Spontaneous symmetry breaking phenomenon in nonlinear Schrödinger equations

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Abstract. In this talk we discuss some results for a class of nonlinear models in Quantum Mechanics. In particular we focus our attention to the nonlinear one-dimensional Schrödinger equation with a symmetric double-well potential. In the semiclassical limit we prove that the ground state of the linear model bifurcates when the strength of the nonlinear perturbation assume a critical value, and the kind of bifurcation depends on the nonlinearity power. This line of research is inspired by Grecchi V. and Martinez A.,"Non-linear Stark effect and molecular localization", Communications in Mathematical Physics (1995).

References:

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1. Grecchi V., Martinez A., Sacchetti A., *Double well Stark effect: crossing and anticrossing of resonances*, Asympt. Anal. **13** (1996), 373-391.

2. Grecchi V., Martinez A., Sacchetti A., *Splitting instability: the unstable double wells*, J. Phys. A: Math. and Gen. **29** (1996), 4561-4587.

3. Grecchi V., Martinez A., Sacchetti A., *Destruction of the beating effect for a non-linear Schrödinger equation*, Comm. Math. Phys. **227** (2002), 191-209.

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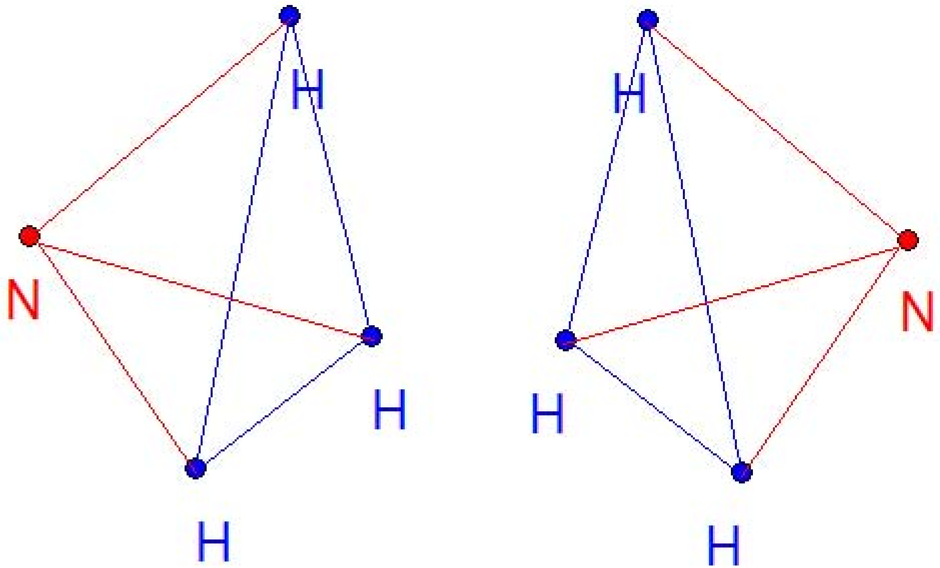
One-dimensional NLS equation with a symmetric double well potential

Physical motivation: Mean field models in quantum chemistry

Let us consider a single ammonia molecule NH^3, and in particular we restrict our attention to the motion of the nitrogen atom N *along the direction* x *perpendicular to the plane containing the three hydrogen atoms* H. The atom N is subjected to a force where its energy potential $V(x)$ has a *symmetric double-well* shape. Classically we have two symmetric equilibrium configurations for the atom N corresponding to the minimum points of the double-well potential.

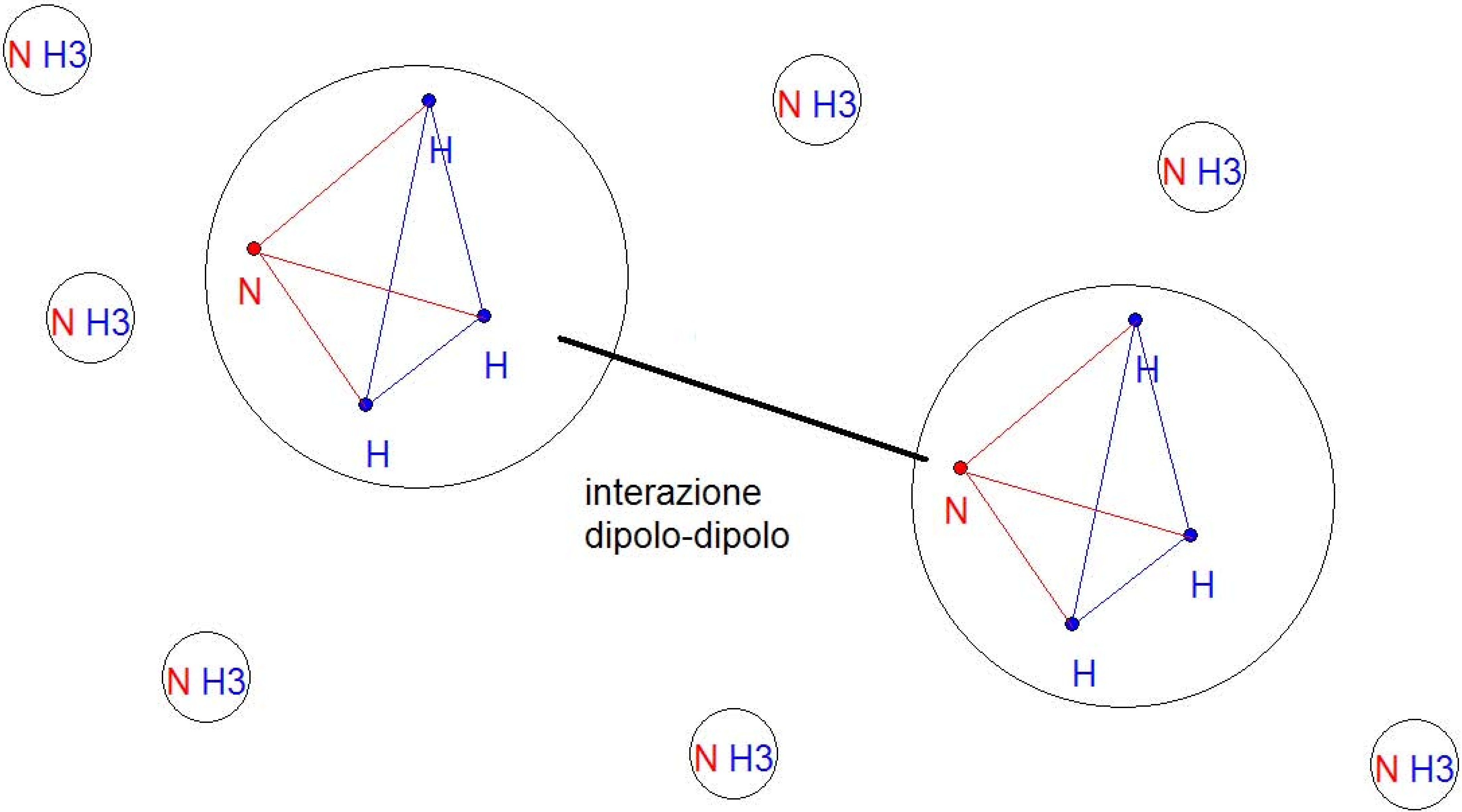


NH3 --- 24 GHz
ND3 --- 1.6 GHz

The *inversion motion* in an *isolated* ammonia molecule (NH_3) is the motion of the nitrogen atom (N) along the line perpendicular to the plane of the 3 hydrogen atoms (H). A potential barrier prevents classical oscillations between equilibrium configurations (L) and (R), but quantal barrier penetration (i.e. tunneling) can produce strong oscillations.
In fact, quantum tunneling effect enable the atom N to pass through the barrier and the atom N periodically moves from one side to the plane to the other side; this is the so called *beating-motion* of the ammonia molecule. This beating motion is actually observed with inversion frequency 24 GHz for ammonia NH_3 and 1.6 GHz for deutered ammonia ND_3.
The wavefunction $\psi(x,t)$ describing the beating motion of the atom N satisfies to the one-dimensional Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

