SINGULAR BOHR-SOMMERFELD CONDITIONS

Yves Colin de Verdière*, ** and Bernard Parisse**

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* Institut Universitaire de France
** Institut Fourier, Unité mixte de recherche CNRS-UJF 5582
BP 74, 38402-Saint Martin d'Hères Cedex (France)
yves.colin-de-verdiere@ujf-grenoble.fr
bernard.parisse@ujf-grenoble.fr

Abstract

The object of this paper is to present a geometrical formulation of the singular Bohr-Sommerfeld conditions given in [8], in a more general context, including characteristic manifolds with several saddle points. Several examples are detailed and numerical checkings of the results are provided.

Keywords: eigenvalues, scattering matrix, Bohr-Sommerfeld conditions, semi-classics, saddle point, Morse lemma.
Mathematical classification: 34E20 - 34L25 - 81Q20

Introduction

Bohr-Sommerfeld conditions allow to describe the semi-classical behavior of eigenvalues for a completely integrable Hamiltonian system; in fact, they are only concerned with the open dense subset of the phase space foliated by invariant Lagrangian tori and are expressed as quantization conditions which select some discrete set of these tori (see [3], [9] or [15]). These conditions make use action integrals and integrals of the sub-principal symbol along the cycles of the invariant torus. It is possible to reinterpret these conditions outside any spectral context as existence conditions for a pseudo-differential operator for which this torus is a characteristic manifold. In dimension 1, if γ is a smooth compact connected component of the characteristic manifold (γ is a topological circle), let us denote by $A_\gamma = \int_\gamma \xi dx$ the action integral and by $I_\gamma = \int_\gamma H_1 dt$ (H_1 is the sub-principal symbol). If $\mathcal{X}_{H_0}$ is the Hamiltonian vector field associated with the principal symbol H_0, dt is defined by $dt(\mathcal{X}_{H_0}) = 1$ and $m(\gamma)$ is the Maslov index. A necessary and sufficient condition for the existence of a function u satisfying $\hat{H}u = O(h^2)$ with L^2 norm bounded from below, can be written as follows:

$$\frac{1}{h}A_\gamma - I_\gamma + \frac{\pi}{2}m(\gamma) \in 2\pi\mathbb{Z} \ . \tag{1}$$

In dimension 1 already, a generic Hamiltonian $H_0(x,\xi)$ admits, in general, critical values with singular corresponding level sets. Near some local non degenerate extremum, it is always possible to regularize the equations using harmonic oscillators (see [4]). This is no more true for saddle points. There exists, however, a microlocal normal form (semi-classical Morse lemma, see [7], [6]). In the paper [8], we described the quantization conditions associated with the singular manifold in the case of a double potential well for the Schrödinger equation.

The aim of the present paper is to reformulate and extend the quantization conditions of [8]. The reformulation is purely geometrical: the action integrals do not need to be regularized, but the integrals of the sub-principal symbol are divergent and need to be regularized using the symplectic geometry of the phase space (see 2.2).

In such a way, it becomes possible to describe the semi-classical spectrum in cases where the characteristic manifold do admit several saddle points: multiple wells with saddle at the same energy, pendulum on the torus. The case of coupled systems (see the local theory in [6]) will be described in [5].

It is also possible to study scattering problems. The case of a potential with one threshold only and the volcano-top are presented (see section 12). In [5], we study the adiabatic limit for a N-levels system with avoided eigenvalues crossings (see [13] and also [11]). For comparison with existing texts, we insist on the fact that our methods are situated in the smooth context and do not use analytic extensions. Subtle combinatorics of Stokes lines is replaced by some algebraic mechanism on the characteristic manifold which is a tetravalent graph.

The paper is organized as follows: microlocal solutions of the pseudo-differential equation are sections of a sheaf on the characteristic manifold Z. The abstract description of these sheafs is provided in section 4. The geometric description (mod $O(h^2)$) of this sheaf is given in terms of the classical invariants of cycles (section 2) and saddle points (section 3). We consider in particular some canonical regularization of the integrals $\int_\gamma H_1 dt$ where γ is a cycle of the characteristic manifold.

After that, we show how to perform the computations on several examples: eigenvalues of the Schrödinger operator with a double well on $\mathbb{R}$ in order to recover results of [8] (section 8), with a triple well (section 9), discriminant and spectra of Hill's equation (sections 10 and 11), computation of the scattering matrix for potential on the real line with 1 (section 12.1) or 2 channels (section 12.2).

