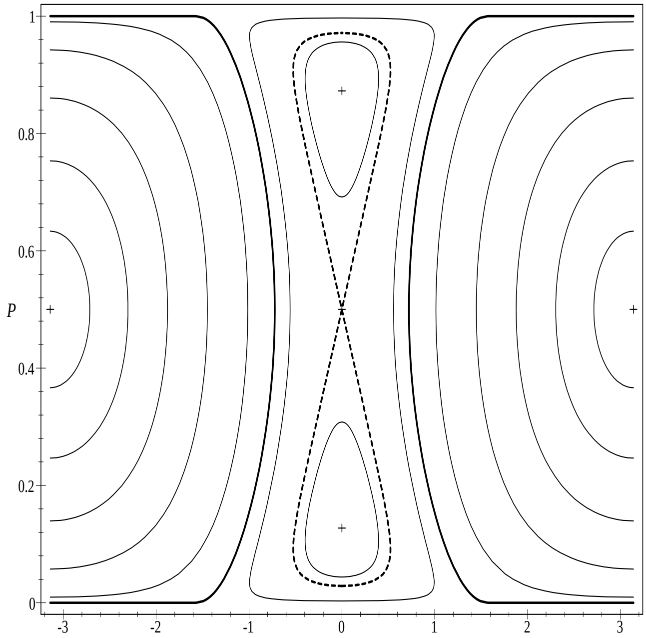

Fig. 2. Integral paths of equation $I(P,z,\mu)=\tilde{I}$ for some values of $\tilde{I}$ and for $\mu=-\frac{3}{2}$ fixed. We observe the stability of the beating motion (bold line) despite the appearance of the bifurcation of one fixed point. Broken lines represent the two sepratrices; inside the region enclosed by these lines we have closed paths, around the asymmetrical stationary state originated from the bifurcation of the fundamentals state, representing periodic oscillations within only one well

(ii) *if* $|\mu|>1$, *let* $\mathcal{D}=\mathcal{D}(\mu)$ *be the bounded open set enclosed by the path with equation*

$$z=\frac{\pi}{2}\left[1+\frac{|\mu|}{\mu}\right]\pm \arccos\left[\frac{1+2\mu P(1-P)-\mu/2}{2\sqrt{P}\sqrt{1-P}}\right] \tag{44}$$

and containing the stationary solutions (III) *and* (IV)*; then for any* $(P_0,z_0)\in\mathcal{D}$, (P_0,z_0) *different from the stationary solutions* (III) *and* (IV), $P(\tau)$ *has a behavior of type* **C2***; in contrast, if* $(P_0,z_0)\notin\bar{\mathcal{D}}$, *where* $\bar{\mathcal{D}}$ *denotes the closure of* $\mathcal{D}$, *and* (P_0,z_0) *is different from the stationary solution* (I), *then* $P(\tau)$ *has a behavior of type* **C1** *(see Figs. 2 and 3).*

Remark 5. Let (P_0,z_0) be such that $P_0=0$ or $P_0=1$. Then $I(P_0,z_0,\mu)=0$ and $(P_0,z_0)\in\mathcal{D}$, if $|\mu|>2$, and $(P_0,z_0)\notin\bar{\mathcal{D}}$, if $|\mu|<2$. Hence, for $|\mu|<2$ we observe the beating motion, such that $P(\tau)$ periodically assumes the values 0 and 1 (see the bold line in Fig. 2). The beating motion corresponds to the path with equation $I(P,z,\mu)=0$; that is:

$$z_{fb}=\frac{\pi}{2}\left[1-\frac{|\mu|}{\mu}\right]\pm \arccos\left[|\mu|\sqrt{P}\sqrt{1-P}\right].$$

In contrast, for $2<|\mu|$ we have that the beating motion between the two wells is not possible (see the bold line in Fig. 3, where $\mu=-\frac{5}{2}$); in particular, if initially $P(0)=1$