where $V(x)$ has a double-well shape and it admits, under some circumstances, an explicit solution which explain the above mentioned beating motion.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In fact, in an ammonia gas we don't have isolated molecules because they interact among them and if one take into account the dipole-dipole interaction the mean field approximation leads to a nonlinear one-dimensional equation for the wave-function of the form (Claviere and Jona Lasinio 1986, Grecchi and Martinez 1995, Jona-Lasinio, Presilla e Toninelli 2002)

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi + \mu\langle\psi, W\psi\rangle W(x)\psi\,.$$

where $W(-x) = -W(x)$ is an odd function and where $\langle\psi, W\psi\rangle$ represents the molecular dipole.

The linear problem.

$$\begin{cases} i\hbar\frac{\partial\psi}{\partial t} = H_{lin}\psi \\ \psi(x,0) = \psi_0(x) \in L^2(\mathbb{R}, dx) \end{cases}$$

where H_{lin} is the (one-dimensional) linear operator formally defined on $L^2(\mathbb{R}, dx)$ as

$$H_{lin} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\,,$$

and where $V(x)$ is a (smooth and bounded) *double-well potential.* In particular, we assume that $V(x)$ is a potential regular enough satisfying the properties:

i. symmetric: $V(-x) = V(x)$;

ii. double well shape: there exists two (non-degenerate) minima at $x_\pm = \pm d$, $d > 0$, such that $V(x) > V(x_\pm)$ $\forall x \neq x_\pm$;

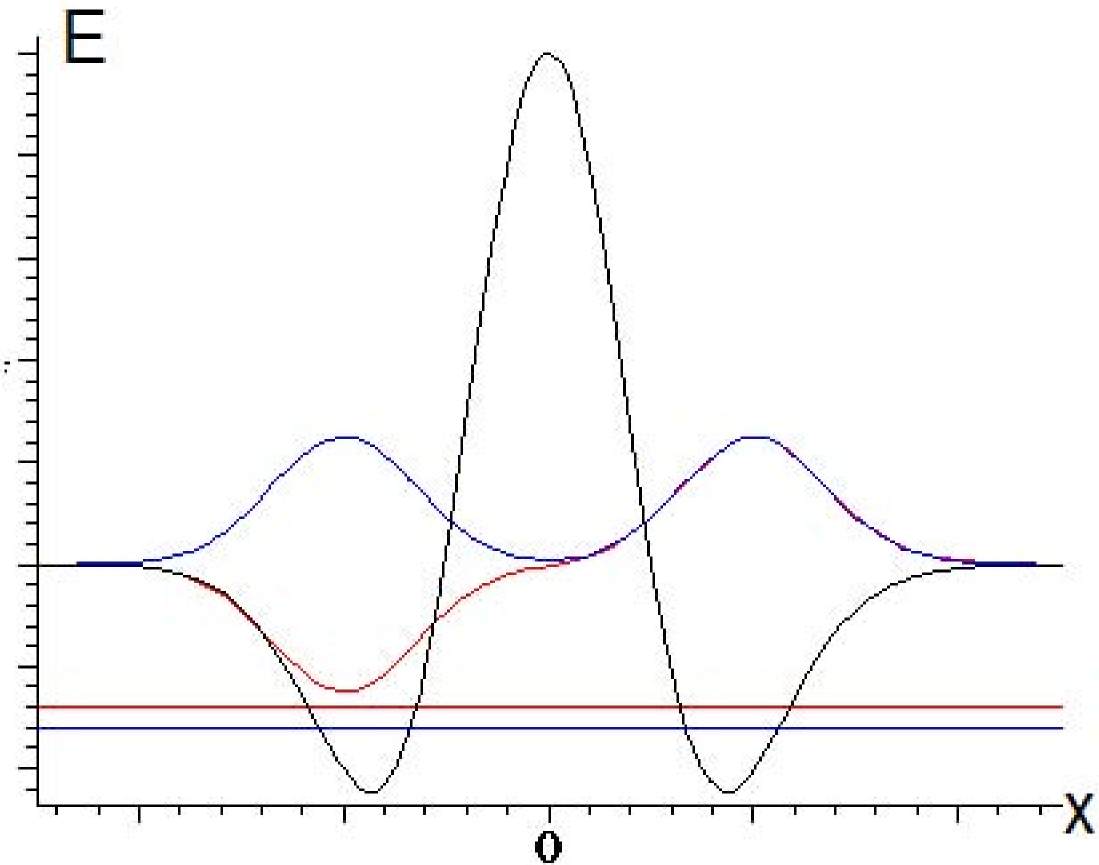
iii. $V_\infty := \liminf_{|x|\to\infty} V(x) > V(x_\pm)$.

The linear operator H_{lin} admits a self-adjoint extension (still denoted H_{lin}) and its spectrum is such that

$$\sigma(H_{lin}) = \sigma_d(H_{lin}) \cup \sigma_{ess}(H_{lin})$$

where $\sigma_{ess}(H_{lin}) = [V_\infty, +\infty)$ and where $\sigma_d(H_{lin}) \subset (-\infty, V_\infty)$ consists of a finite number of isolated eigenvalues.
If $\hbar$ is small enough then $\#\sigma_d(H_{lin}) \geq 2$ and let $E_+ < E_-$ be the two lowest eigenvalues of H_{lin} with associated normalized eigenvectors φ_+ and φ_-.
It is a well known result that $\varphi_\pm$ are real-valued (up to a constant phase factor) functions, φ_+ is a positive even function $\varphi_+(-x) = \varphi_+(x) > 0$, and φ_- is an odd function $\varphi_-(-x) = -\varphi_-(x)$ with only just one zero at $x = 0$.
Furthermore

$$\varphi_+(x) \sim \varphi_-(x) \ \text{ if } x > 0 \ \text{ and } \ \varphi_+(x) \sim -\varphi_-(x) \ \text{ if } x < 0$$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If we assume that the initial wave-function ψ_0 is prepared in the space $F = \text{span}\,(\varphi_+, \varphi_-)$, that is:

$$\Pi_c \psi_0 = 0$$

where

$$\Pi_c = \mathbf{1} - \Pi\,,\ \Pi = \Pi_- + \Pi_+,\quad \Pi_\pm = \langle \varphi_\pm, \cdot \rangle \varphi_\pm\,,$$