At the end, in the appendices (section A), the theoretical results are compared with direct numerical computations.

The cases of systems of Schrödinger equations (Born-Oppenheimer approximation) and of the adiabatic limit for avoided crossings for an N-levels system will be described in [5].

The case of dimensions ≥ 2 will be studied in some future work with application to semi-excited states in the resonant $2d$ case (see [12] and [2]). *Focus-focus* singularities are discussed in [18] and [19].

1 The context

1.1 Classics

Let (X, ω) be a 2-dimensional symplectic manifold (X is the phase space) and $H_0 : X \to \mathbb{R}$ a smooth Hamiltonian. Very often, X is the cotangent bundle of $M = \mathbb{R}$ or of $M = \mathbb{R}/\mathbb{Z}$, but it is also possible to work with a Riemann surface X (Toeplitz operators).

Let us assume that 0 is a critical value of H_0 and let Z be some connected component of the characteristic manifold $H_0^{-1}(0)$. Let us assume that all critical points of H_0 located on Z are non degenerated saddle points. For eigenvalues problems, Z is a compact set, while Z admits some open edges for the scattering problems. Let us denote by m_∞ the number of open edges of Z, Z_0 the set of all critical points and $n = \#Z_0$. The set Z is a tetravalent graph embedded in X. We will denote by $s_j,\ j = 1, \cdots, n$ the points of Z_0 (vertices of Z), $e_l,\ l = 1, \cdots, m$ the edges of Z (compact or open), let us define $m = m_b + m_\infty$. Let $\gamma_j,\ j = 1, \cdots, N$ be a basis of cycles of Z, i.e. a basis of $\mathbf{H}_1(Z, \mathbb{Z})$ (free $\mathbb{Z}-$module of rank N) which consists of geometric oriented cycles. Euler-Poincaré formula implies:

$$N = b_1(Z) = 1 - n + m_b \ , \tag{2}$$

with $4n = 2m - m_\infty$. In the compact case $N = 1 + n$.

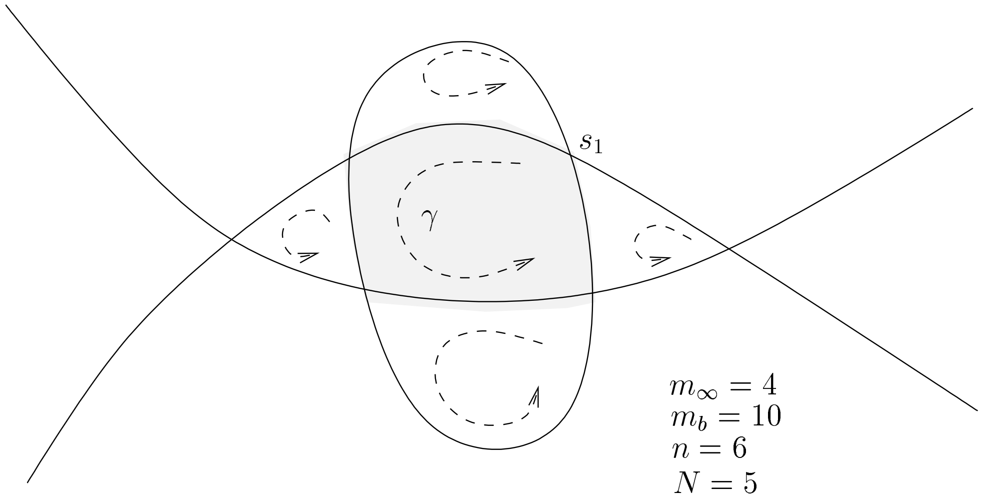

Figure 1: the characteristic manifold Z

1.2 Semi-classics

Let $\hat{H}$ be a quantum Hamiltonian (semi-classical) on X whose principal symbol is H_0. We do not assume that $\hat{H}$ is a self-adjoint operator. Let us denote by $H_1 : X \to \mathbb{C}$ its sub-principal symbol (see [9]). If $X = T^\star\mathbb{R}$, we have:

$$\hat{H} = \mathrm{Op_W}(H_0 + hH_1) + O(h^2) \ , \tag{3}$$

where Op_W denotes the *Weyl quantization* which is defined by

$$\mathrm{Op_W}(H)u(x) = \frac{1}{2\pi h}\int e^{\frac{i}{h}(x-y)\xi} H(\frac{x+y}{2}, \xi) u(y)|dyd\xi| \ .$$

The previous formula may be used as a definition of the sub-principal symbol H_1.