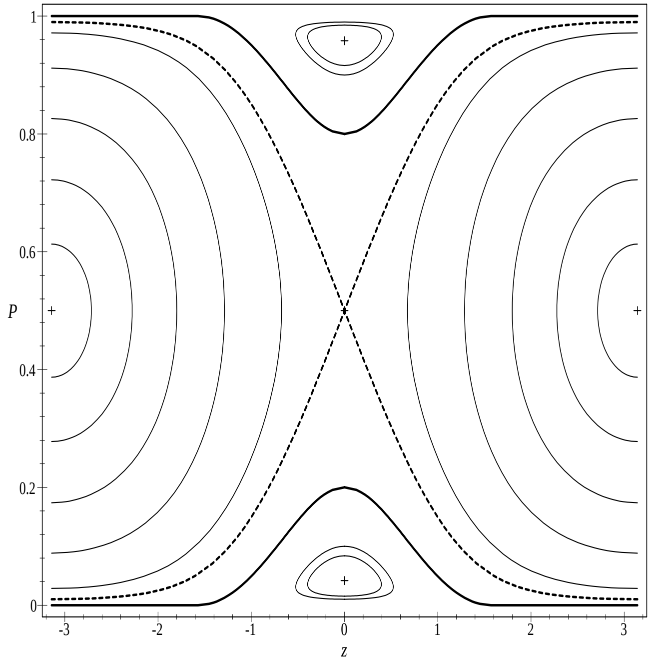

Fig. 3. Integral paths of equation $I(P, z, \mu) = \tilde{I}$ for some values of $\tilde{I}$ and for $\mu = -\frac{5}{2}$ fixed. We observe the destruction of the beating motion. The trajectory (bold line) starting from the localization point corresponding to $P = 1$ (respectively $P = 0$) stays in the region $P > \frac{1}{2}$ (respectively $P < \frac{1}{2}$) and it encircles one asymmetrical stationary state originated from the bifurcation of the fundamental state

(respectively $P(0) = 0$) then during the motion we have that $P(\tau) > \frac{1}{2}$ (respectively $P(\tau) < \frac{1}{2}$) for any τ.

As a result of Lemma 3, it follows that we generically observe a periodic motion with period τ_B that depends on the parameter μ and on the initial condition (P_0, z_0). In particular:

Lemma 4. *If $(P_0, z_0) \notin \bar{\mathcal{D}}$, where the set $\mathcal{D}$ is defined in Lemma 3, then the beating motion between the two wells has period given by*

$$\tau_B = \tau_B(I, \mu) = 4\frac{E_K\left(\mu\frac{\sqrt{(\mu-4I+2)(\mu-4I-2)}}{\mu^2-(1+\sqrt{1+4\mu I})^2}\right)}{\sqrt{(1+\sqrt{1+4\mu I})^2-\mu^2}}, \tag{45}$$

where $I = I(P_0, z_0; \mu)$ and E_K is the complete elliptic integral of the first kind.

We close this section with the following remarks.

Remark 6. If $(P_0, z_0) \in \mathcal{D}$ then we have a periodic motion within one well with period:

$$\tau_B = -2i\frac{\sqrt{x_2}}{\mu\sqrt{x_1}}\left[E_F\left(\frac{\mu\sqrt{x_1}}{x_2}, \frac{x_2}{\mu\sqrt{x_1}}\right) - E_K\left(\frac{x_2}{\mu\sqrt{x_1}}\right)\right], \tag{46}$$

where E_F denotes the incomplete elliptic integral of the first kind and where

$$x_1 = \mu^2 - 4 - 8\mu I + 16I^2 \quad \text{and} \quad x_2 = \mu^2 - (1 + \sqrt{4\mu I + 1})^2.$$

Remark 7. The frequency $\nu^{fb} = 1/\tau^{fb}$ of the beating motion, corresponding to the value $I = 0$ of the integral of motion, depends on $|\mu|$ and monotonically decreases and vanishes at $|\mu| = 2$; indeed, we have that

$$\nu^{fb} = \frac{\sqrt{4-\mu^2}}{4E_K\left(i\mu/\sqrt{4-\mu^2}\right)}$$

which is a monotone decreasing function as $\mu \in [0, 2)$. From formulas (106.02) and (112.01) [3], it follows that

$$\nu^{fb} \sim \frac{1}{2}\frac{1}{\ln(8/\sqrt{4-\mu^2})} \quad \text{as} \quad |\mu| \to 2^-.$$

We remark also that the range of frequencies is given by $(\nu_{\min}, \nu_{\max}]$, where

$$\nu_{\min} = \begin{cases} \frac{1}{\pi}\sqrt{1-|\mu|}, & \text{if } |\mu| < 1 \\ 0, & \text{if } |\mu| \geq 1 \end{cases}$$

and

$$\nu_{\max} = \frac{1}{\pi}\sqrt{1+|\mu|}, \quad \text{for any } \mu.$$

In particular we observe that the interval $(\nu_{\min}, \nu_{\max}]$ broadens as μ increase.