then

$$\psi(x,t) = c_+ e^{-iE_+ t/\hbar} \varphi_+(x) + c_- e^{-iE_- t/\hbar} \varphi_-(x)$$

and the mean value of the position observable x defined as

$$\begin{aligned} \langle x \rangle^t &= \langle \psi(\cdot,t), x\psi(\cdot,t) \rangle \\ &= \overline{c_+} c_- e^{i(E_+ - E_-)t/\hbar} \langle \varphi_+, x\varphi_- \rangle + \overline{c_-} c_+ e^{-i(E_+ - E_-)t/\hbar} \langle \varphi_-, x\varphi_+ \rangle \end{aligned}$$

is a periodic function with period

$$T = \frac{\pi\hbar}{\omega}, \quad \omega = \frac{E_- - E_+}{2}$$

In order to better understand the *beating motion* let us introduce the two vectors

$$\varphi_R = \frac{1}{\sqrt{2}}\left[\varphi_+ + \varphi_-\right], \quad \varphi_L = \frac{1}{\sqrt{2}}\left[\varphi_+ - \varphi_-\right]$$

where φ_R is a normalized vector localized (up to a tail which is exponentially small as $\hbar$ goes to zero) on one well (say the hand right one), and φ_L is a normalized vector localized (up to a tail which is exponentially small as $\hbar$ goes to zero) on the other well (say the hand left one). Hence,

$$\begin{aligned}
\psi(x,t) &= e^{-i\Omega t/\hbar}\frac{c_+ e^{i\omega t/\hbar} + c_- e^{-i\omega t/\hbar}}{\sqrt{2}}\varphi_R(x) + \\
&\quad + e^{-i\Omega t/\hbar}\frac{c_+ e^{i\omega t/\hbar} - c_- e^{-i\omega t/\hbar}}{\sqrt{2}}\varphi_L(x)\,,
\end{aligned}$$

where $\Omega = \frac{E_+ + E_-}{2}$. If we assume, for argument's sake, that $c_+ = c_- = 1/\sqrt{2}$ (that is $\psi_0(x) = \varphi_R(x)$ is localized on the right hand well) then

$$\psi(x,t) = \sqrt{2}e^{-i\Omega t/\hbar}\left[\cos(\omega t/\hbar)\varphi_R(x) + i\sin(\omega t/\hbar)\varphi_L(x)\right]$$

and

$$\langle x\rangle^t = 2\langle\varphi_R, x\varphi_R\rangle\left[\cos^2(\omega t/\hbar) - \sin^2(\omega t/\hbar)\right]\,.$$

Semiclassical results.

Here, we assume to be in the *semiclassical limit*

$$\hbar \ll 1 \, .$$

In such a case one can give an asymptotic expression of the eigenvalues $E_\pm$ and of the associated normalized eigenvectors $\varphi_\pm$. In particular one can prove that

$$\omega \sim e^{-S_0/\hbar} \quad \text{and} \quad \int_0^{+\infty} |\varphi_L(x)|^2 dx = \int_{-\infty}^0 |\varphi_R(x)|^2 dx = O(e^{-S_0/\hbar})$$

as $\hbar \ll 1$, where S_0 is the Agmon distance between the two wells:

$$S_0 = \int_{x_-}^{x_+} \sqrt{V(x) - V(x_+)} dx \, .$$

In this sense we can say that the vector φ_R (resp. φ_L) is *localized* on the right (resp. left) hand side well.

Nonlinear Perturbation

We consider two different situations:

- *Non local perturbation:*

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) + \mu W(x) \langle \psi, W \psi \rangle \right] \psi \, , \ n = 1$$

where $W(-x) = -W(x)$ [V.Grecchi, A.Martinez, Comm. Math. Phys. (1995); V.Grecchi, A.Martinez, A.S., Comm. Math. Phys. (2002)]. This model is inspired by analysis of the ammonia molecule.

- *Local perturbation:*

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) + \mu |\psi|^{2\sigma} \right] \psi \, , \ n = 1 \, , \ \sigma > 0$$

[A.S., J. Stat. Phys. (2005); D.Bambusi, A.S., Comm. Math. Phys. (2007); A.S., Phys. Rev. Lett. (2009); R.Fukuizumi, A.S. (2011)]. In such a case we study the Gross-Pitaevskii equation, useful for Bose-Einstein condensates. In the following we restrict ourselves to the case of local perturbation.

Parameters

We fix the units such that $2m = 1$.

Concerning the strength μ of the non-linear perturbation we assume that it *goes to zero as $\hbar$ goes to zero* in a suitable way. That is, we assume that

$$\hbar \to 0 \text{ and } \ \mu \to 0 \ \text{ such that } \eta := \frac{\hbar^{-\sigma/2} \mu}{\omega} \sim 1.$$

The parameter η will play the role of *effective nonlinearity strength.*

General results

- Existence of the global solution;
- Stationary solutions: bifurcation phenomenon and stability results;
- Asymptotic behavior of the wavefunction $\psi(x,t)$, with a rigorous estimate of the error, for times of the order of the beating period;
- Destruction of the beating motion for effective non-linearity strength η larger than a critical value.

Existence Result and conservation laws

Let

$$\Pi_c \psi_0 = 0\,;$$

this fact implies that ψ_0 is regular enough, i.e. $\psi_0 \in H^1(\mathbb{R})$. Then there exist $\hbar^\star > 0$ and $\mu_0 > 0$ such that for any $\hbar \in (0, \hbar^\star]$ and $\mu \in [-\mu_0, \mu_0]$ then the Cauchy problem admits a unique solution $\psi(x,t) \in H^1$ for any $t \in [0, T^\star)$, for some $T^\star > 0$. Moreover, the following conservation laws hold:

- Conservation of the norm

$$\mathcal{N}(\psi) := \|\psi(\cdot, t)\| = \|\psi_0(\cdot)\| = 1$$

- Conservation of the energy

$$\mathcal{E}(\psi) = \mathcal{E}(\psi_0)$$

where

$$\mathcal{E}(\psi) = \hbar^2 \left\|\nabla \psi\right\|^2 + \langle V\psi, \psi\rangle + \frac{\mu}{\sigma+1} \|\psi\|^{2\sigma+2}_{L^{2\sigma+2}(\mathbb{R})}$$

A local existence result, with the *blow-up alternative*, holds true even in presence of a bounded potential $V(x)$. That is there exists $T^\star > 0$ and an unique solution $\psi(x,t) \in H^1$ for any $t \in [0, T^\star)$ where $T^\star = +\infty$ or $\|\nabla \psi\|_{L^2(\mathbb{R})} \to +\infty$ as $t \to T^\star$. A *priori estimate* will follow:

Lemma. *Let*

$$\Lambda = \frac{\mathcal{E}(\psi_0) - V_{min}}{\hbar^2} \sim \hbar^{-1}$$

where $\mathcal{E}(\psi_0) \sim \hbar$ is the energy defined above. The solution $\psi(x,t)$ satisfies to the following a priori estimates

$$\|\nabla \psi\|_{L^2(\mathbb{R})} \le C\sqrt{\Lambda} \le C\hbar^{-1/2} \tag{1}$$

and

$$\|\psi\|_{L^p(\mathbb{R})} \le C\Lambda^{\frac{p-2}{4p}} \le C\hbar^{-\frac{p-2}{8p}}$$

where

$$p \in [2, +\infty] .$$

Hence $T^\star = +\infty$!