1.3 Spectrum

Let us assume that Z is a compact set. *Singular Bohr-Sommerfeld conditions* are geometric conditions which are equivalent to the existence of functions u which satisfies

$$\hat{H}u = O(h^2), \tag{4}$$

are microlocalized on Z and satisfy the lower bound $\int |u(x)|^2 dx \sim 1$.

In [8], we described the case where $\hat{H} = \hat{K} - \lambda h$ ($\hat{K}$ is a Schrödinger operator with $K_1 = 0$) and then $H_1 = -\lambda$. The values of λ for which the Bohr-Sommerfeld conditions hold correspond to eigenvalues $h\lambda$ of $\hat{K}$.

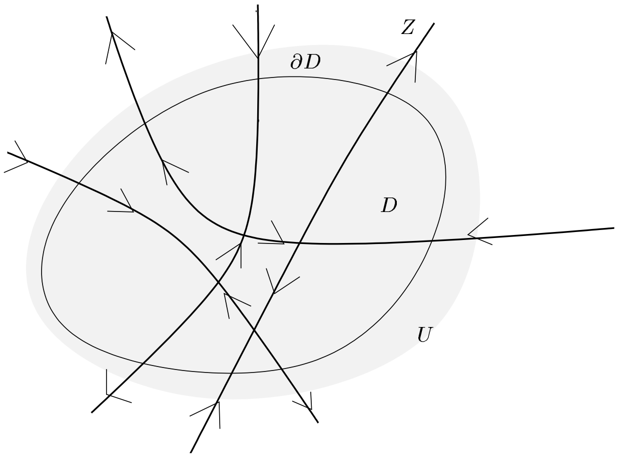

Figure 2: $\mathcal{S}$ matrix

1.4 $\mathcal{S}$ matrix

Let us assume that Z admits open edges. Each one is oriented by the Hamiltonian flow of H_0. There are as many out-going edges as in-going edges. Let us denote by $\mathcal{H}_\infty$ the direct sum for all open edges of the microlocal solutions of $\hat{H}u = 0$ on these edges. $\mathcal{H}_\infty$ is a $\mathbb{C}(h)-$module of rank m_∞. The space $\mathcal{H}_\infty$ admits a natural decomposition into a sum of 2 subspaces of the same dimension $\mathcal{H}_\infty = \mathcal{H}_{in} \oplus \mathcal{H}_{out}$. We call *$\mathcal{S}$-matrix* of $\hat{H}$ the subspace of $\mathcal{H}_\infty$ defined as the set of microlocal solutions of $\hat{H}u = 0$ on open edges which admit an extension as solutions on the whole set Z. This space is in general the graph of a linear mapping from $\mathcal{H}_{in}$ into $\mathcal{H}_{out}$.

Unitarity.

Let us assume that $\hat{H}$ is self-adjoint, we want to define some Hermitian form J on $\mathcal{H}_\infty$. Let D be a domain with boundary ∂D in X which contains the compact edges of Z and such that ∂D intersects transversally each open edge at 1 point. Let Ω be a neighborhood of ∂D in X which intersects only open edges and $U = D \cup \Omega$. Let Π be a self-adjoint PDO of order 0 whose microsupport is contained in U and which is microlocally equal to Id in some neighborhood of $D \setminus \Omega$. Let Σ be another self-adjoint PDO which vanishes microlocally in some other neighborhood of $D \setminus \Omega$ and which coincides with Id where Π does not. Let us put:

$$J(u,v) = \frac{i}{h}(< \Sigma\hat{H}\Pi u \mid \Pi v > - < \Pi u \mid \Sigma\hat{H}\Pi v >) \ .$$

The microlocal solutions on different open edges are $J-$orthogonals and the form J is positive (resp. negative) definite on the in-going (resp. out-going) edges. In fact, we have:

$$J(u,v) = \frac{i}{h} < \Pi[\Sigma, \hat{H}]\Pi u | v > = \frac{i}{h} < [\Sigma, \hat{H}] u | v > + O(h^\infty) \ .$$

It is possible to compute $J(u,u)$ for any microlocal solution u on the edge e in terms of his principal symbol $\sigma_0(u)$ which is an half-density on e invariant by the Hamiltonian flow of H_0.