3.4. Beating destruction for large non-linearity. Now, we complete the proof of Theorem 2 and of the corollary. To this end we remark that the *energy* has the form

$$\mathcal{H} = \langle\psi, H_0\psi\rangle + \frac{1}{2}\epsilon\langle\psi, W\psi\rangle^2,$$

where, in order to take into account the contribution due to the term ψ_c, we observe that

$$\langle W\rangle^t = \langle\psi, W\psi\rangle = \left(|a_R|^2 - |a_L|^2\right)\langle\varphi_R, W\varphi_R\rangle + R_1 + R_2,$$

where

$$\begin{aligned} R_1 &= a_R\bar{a}_L\langle\varphi_R, W\varphi_L\rangle + \bar{a}_R a_L\langle\varphi_L, W\varphi_R\rangle \\ &\quad + |a_L|^2\left(\langle\varphi_L, W\varphi_L\rangle + \langle\varphi_R, W\varphi_R\rangle\right), \\ R_2 &= \langle\psi_c, W\psi_c\rangle + a_R\langle\varphi_R, W\psi_c\rangle + \bar{a}_R\langle\psi_c, W\varphi_R\rangle \\ &\quad + a_L\langle\varphi_L, W\psi_c\rangle + \bar{a}_L\langle\psi_c, W\varphi_L\rangle, \end{aligned}$$

and

$$\langle\psi, H_0\psi\rangle = \Omega(|a_R|^2 + |a_L|^2) - \frac{1}{2}\omega(a_R\bar{a}_L + a_L\bar{a}_R) + R_3,$$

where

$$R_3 = \langle\psi_c, H_0\psi_c\rangle.$$

From Theorem 3 we have that $a_R(t)$ and $a_L(t)$ are such that for any $\alpha < 1$,

$$1 - \left(|a_R(t)|^2 + |a_L(t)|^2 \right) = \|\psi_c(t, \cdot)\|^2 = \mathcal{O}(\tilde{\omega}^{2\alpha})$$

for any $t \in [0, (\tau^\star/\tilde{\omega}) \ln(1/\tilde{\omega})]$, for some fixed $\tau^\star$, and

$$\sup_{t \in [0, (\tau^\star/\tilde{\omega}) \ln(1/\tilde{\omega})]} \left| |a_{R,L}(t)| - |A_{R,L}(t\tilde{\omega}/2)| \right| = \mathcal{O}(\tilde{\omega}^\alpha),$$

where $A_{R,L}(\tau)$ are computed in Sects. 3.3. From (3) and since the wave-functions $\varphi_{R,L}$ are localized on just one well [8], it follows that

$$R_1 = \mathcal{O}(\omega), \quad \text{as } \hbar \to 0, \tag{47}$$

for any $t \geq 0$. Moreover, making use of Theorem 3, we have that

$$R_2 = \mathcal{O}(\tilde{\omega}^\alpha) \quad \text{and} \quad R_3 = \mathcal{O}(\tilde{\omega}^{2\alpha}) \tag{48}$$

for any $\tau \in [0, (\tau^\star/\tilde{\omega}) \ln(1/\tilde{\omega})]$ and for some $\tau^\star > 0$. From these facts and from (41) then it follows that for any $t \in [0, (\tau^\star/\tilde{\omega}) \ln(1/\tilde{\omega})]$ we have that

$$\langle W \rangle^t = (2P - 1) \langle \varphi_R, W\varphi_R \rangle + \mathcal{O}(\tilde{\omega}^\alpha),$$

where $P = |A_R|^2$ is the periodic solution given in Lemma 3. Then $\langle W \rangle^t$ is, up to an error of order $\mathcal{O}(\tilde{\omega}^\alpha)$, a periodic function with period T given in Lemma 4. If we remark that

$$\mathcal{H} = \Omega + \frac{1}{4}\omega\mu - \omega I(P, z, \mu) + \mathcal{O}(\tilde{\omega}^{2\alpha}),$$

where we choose $\alpha > \frac{1}{2}$, then we have that (11) implies that $(P_0, z_0) \notin \bar{\mathcal{D}}$. From this fact and from the stability result the beating motion between the two wells follows. In contrast, (10) implies that $(P_0, z_0) \in \mathcal{D}$; hence, the beating motion disappears.

In particular, we observe that the *energy* corresponding to the beating motion with initial condition $P_0 = 0$ (or $P_0 = 1$) is such that $\mathcal{H}_{fb} \approx \Omega + \frac{1}{4}\mu\omega$. Hence, the beating motion disappears for $|\mu| > 2$. Theorem 2 and the corollary are proved.

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