Proof: We make use of the conservation of the energy

$$\begin{aligned} \hbar^2 \|\nabla \psi\|_{L^2(\mathbb{R})}^2 &= \mathcal{E}(\psi_0) - \frac{\mu}{\sigma+1} \langle \psi^{\sigma+1}, \psi^{\sigma+1} \rangle - \langle V\psi, \psi \rangle \\ &\leq \mathcal{E}(\psi_0) - V_{min}\mathcal{N}(\psi_0) + \frac{|\mu|}{\sigma+1} \|\psi\|_{L^{2(\sigma+1)}(\mathbb{R})}^{2(\sigma+1)} \end{aligned}$$

where $V_{min} = \min_x V(x) = V(x_\pm) > -\infty$ and $\mathcal{N}(\psi_0) = 1$. Hence

$$\|\nabla \psi\|_{L^2(\mathbb{R})}^2 \leq \Lambda + \rho^2 \|\psi\|_{L^{2(\sigma+1)}(\mathbb{R})}^{2(\sigma+1)}$$

where

$$\rho^2 = \frac{|\mu|}{(\sigma+1)\hbar^2} \leq C|\mu|\hbar^{-2} \ll 1 \quad \text{and} \quad \hbar|\Lambda| = C + o(1)$$

We apply the Gagliardo-Nirenberg inequality obtaining

$$\|\nabla \psi\|_{L^2(\mathbb{R})}^2 \leq \Lambda + C\rho^2 \|\nabla \psi\|_{L^2(\mathbb{R})}^{\sigma} \|\psi\|_{L^2(\mathbb{R})}^{2+\sigma(2-d)} \leq \Lambda + C\rho^2 \|\nabla \psi\|_{L^2(\mathbb{R})}^{\sigma}$$

from which and from *bootstrap*(-fixed point) argument (remember that $\rho \ll 1$ and that $\Lambda \gg 1$) the estimate (1) follows. Making use of the Gagliardo-Nirenberg inequality again, we obtain that

$$\|\psi\|_{L^p(\mathbb{R})} \leq C \|\nabla \psi\|_{L^2(\mathbb{R})}^{\delta} \|\psi\|_{L^2(\mathbb{R})}^{1-\delta} \leq C\Lambda^{\frac{1}{2}\delta}, \quad \delta = \frac{(p-2)}{2p} .$$

Two-level approximation

Let

$$\psi \to \psi(x,\tau) = e^{-i\Omega t/\hbar}\psi(x,t), \quad \Omega = \frac{E_+ + E_-}{2}, \ \tau = \frac{\omega t}{\hbar}$$

then

$$\psi(x,\tau) = a_R(\tau)\varphi_R(x) + a_L(\tau)\varphi_L(x) + \psi_c(x,\tau)$$

where $\psi_c e^{-i\Omega\tau/\hbar} = \Pi_c \psi$, $\Pi_c = \mathbf{1} - \Pi$, and Π is the projection operator on the space F spanned by the first two ground states of the linear problem ($F = \text{span}\,\{\varphi_+, \varphi_-\} = \text{span}\,\{\varphi_R, \varphi_L\}$). Then the Cauchy problem

$$\begin{cases} i\frac{\partial \psi}{\partial \tau} = \frac{1}{\omega}\left[H_{lin} - \Omega\right]\psi + \frac{\mu}{\omega}|\psi|^{2\sigma}\psi \\ \psi(x,0) = \psi_0(x), \quad \Pi_c\psi_0 = 0 \end{cases}$$

takes the form (hereafter $\dot{} = \frac{\partial}{\partial \tau}$)

$$\begin{cases} i\dot{a}_R &= & -a_L + r_R, & r_R = r_R(a_R, a_L, \psi_c) = \frac{\mu}{\omega}\langle \varphi_R, |\psi|^{2\sigma}\psi\rangle \\ i\dot{a}_L &= & -a_R + r_L, & r_L = r_L(a_R, a_L, \psi_c) = \frac{\mu}{\omega}\langle \varphi_L, |\psi|^{2\sigma}\psi\rangle \\ i\dot{\psi}_c &= & \frac{1}{\omega}\left[H_{lin} - \Omega\right]\psi_c + r_c, & r_c = r_c(a_R, a_L, \psi_c) = \frac{\mu}{\omega}\Pi_c\psi \end{cases} \tag{2}$$

$$a_{R,L}(0) = \langle \varphi_{R,L}, \psi_0\rangle, \ \psi_c^0 = 0$$

Lemma. *$r_X(a_R, a_L, \psi_c)$, $X = R$ or $X = L$, is such that for any $\Gamma < S_0$*

$$r_X(a_R, a_L, 0) = \eta C_X |a_X|^{2\sigma} a_X + \mathcal{O}(e^{-\Gamma/\hbar}) \, , \ \eta = \frac{\mu}{\omega} \hbar^{-\sigma/2} \, ,$$

where

$$C_X = \hbar^{\sigma/2} \langle \varphi_X, |\varphi_X|^{2\sigma} \varphi_X \rangle \, , \ X = R, L \, ,$$

are such that $C_R = C_L \sim C$ (say $C = 1$) as $\hbar$ goes to zero.

We call **two-level approximation** the system of differential equations given by

$$\left\{ \begin{array}{lcl} i\dot{b}_R & = & -b_L + \eta |b_R|^{2\sigma} b_R \\ i\dot{b}_L & = & -b_R + \eta |b_L|^{2\sigma} b_L \end{array} \right. , \quad b_{R,L}(0) = a_{R,L}(0) \, . \tag{3}$$

Strategy: The solutions to (3) approximate the solutions to (2).

Main Results
Stationary solutions

Theorem 1. *Let* $\psi = a_R\varphi_R + a_L\varphi_L + \psi_c$, *where* $|a_R|^2 + |a_L|^2 + \|\psi_c\|^2_{L^2(\mathbb{R})} = 1$. *Let*

$$a_R = pe^{i\theta}\,,\ a_L = q\,, \quad \text{where} \ \ p,q \in [0,1] \ \ \text{and} \ \ \theta \in [0,2\pi)\,,$$

and let $z = p^2 - q^2$ *be the imbalance function. Let* $\hbar \in (0,\hbar^\star)$, *where* $\hbar^\star$ *is small enough, let* S_0 *be the Agmon distance between the two wells, let* Γ *any positive number such that* $\Gamma < S_0$ *and let* η *be the effective nonlinearity strength. Then the stationary problem associated to (2) always has stationary solutions* $\psi(x,\tau) = e^{i\lambda^2\tau}\phi(x)$ *with the following properties:*

- *a* symmetric solution ψ^s *such that* $\theta = 0$ *and* $z = 0$ *with energy* $\lambda^2 = \Omega + \omega\left[-1 + \eta\frac{1}{2^\sigma} + \mathcal{O}(e^{-\Gamma/\hbar})\right]$;
- *an* antysymmetric solution ψ^{as} *such that* $\theta = \pi$ *and* $z = 0$ *with energy* $\lambda^2 = \Omega + \omega\left[+1 + \eta\frac{1}{2^\sigma} + \mathcal{O}(e^{-\Gamma/\hbar})\right]$.