Lemma 1

$$J(u,u) = \pm \frac{|\sigma_0|^2}{|dt|} + O(h) \ ,$$

with the + sign for an out-going edge and the − sign for an in-going edge. Here $|\sigma_0|^2/dt$ *denotes the quotient of a density (square of an half-density) by dt and not a derivative.*

This lemma comes from the computation of the symbol of the bracket $[\Sigma, \hat{H}]$ which is $\frac{h}{i}\frac{d\sigma}{dt}$ if we denote by σ the principal symbol of Σ.

We have then the:

Theorem 1 *Let us put* $\mathcal{H}_\infty = \mathcal{H}_{in} \oplus \mathcal{H}_{out}$*, then, up to* $O(h^\infty)$*, the* $\mathcal{S}$*-matrix is the graph of an unitary mapping from* $\mathcal{H}_{in}$ *to* $\mathcal{H}_{out}$ *with respect to the metrics induced respectively by* J *on* $\mathcal{H}_{out}$ *and* $-J$ *on* $\mathcal{H}_{in}$ *.*

Isotropy is clear, because if u is a solution in U, $\Sigma \hat{H}\Pi u = \hat{H}\Pi u$. The theorem is then proved by induction on the number of compact edges. If there are no compact edges, we know already that the dimension of the space of solutions is half the number of open edges because in that case, Z is an union of simple crosses. Gluing boundaries of a cut edge can be identified with a reduction on the $\mathcal{S}$-matrix. More precisely, we use the:

Lemma 2 *Let* $H = H_+ \oplus H_-$ *where* H_+ *and* H_- *are 2 Hilbert spaces of the same finite dimension and* $U : H_- \to H_+$ *be a linear isometry whose graph is* Γ*.* $e_\pm \in H_\pm$ *are 2 vectors of length 1 and* $K_\pm$ *are the orthogonals of* $\mathbb{C}e_\pm$*. Let* $e^{i\alpha}$ *be a complex number of modulus* 1 *and*

$$\Gamma_1 = \{(z_-, z_+) \in K_- \oplus K_+ | \ \exists y \in \mathbb{C}, \ (z_- + ye_-, z_+ + e^{i\alpha} y e_+) \in \Gamma\} \ .$$

Then Γ_1 *is the graph of an unitary mapping from* K_- *into* K_+*.*

The proof is elementary.

We then apply the lemma. Given Z, Z_1 is obtained by cutting some compact edge of Z and replacing it by one in-going and one out-going edge of Z_1. $H_\pm$ are related to Z_1 and $K_\pm$ are related to Z. The functions $e_\pm$ are J-normalized microlocal solutions at both ends of the cut edge and $y_+ = e^{i\alpha} y_-$ expresses the gluing of both solutions.

2 Semi-classical invariants of cycles

To each cycle γ of Z, we associate 3 numbers: the *principal action* A_γ (more precisely $\exp(\frac{i}{h}A_\gamma)$), the *sub-principal action* I_γ and the *Maslov index* $m(\gamma)$.

2.1 Principal actions A_γ

If γ is a cycle of Z, we put:

$$A_\gamma = \int_\gamma \xi dx \ . \tag{5}$$

If $\gamma = \partial D$ is the boundary of a compact domain D of the phase space, the number A_γ is the symplectic area of the D.

2.2 Sub-principal actions I_γ

If $\mathcal{X}_{H_0}$ is the symplectic gradient of H_0, we denote by dt the associated differential form on $Z \setminus Z_0$ defined by:

$$dt(\mathcal{X}_{H_0}) = 1 \ . \tag{6}$$

The numbers I_γ are *principal parts* of the divergent integrals $\int_\gamma H_1 dt$. It is enough to described how principal parts should be derived near saddle points.

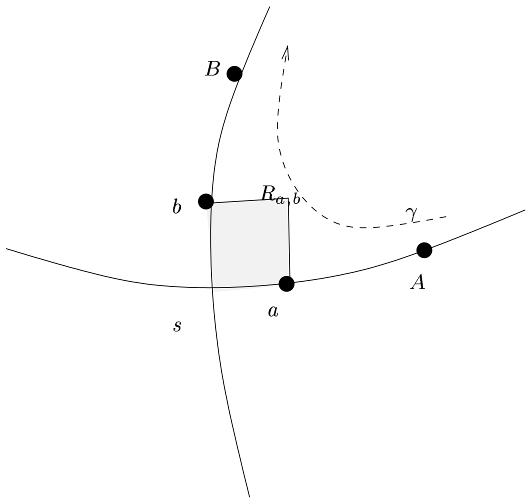

Figure 3: computation of the principal part of $\int_\gamma H_1 dt$

Let AB be an arc of γ on which the unique singularity is s_j. We define

$$\mathrm{vp}\int_A^B H_1 dt = \lim_{a,b\to 0}\left(\int_A^a H_1 dt + \int_b^B H_1 dt + a(s_j)\ln\left|\int_{R_{a,b}}\omega\right|\right) \ , \tag{7}$$

where

$$a(s_j) = \frac{\pm H_1(s_j)}{|\mathrm{det} H_0"(s_j)|^{1/2}} \ , \tag{8}$$

and $R_{a,b}$ is the parallelogram built on the vectors $\vec{s_j a}$ and $\vec{s_j b}$ drawn on the figure. The sign $\pm$ is $+$ if AB is oriented in the same direction as dt and $-$ otherwise.

Lemma 3 *The previous limit exists and is independent of the choices.*

Proof.–

> Performing first a canonical transformation, we may assume that $H_0(z) = Wx\xi + O(|z|^3)$. Of course, we have $W = \pm|\mathrm{det} H"_0(s_j)|^{1/2}$ with the same sign convention as in formula (8). We can then compute $(\int_A^a + \int_b^B) H_1 \, dt$ by replacing H_0 by $Wx\xi$ (then $dt = \frac{dx}{Wx} = -\frac{d\xi}{W\xi}$), which gives the following divergent part of the integral: $-H_1(s_j)/W \ln(ab)$.

□

If the cycle γ is smooth at s_j, we define

$$\tilde{\int}_B^A H_1 dt = \lim_{\varepsilon \to 0^+} \left(\int_B^{\gamma(-\varepsilon)} + \int_{\gamma(\varepsilon)}^A \right) H_1 dt \ , \tag{9}$$

where $u \to \gamma(u)$ is a C^1 parameterization of γ and with $\gamma(0) = s_j$. This choice is compatible with the previous ones: $\gamma \to I_\gamma$ is a $\mathbb{Z}-$linear mapping.

Remark: sub-principal actions I_γ do admit a natural interpretation in symplectic geometry. Let us assume that γ is a simple cycle of $Z = \{H_0 = 0\}$ such that $\gamma = \partial D$ and that H_0 is ≤ 0 inside D. Denote by $s_j, \ j = 1, \cdots N$ the saddle points of Z located on γ. Let $H_1 : X \to \mathbb{R}$ be such that $\forall j, \ 1 \leq j \leq N$, we have $H_1(s_j) < 0$. For $\tau < 0$, let us define

$$A(\tau) = \int_{H_0 + \tau H_1 \leq 0} |dx d\xi| \ .$$

Then, if $\tau \to O^-$, $A(\tau)$ admits the following expansion:

$$A(\tau) = A(0) + \tau \Big(\sum_{j=1}^N \varepsilon_0(s_j)(1 - \ln|\tau \varepsilon_0(s_j)|) \Big) - \tau I_\gamma + O(\tau^2 \ln|\tau|) \ . \tag{10}$$

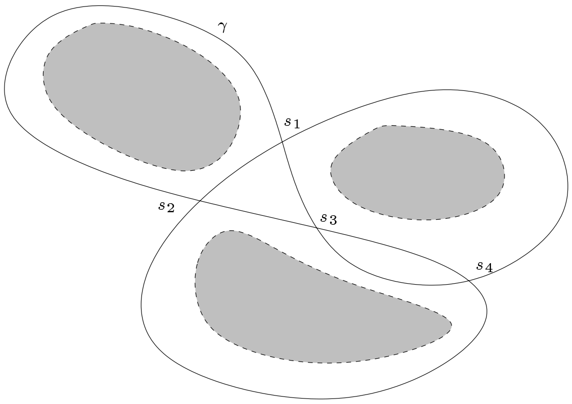

Figure 4: area $A(\tau)$

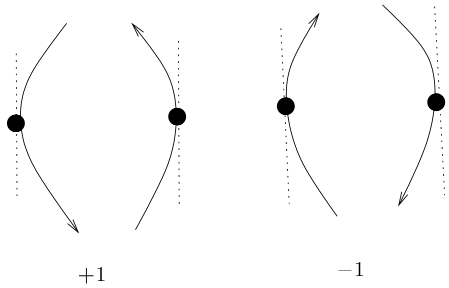

Figure 5: recipes for Maslov indices .

2.3 Maslov indices $m(\gamma)$

Assume now that the tangent vectors to edges at singular points are never vertical, i.e. contained in the kernel of the differential of the projection from $T^\star M$ onto M. We define the Maslov index of an oriented arc e_j following the usual recipe which is summarized on figure 5.