Furthermore, in the case of negative (resp. positive) η, then asymmetrical solutions ψ^{as} *corresponding to* $\theta^{as} = 0$ *(resp.* $\theta^{as} = \pi$*) there exists because a spontaneous symmetry bifurcation phenomenon occurs:*
- for $\sigma \leq \sigma_{threshold}$ *the symmetric (resp. antisymmetric) state corresponding to* $z_s = 0$ *bifurcates showing a pitchfork bifurcation when the adimensional nonlinear parameter* $|\eta|$ *is larger than the critical value* $\eta^\star = \frac{2^\sigma}{\sigma}$
- for $\sigma > \sigma_{threshold}$ *two couples of new asymmetrical stationary states appear as saddle-node bifurcations when* $|\eta|$ *is equal to a given value* η^+ *such that* $\eta^+ < \eta^\star$*; then, for increasing values of* $|\eta|$ *two branches of the solutions disappear at* $|\eta| = \eta^\star$ *showing a pitchfork bifurcation. The critical value* η^+ *is given by* $\eta(z^+)$ *where*

$$\eta(z) = \frac{2z}{\sqrt{1-z^2}} \left[\left(\frac{1+z}{2} \right)^\sigma - \left(\frac{1-z}{2} \right)^\sigma \right]^{-1}$$

and where $z^+ \in (0,1)$ *is the nonzero solution to* $\frac{d\eta}{dz} = 0$*.*
In all the cases, the remainder term ψ_c *of the stationary solution is such that* $\|\psi_c\|_{H^1(\mathbb{R})} = \mathcal{O}(e^{-\Gamma/\hbar})$*.*

Remark. *The critical value $\sigma_{threshold}$ is given by*

$$\sigma_{threshold} = \frac{1}{2}\left[3+\sqrt{13}\right]$$

and it is universal *in the sense that it does not depend on the shape of the double-well potential as well as on the dimension (in fact, the previous result holds true even in dimension d bigger than one).*
The proof makes use of the Lyapunov-Schmidt method and of some results of the theory of numbers in order to count the number of solutions of equations coming from the two level approximation.

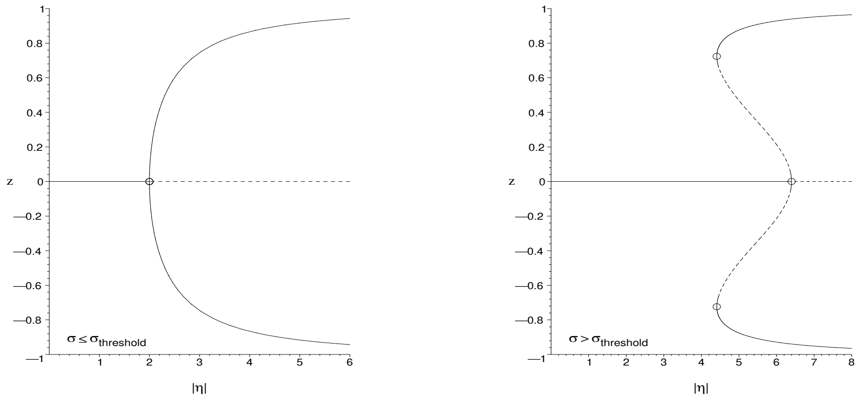

Figure 1: In this figure we plot the graph of the stationary states of the nonlinear Schrödinger equation (2) as function of the nonlinearity parameter η for nonlinearity $\sigma = 1 < \sigma_{threshold}$ (panel (a)) and for nonlinearity $\sigma = 5 > \sigma_{threshold}$ (panel (b)); here $z = |a_R|^2 - |a_L|^2$ is the imbalance function. Full lines represent stable stationary states and broken lines represent unstable stationary states.

Concerning the *orbital stability* of the stationary solutions we restrict ourselves to the case

$$\eta < 0 \,.$$

Where orbital stability means that for any $\epsilon > 0$ there exists $\delta > 0$ such that if the initial wavefunction ψ_0 is "closed" to the stationary solution ϕ

$$\inf_{\theta\in\mathbb{R}} \|\psi_0(\cdot) - e^{i\theta}\phi(\cdot)\|_{H^1(\mathbb{R})} < \delta \,,$$

then the solution $\psi(x,t)$ satisfies

$$\inf_{\theta\in\mathbb{R}} \|\psi(\cdot,t) - e^{i\theta}\phi(\cdot)\|_{H^1(\mathbb{R})} < \epsilon \,.$$

The following results hold true:

Theorem 2. *Fix any $\hbar > 0$ be sufficiently small. Then:*

- *Let $\sigma \leq \sigma_{threshold}$. The symmetric solution corresponding to $z = 0$ is orbitally stable in H^1 for $|\eta| < \eta^\star$. At the bifurcation point $\eta = \eta^\star$, there is an exchange of stability, that is, for $|\eta| > \eta^\star$, the asymmetric solution is orbitally stable in H^1 and the symmetric solution is unstable.*

- *Let $\sigma \leq \sigma_{threshold}$. By Theorem 1, a couple of new asymmetric stationary states, denoted by ψ^{as1} and ψ^{as2} appears at $|\eta| = \eta^+$. For $|\eta| > \eta^+$, ψ^{as1} is orbitally stable in H^1, ψ^{as2} is unstable. On the other hand, the symmetric state is orbitally stable in H^1 for $|\eta| < \eta^\star$, and unstable for $|\eta| > \eta^\star$.*

Let us rescale ψ as $\phi = |\mu|^{1/2\sigma}\psi$; then the GPE is equivalent to

$$i\hbar\frac{\partial\phi}{\partial t} = H_{lin}\phi - |\phi|^{2\sigma}\phi\,,\ \|\phi\|_{L^2(\mathbb{R})} = |\mu|^{1/2\sigma}\,.$$

The proof is based on the spectral analysis of the real and imaginary part of the linearized operator around the stationary solution $\phi := \phi_{\lambda^2}$:

$$\begin{aligned} L_+ &= H_{lin} - E - (2\sigma+1)|\phi_{\lambda^2}|^{2\sigma} \\ L_- &= H_{lin} - E - |\phi_{\lambda^2}|^{2\sigma} \end{aligned}$$

and on the analysis of the sign of the derivative of $F(\lambda^2) := \|\phi_{\lambda^2}\|^2_{L^2(\mathbb{R})}$. More precisely, we make use of the following criterion due to Weinstein.