If some of these tangent vectors are vertical, we first perform some small move in order to put them in generic position before performing the calculus. The same move will be used for the choice of the canonical transformation χ, see figure 7, p. 13.

3 Semi-classical invariants of the saddle points

We may reformulate the semi-classical Morse lemma (see [7] pages 1546- and [6]) in the following way:

Theorem 2 *Let us denote by χ a (germ of) canonical transformation defined on $(\mathbb{R}^2, O)$, $(x,\xi) = \chi(y,\eta)$ which satisfy $H_0 \circ \chi = W(y\eta)y\eta$ and $\chi(O) = s,\ s \in Z_0$. Then there exists a unitary FIO U associated with χ, a PDO $\hat{W}$, elliptic at the point O, and a unique formal series*

$$\varepsilon(h) \sim \sum_{j=0}^{\infty} \varepsilon_j h^j \tag{11}$$

such that:

$$\hat{H}U = U\hat{W}(\hat{y\eta} - h\varepsilon(h)) \ , \tag{12}$$

microlocally near O.

$$\hat{y\eta} = \frac{h}{i}\left(y\frac{d}{dy} + \frac{1}{2}\right) \tag{13}$$

is the Weyl quantization of $y\eta$. We have:

$$\varepsilon_0 = \pm \frac{H_1(s)}{|\det(H_0"(s))|^{1/2}} \ . \tag{14}$$

The sign $\pm$ is the opposite of that of $W(0)$.

Proof.–

The proof given in [6] is very close to the argument given in [7], but because we do not assume that $\hat{H}$ is self-adjoint, we cannot use the functional calculus, which leads us to (12). Uniqueness of the formal series $\varepsilon(h)$ is proved in a geometrical way in [6]: we associate to the microlocal situation a natural invariant using a cross-ratio.

We will only comment on the formula (14). Because H_0 vanishes and is critical at the point s_j, the sub-principal symbol $H_1(s_j)$ of $\hat{H}$ at s_j is the same as that of $\hat{W}(\hat{y\eta} - h\varepsilon_0)$ at O. The last one is $-W(O)\varepsilon_0$. In order to evaluate $W(O)$, we compute the determinant of the Hessian of H_0 at the critical point which is preserved by χ. We find:

$$|W(O)| = |\det(H"_0(s_j))|^{\frac{1}{2}} \ . \tag{15}$$

For applications, it may be better not to assume $W(0) > 0$. We prefer to assume that the image by χ of the first quadrant is pointing to the top, see figure 9), then $W(0)$ is > 0 or < 0 according to the sign of H_0 in that domain. ε_0 has to be exchanged according to the same rule.

□

Definition 1 *The formal series $\varepsilon_j(h) = \varepsilon_{0,j} + O(h)$ is the* semi-classical invariant *of the saddle point s_j.*

4 Sheafs on Z

4.1 Linear algebra

Let Z be a connected tetravalent graph which may have some open edges. Let us denote by e the generic edge. We also assume that we have chosen for each vertex some labeling of the four attached edges: e_1, e_2, e_3, e_4 (for example, by following the convention of the figure 7, p. 13).

Definition 2 *We define a sheaf $\mathcal{F} = (Z, E_e, F_s)$ on Z in the following way: to each edge e, we associate a 1-dimensional vector space E_e over a field K (or a free modulus over some ring) and, to each vertex s, we associate a generic 2-dimensional subspace F_s of the direct sum $\oplus_{i=1}^4 E_{e_i}$. Generic means that F_s is not included into a sum of 3 of the E_{e_j} and does not contain any lines $E_{e_j} \oplus 0$.*

We can interpret F_s as the graph of a linear mapping $T_s : E_{e_1} \oplus E_{e_2} \to E_{e_3} \oplus E_{e_4}$. There exists some basis of the E_{e_i} such that the matrix of T satisfies $T_{i,j} = 1$ for $(i,j) = (1,4), (2,3), (2,4)$ and $T_{1,3} = \rho_s$.

$$T = \begin{pmatrix} \rho_s & 1 \\ 1 & 1 \end{pmatrix} \ . \tag{16}$$

ρ_s is a non-zero scalar which is independent of the chosen basis: $\rho_s = \frac{T_{1,3}T_{2,4}}{T_{1,4}T_{2,3}}$. We may interpret it using some cross-ratio as in [6]. Let us define the lines $D_i \subset F_s$ as the vectors whose projection on E_{e_i} vanishes. Then ρ_s is the cross-ratio of the four lines D_i. Such bases are unique up to some global similarity.. Such a choice of basis can be interpreted as a sub-sheaf $\mathcal{F}_1$ of $\mathcal{F}$ on Z. The germs of $\mathcal{F}_1$-sections at each vertex is now of dimension 1. Let γ be a cycle of Z. We associate with it a non zero scalar h_γ which is the holonomy along γ of the sheaf $\mathcal{F}_1$ defined using the following prescription: if ϕ_+ is a section on the edge e ($\phi_+ \in E_e \setminus 0$) which we follow as section of $\mathcal{F}_1$ along γ, we get a new vector ϕ_- in E_e and we put:

Definition 3 *The holonomy of γ is then defined by:*

$$\phi_+ = h_\gamma \phi_- \ .$$

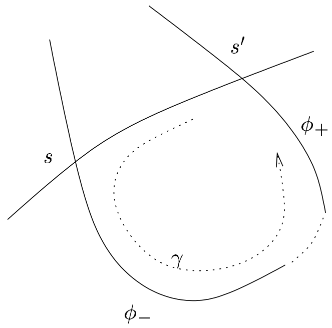

Figure 6: recipe for the holonomies

We then have the:

Theorem 3 *The $n+N$ non-zero scalars ρ_s and h_γ define the sheaf $\mathcal{F} = (Z, E_e, F_s)$ up to isomorphism. If we call* section *of $\mathcal{F}$ the data of one vector of $\oplus E_e$ which belongs to F_s for each vertex, the dimension of the space of sections $b_0(\mathcal{F})$ is only dependent of these invariants. The same statement is true for the $\mathcal{S}$-matrix (up to conjugacy by diagonal matrices) in case where Z admits some open edges.*

Proof.–

By cutting some edges of Z, we get a maximal tree T of Z. Each *oriented* cut edge is associated to some unique cycle $\gamma \in H_1(Z, \mathbb{Z})$ and that way we get a bijection between the set of cut edges and a basis of cycles of Z. The data permit to trivialize the sheaf $\mathcal{F}_1$ on T and rebuilding $\mathcal{F}$ on T. Holonomies h_γ can then be read on the cut edges using the definition 3.

□

4.2 The semi-classical case

Let $\mathbb{C}(h)$ be the ring of formal power series in h. In what follows, E_e is the $\mathbb{C}(h)-$modulus of microlocal solutions along e modulo $O(h^\infty)$. Moduli F_s are given by microlocal solutions near the saddle point s. The number ρ is computed in terms of the series $\varepsilon(h)$ associated to the saddle point by the theorem 2. More precisely, we get

$$\rho_s = -e^{2\pi\varepsilon} \ . \tag{17}$$

Of course, we may have used another normal form in order to define the sub-sheaf $\mathcal{F}_1$.

The e_i's are chosen near s as in figure 7.

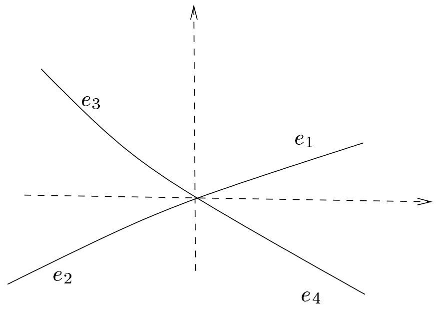

Figure 7: choice of the e_i's

We then take as normal form:

$$T(\varepsilon) = \mathcal{E}\begin{pmatrix} 1 & ie^{-\varepsilon\pi} \\ ie^{-\varepsilon\pi} & 1 \end{pmatrix}, \tag{18}$$

where:

$$\mathcal{E} = \frac{1}{\sqrt{2\pi}}\Gamma(\frac{1}{2} + i\varepsilon)e^{\varepsilon(\frac{\pi}{2}+i\ln h)} \tag{19}$$

$$= \frac{1}{\sqrt{1+e^{-2\pi\varepsilon}}}e^{i\arg\Gamma(1/2+i\varepsilon)+i\varepsilon\ln(h)} \ . \tag{20}$$

As $\varepsilon \to \pm\infty$, Stirling's formula allows to show the following asymptotics

$$T(\varepsilon) = e^{i\varepsilon\ln|h\varepsilon|}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}(1 + O(\frac{1}{\varepsilon})), \ \varepsilon \to +\infty \ , \tag{21}$$

and

$$T(\varepsilon) = e^{i\varepsilon\ln|h\varepsilon|}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}(1 + O(\frac{1}{\varepsilon})), \ \varepsilon \to -\infty \ . \tag{22}$$

These asymptotics describe the transition between the singular and the smooth case. They allow in particular to check the validity of the quantization formula!