Proposition. *Suppose that L_- is a nonnegative operator. If:*

- *L_+ has only one negative eigenvalue, and $\frac{dF}{d\lambda^2} < 0$ then ϕ_{λ^2} is orbitally stable in $H^1(\mathbb{R})$;*

- *L_+ has only one negative eigenvalue, and $\frac{dF}{d\lambda^2} > 0$ then ϕ_{λ^2} is orbitally unstable in $H^1(\mathbb{R})$;*

- *L_+ has at least two negative eigenvalues then ϕ_{λ^2} is orbitally unstable in $H^1(\mathbb{R})$.*

Behaviour of the wavefunction
Validity of the two-level approximation

Theorem 3. *Let ψ_c, a_R and a_L be the solutions to*

$$\left\{ \begin{array}{lcll} i\dot{a}_R & = & -a_L + r_R, & r_R = r_R(a_R, a_L, \psi_c) = \frac{\mu}{\omega}\langle \varphi_R, |\psi|^{2\sigma}\psi\rangle \\ i\dot{a}_L & = & -a_R + r_L, & r_L = r_L(a_R, a_L, \psi_c) = \frac{\mu}{\omega}\langle \varphi_L, |\psi|^{2\sigma}\psi\rangle \\ i\dot{\psi}_c & = & \frac{1}{\omega}\left[H_{lin} - \Omega\right]\psi_c + r_c, & r_c = r_c(a_R, a_L, \psi_c) = \frac{\mu}{\omega}\Pi_c\psi \end{array} \right. .$$

Let b_R and b_L be the solution of the two-level approximation

$$\left\{ \begin{array}{lcl} i\dot{b}_R & = & -b_L + \eta|b_R|^{2\sigma}b_R \\ i\dot{b}_L & = & -b_R + \eta|b_L|^{2\sigma}b_L \end{array} \right. , \quad b_{R,L}(0) = a_{R,L}(0)\, .$$

Then, for any fixed $\Gamma \in (0, S_0)$ and any $\tau' > 0$

$$|b_{R,L}(\tau) - a_{R,L}(\tau)| = \mathcal{O}(e^{-\Gamma/\hbar})$$

$$\|\psi_c(\cdot,\tau)\|_{L^2(\mathbb{R})} = \mathcal{O}(e^{-\Gamma/\hbar})$$

as $\hbar \to 0$, for any $\tau \in [0, \tau']$.

Remark. The time behavior, at least for times of the order of the beating period, of the wavefunction ψ, initially prepared on the two lowest states, is practically described by means of the solutions of the two-level approximation for times of the order of the beating period, with a precise estimate of the remainder term.

The proof of the Theorem is splitted in several steps.

Step 1.

$$\varphi(x,\tau) = a_R(\tau)\varphi_L(x) + a_L(\tau)\varphi_L(x) \quad \text{and} \quad \psi = \psi_c + \varphi$$

$$W^I = |\varphi(x,\tau)|^{2\sigma}\varphi(x,\tau) \quad \text{and} \quad W^{II} = |\psi(x,\tau)|^{2\sigma}\psi(x,\tau) - W^I$$

$$\|W^I\|_{L^2(\mathbb{R})} \leq C\hbar^{-\sigma/2} \quad \text{and} \quad \|W^{II}\|_{L^2(\mathbb{R})} \leq C\hbar^{-\sigma/2}\|\psi_c\|_{L^2(\mathbb{R})} \, .$$

for some positive constant C independent on τ and $\hbar$.

Step 2.

$$W^I \in C^1(\mathbb{R}, L^2(\mathbb{R}^d)), \quad \left\| \frac{\partial W^I}{\partial \tau} \right\|_{L^2(\mathbb{R})} \leq C\hbar^{-\sigma/2}, \quad \forall \tau \geq 0$$

Step 3. $\psi_c = \Pi_c \psi$ satisfies to the following estimate

$$e^{-C\tau} \|\psi_c\|_{L^2(\mathbb{R})} = \mathcal{O}(e^{-\Gamma/\hbar}), \quad \forall \tau \geq 0,$$

for some positive constant $C > 0$ independent of $\hbar$ and τ. Indeed,

$$\psi_c(\cdot, \tau) = -i \frac{\mu}{\omega} \int_0^\tau e^{-i(H_{lin}-\Omega)(\tau-s)/\omega} \Pi_c \left[W^I + W^{II} \right] ds = I + II$$

By integrating by part,

$$\begin{aligned} I &= \left[-i\omega e^{-i(H_{lin}-\Omega)(\tau-s)/\omega} [H_{lin} - \Omega]^{-1} \Pi_c W^I \right]_0^\tau + \\ &\quad + i\omega \int_0^\tau e^{-i(H_{lin}-\Omega)(\tau-s)/\omega} [H_{lin} - \Omega]^{-1} \Pi_c \frac{\partial W^I}{\partial s} ds \end{aligned}$$

recalling that $\left\| e^{-i(H_{lin}-\Omega)(\tau-s)/\omega} \right\| = 1$ and $\|\hbar [H_{lin} - \Omega]^{-1} \Pi_c\| \leq C$ then

$$\|I\|_{L^2(\mathbb{R})} \leq C \frac{\omega}{\hbar} \max_{s \in [0,\tau]} \left\{ \|W^I\|_{L^2(\mathbb{R})} + \tau \left\| \frac{\partial W^I}{\partial s} \right\|_{L^2(\mathbb{R})} \right\} \leq C \frac{\omega}{\hbar} \hbar^{-\sigma/2} (1 + \tau)$$

$$\|II\|_{L^2(\mathbb{R})} \leq \int_0^\tau \|W^{II}\|_{L^2(\mathbb{R})} ds \leq C \hbar^{-\sigma/2} \int_0^\tau \|\psi_c\|_{L^2(\mathbb{R})} ds$$

Let us set $h(\tau) = \|\psi_c(\cdot, \tau)\|_{L^2(\mathbb{R})}$, then it satisfies to the following inequality

$$\begin{aligned} h(\tau) &\le \frac{\mu}{\omega}\left\{ C\omega\hbar^{-1-\sigma/2}(1+\tau) + C\hbar^{-\sigma/2}\int_0^\tau h(s)ds \right\} \\ &\le a\int_0^\tau h(s)ds + b(1+\tau), \end{aligned}$$

where

$$a = C\frac{\mu\hbar^{-\sigma/2}}{\omega} = C\eta \sim 1 \quad \text{and} \quad b = C\mu\hbar^{-1-\sigma/2} = \mathcal{O}\left(e^{-\Gamma/\hbar}\right) .$$

Then, the Gronwall's Lemma gives that

$$h(\tau) \le be^{a\tau} + \frac{b}{a}\left[e^{a\tau} - 1\right] \le Cbe^{C\tau}$$

That is

$$\|\psi_c(\cdot, \tau)\|_{L^2(\mathbb{R})} = \mathcal{O}\left(e^{-\Gamma/\hbar}\right) .$$

Step 4. Let

$$J=\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix},\ A=\begin{pmatrix} a_R \\ a_L \end{pmatrix},\ B=\begin{pmatrix} b_R \\ b_L \end{pmatrix},\ A,B\in S^2$$

$$S^2=\left\{A=\begin{pmatrix} a_R \\ a_L \end{pmatrix},\ a_R,\ a_L\in\mathbb{C}\ :\ |A|:=\sqrt{|a_R|^2+|a_L|^2}\le 1\right\}.$$

Let $R(A)=\begin{pmatrix} |a_R|^{2\sigma}a_R \\ |a_L|^{2\sigma}a_L \end{pmatrix}$ and $\tilde{R}$ such that

$$\eta\tilde{R}=\frac{\mu}{\omega}\begin{pmatrix} \langle\varphi_R,|\psi|^{2\sigma}\psi\rangle \\ \langle\varphi_L,|\psi|^{2\sigma}\psi\rangle \end{pmatrix}-\eta R(A)$$

Then (2) and (3) may be written as

$$\left\{\begin{array}{lcl} \dot{A} & = & F(A)+\eta\tilde{R} \\ \dot{\psi}_c & = & -\frac{i}{\omega}\left[H_{lin}-\Omega\right]\psi_c-ir_c \end{array}\right.,\quad \left\{\begin{array}{lcl} \dot{B} & = & F(B) \\ B(0) & = & A(0) \end{array}\right.$$

where $F(A)=JA+\eta R(A)$ is such that

$$|F(A)-F(B)|\le C|A-B|$$

and where

$$\eta|\tilde{R}|\le Ce^{-\Gamma/\hbar}e^{C\tau},\quad \forall\tau\ge 0,\ \forall\hbar\in(0,\hbar^\star).$$

Then

$$A(\tau) - B(\tau) = \int_0^\tau \left[F[A(s)] - F[B(s)]\right] ds + \eta \int_0^\tau \tilde{R} ds$$

If we set $q(\tau) = |A(\tau) - B(\tau)|$ then it satisfies to the following inequality

$$q(\tau) \leq C \int_0^\tau q(s)ds + Ce^{-\Gamma/\hbar}\left[e^{C\tau} - 1\right],$$

and then the Gronwall's Lemma prove the result:

$$q(\tau) \leq Ce^{-\Gamma/\hbar}e^{C\tau}.$$

Analysis of the two-level approximation.

Here, we are going to discuss the solutions to the two-level approximation

$$\begin{cases} i\dot{b}_R = -b_L + \eta C |b_R|^{2\sigma} b_R \\ i\dot{b}_L = -b_R + \eta C |b_L|^{2\sigma} b_L \end{cases}, \quad b_R(0) = a_R(0), \ b_L(0) = a_L(0)$$

Recalling that $|b_R(0)|^2 + |b_L(0)|^2 = |a_R(0)|^2 + |a_L(0)|^2 = 1$ we set

$$b_R = pe^{i\alpha}, \ b_L = qe^{i\beta}, \ z = p^2 - q^2, \ p^2 + q^2 = 1, \ \theta = \alpha - \beta$$

The *imbalance function* z takes value in the interval $[-1, 1]$; when $z = 1$ then $|b_R| = 1$ and $|b_L| = 0$ and the wavefunction $\psi = b_R \varphi_R + b_L \varphi_L + \mathcal{O}(e^{-\Gamma/\hbar})$ is practically localized on the *right-side* well, in contrast, when $z = -1$ then $|b_R| = 0$ and $|b_L| = 1$ and the wavefunction ψ is practically localized on the *left-side* well.

The functions $z(\tau)$ and $\theta(\tau)$ are solutions to the following Hamiltonian two-dimensional system

$$\left\{ \begin{array}{rcl} \dot{z} & = & -\partial_\theta \mathcal{H} = 2\sqrt{1-z^2}\sin\theta \\ \dot{\theta} & = & \partial_z \mathcal{H} = \frac{-2z}{\sqrt{1-z^2}}\cos\theta - C\eta\left[\left(\frac{1+z}{2}\right)^\sigma - \left(\frac{1-z}{2}\right)^\sigma\right] \end{array} \right. \tag{4}$$

with Hamiltonian function

$$\mathcal{H} = \mathcal{H}(z,\theta) = 2\left\{\sqrt{1-z^2}\cos\theta - \frac{C\eta}{\sigma+1}\left[\left(\frac{1+z}{2}\right)^{\sigma+1} + \left(\frac{1-z}{2}\right)^{\sigma+1}\right]\right\}$$

Since the Hamiltonian function $\mathcal{H}(z,\theta)$ is an integral of motion then one can plot the trajectories (z,θ) of the solution for different values of $\mathcal{H}(z_0,\theta_0)$

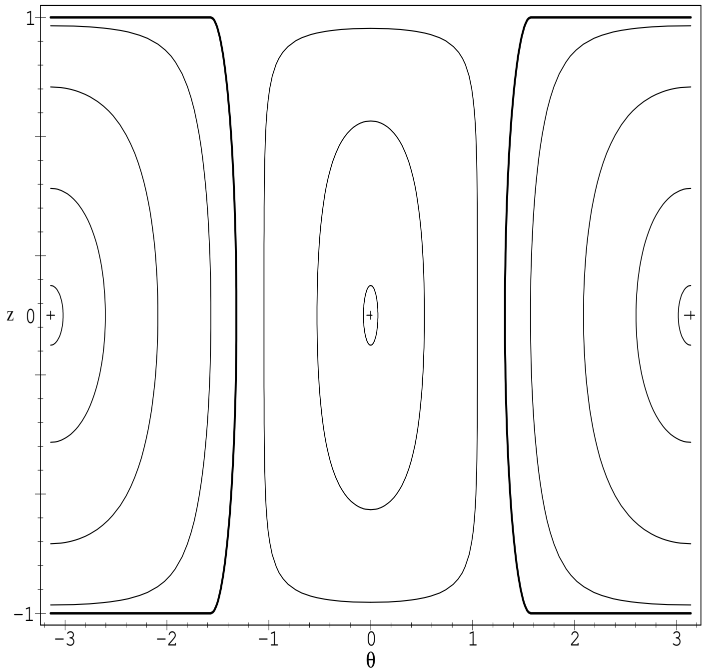

Figure 2: $|\eta| < \eta^{\star}$ — small perturbation regime. Same picture as in the unperturbed case.

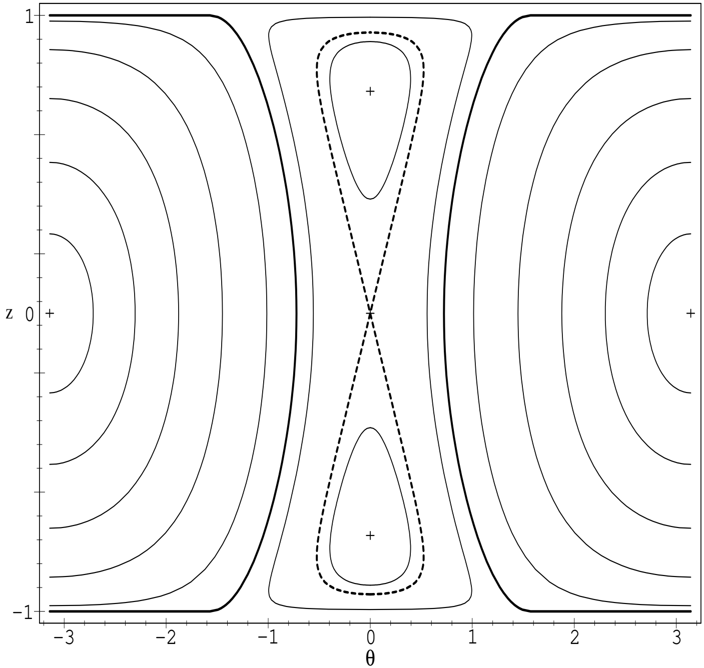

Figure 3: $\eta^\star < |\eta|$ — critical perturbation regime. Bifurcation of the stationary solutions. The beating motion still persists.

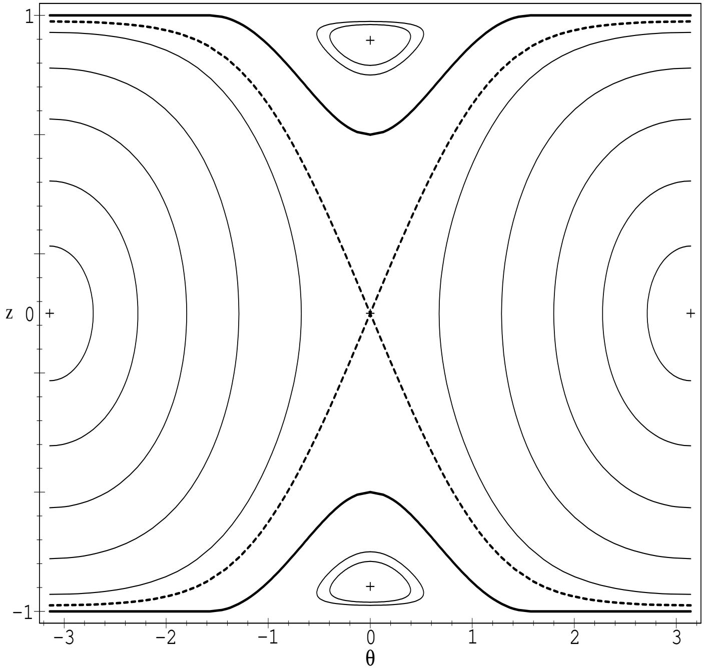

Figure 4: $\eta^\star \ll |\eta|$ — large perturbation regime. Tunneling destruction between the two wells. The beating motion is forbidden.

Explicit solutions for $\sigma = 1, 2$.

In fact, equation (4) admits an explicit solution when $\sigma = 1$ or $\sigma = 2$ by means of Weierstrass's elliptic functions; in particular, let us consider a more general case where the Hamiltonian function has the form

$$\mathcal{H}_\rho = -2\sqrt{1-z^2}\cos\theta + \frac{1}{2}\eta z^2 + 2\rho z\,,\ \mathcal{H} = \mathcal{H}_0\,. \tag{5}$$

Since the Hamiltonian function is an integral of motion, that is

$$\mathcal{H}_\rho\left[z(\tau),\theta(\tau)\right] = \mathcal{H}_\rho\left[z_0,\theta_0\right] = E = \ \mathit{constant}\,, \tag{6}$$

then (4) can be reduced to a first order ODE of the form

$$\dot{z}^2 = f(z)\,,\ z(0) = z_0\,, \tag{7}$$

where $f(z) = az^4+bz^3+cz^2+dz+e$ is a four degree polynomial with constant coefficients

$$a = -\frac{1}{4}\eta^2\,,\ b = -2\eta\rho\,,\ c = -\left(4+\frac{1}{2}\eta^2 - E\eta + 4\rho^2\right)\,,$$
$$d = -(-4E+2\eta)\rho \ \text{ and } \ e = -\left(E^2 - 4 - E\eta + \frac{1}{4}\eta^2\right)\,.$$

One can show that equation (7) has solutions of the form $z(\tau) = \zeta(\pm\tau)$ where

$$\zeta(\tau) = z_0 + \frac{\sqrt{f(z_0)}\dot{P}(\tau) + \frac{1}{2}f'(z_0)\left[P(\tau) - \frac{1}{24}f''(z_0)\right] + \frac{1}{24}f(z_0)f'''(z_0)}{2\left[P(\tau) - \frac{1}{24}f''(z_0)\right]^2 - \frac{1}{48}f(z_0)f^{(IV)}(z_0)} \tag{8}$$

where $' = \frac{d}{dz}$ denotes the derivative with respect to z, $\dot{}$ the derivative with respect to τ, and where $P(\tau) = P(\tau; g_2, g_3)$ is the Weierstrass's elliptic function with parameters

$$g_2 = ae - \frac{1}{4}bd + \frac{1}{12}c^2$$

and

$$g_3 = -\frac{1}{16}eb^2 + \frac{1}{6}eac - \frac{1}{16}ad^2 + \frac{1}{48}dbc - \frac{1}{216}c^3 \, .$$

In particular, the solution $z(\tau)$ is a periodic solution; in order to give an expression of the period T let s_j, $j = 1, 2, 3$, be the complex-valued roots of the trinomial $4s^3 - g_2 s - g_3$, and let $\delta = g_2^3 - 27g_3^2$.
We consider at first the case where $g_3 > 0$. If:

1. $\delta > 0$ then s_j are real-valued roots such that $s_3 < s_2 \leq 0 < s_1$ and the period T is given by

$$T = \frac{2K(m)}{\sqrt{s_1 - s_3}}\,, \; m = \frac{s_2 - s_3}{s_1 - s_3}\,, \tag{9}$$

   where K denotes the complete elliptic integral defined as

$$K(m) = \int_0^1 \left[(1 - q^2)(1 - mq^2)\right]^{-1/2} dq\,;$$

2. $\delta < 0$ then $s_2 \in \mathbb{R}$ and $s_3 = \overline{s_1}$, with $\Im s_1 \neq 0$, and the period T is given by

$$T = \frac{2K(m)}{\sqrt{H_2}}\,, \; m = \frac{1}{2} - \frac{3s_2}{4H_2}\,, \; H_2 = \sqrt{2s_2^2 + s_1 s_3}\,. \tag{10}$$

The case $g_3 < 0$ similarly follows because $P(\tau; g_2, -g_3) = -P(i\tau; g_2, g_3)$ and then we consider the trinomial $4s^3 - g_2 s - (-g_3)$ with roots $s'_j = -s_{4-j}$, $j = 1, 2, 3$; we can conclude that if:

1. $\delta > 0$ then s'_j are real-valued roots such that $s'_3 < s'_2 \leq 0 < s'_1$ and the period T is given by

$$T = \frac{2K'(m)}{\sqrt{s'_1 - s'_3}}\,, \ m = \frac{s'_2 - s'_3}{s'_1 - s'_3}\,, \tag{11}$$

   where $K'(m) = K(1 - m)$.

2. $\delta < 0$ then $s'_2 \in \mathbb{R}$ and $s'_3 = \overline{s'_1}$, with $\Im s_1 \neq 0$, and the period T is given by

$$T = \frac{2K'(m)}{\sqrt{H_2}}\,, \ m = \frac{1}{2} - \frac{3s'_2}{4H_2}\,, \ H_2 = \sqrt{2(s'_2)^2 + s'_1 s'_3}\,. \tag{12}$$

Thank you very much for your kind attention.

And thank you very much André for what you taught me!