Problem: how should we write the condition $b_0(\mathcal{F}) \neq 0$ in terms of these invariants? How should we compute the scattering matrix?

Here is a possible way to derive the quantization conditions. We first cut b_1 edges of Z in order to get a maximal tree T. We choose a non zero section ϕ of $\mathcal{F}_1$ on T. We then try to get a solution $\psi = x\phi : x = (x_e,\ e \in E(T)\ ;\ (x_e^+, x_e^-),\ e \in E(Z \setminus T))$ which satisfy at each vertex $(x_3, x_4) = T(\varepsilon)(x_1, x_2)$ and $x_e^+ = (h_\gamma)^{-1} x_e^-$. Putting these last equations in the first system produces a system of $\nu = 2n$ homogeneous linear equations with ν unknown. The quantization condition can then be written as the vanishing of a $\nu \times \nu$ determinant where $\nu = 2n$.

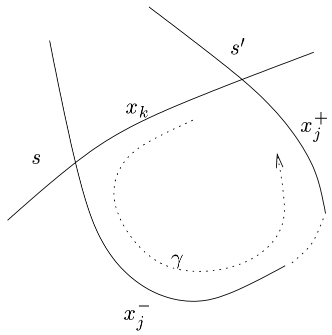

Figure 8: The $x_k,\ x_j^\pm$.

The metric case:

if each space E_e is equipped with an Hermitian metric and if the T_s are unitary maps, it is possible to choose as a normal form for T_s a unitary matrix, for example:

$$T_s = \begin{pmatrix} \cos\theta_s & -\sin\theta_s \\ \sin\theta_s & \cos\theta_s \end{pmatrix} , \tag{23}$$

with $0 < \theta < \frac{\pi}{2}$ and $\tan^2\theta_s = -\rho_s$. In that case, the modulus of holonomies h_γ are 1: they are just phase shifts. It is easy to check that the condition $b_0 \neq 0$ can be rewritten as follows
“1 is an eigenvalue of a unitary matrix”.

Let us assume that we are looking at eigenvalues of a Schrödinger operator K (cf. section 1.3). The equation $b_0 \neq 0$ is equivalent to 1 is an eigenvalue of a unitary matrix which depends of the spectral parameter λ. This equation with complex entries depends on a real parameter. Let us show that in fact this equation is equivalent to a real one: the singular Bohr-Sommerfeld condition.

Let U be a $n \times n$ unitary matrix, we have:

$$\det(I - U) = \det(UU^* - U) = \det(U)\det(U^* - I) = (-1)^n \det(U)\overline{\det(I - U)}$$

Let us write $\det(I-U) = a+ib$ and $(-1)^n \det(U) = c$, we have:

$$(a+ib) = c(a-ib)$$

If $c \neq 1$, then:

$$a = -i\frac{1+c}{1-c}b$$

and $a+ib=0 \Leftrightarrow b=0$. If $c=1$, then $b=0$ and $a+ib=0 \Leftrightarrow a=0$. In both cases, we have got an equation with real entries.

5 Computation of the holonomies up to $O(h)$

We should first compute ρ_s and the holonomies h_γ as in §4. We have already seen that $\rho_s = -e^{2\pi\varepsilon}$. We are left with the computation of holonomies, which is the main statement of this paper:

Theorem 4 *Assuming the choice of the normal form given by the equation (18) and the conventions of figure 7, the holonomies h_γ are given by:*

$$h_\gamma^{-1} = e^{\frac{i}{h}A_\gamma - iI_\gamma + i\frac{\pi}{2}m_\gamma}(1+O(h)) \ . \tag{24}$$

6 Justification

Let $\varphi_\pm(y)$ and $\psi_\pm(y)$ the functions defined by:

$$\varphi_\pm(y) = Y(\pm y)|y|^{-1/2}e^{i\varepsilon \ln|y|} \ , \tag{25}$$

and

$$\psi_\pm(y) = \int^\star Y(\pm\eta)|\eta|^{-1/2}e^{i\frac{y\eta}{h}}e^{-i\varepsilon\ln|\eta|}d\eta \ , \tag{26}$$

where

$$\int^\star = (2\pi h)^{-1/2}e^{-i\pi/4}\int \tag{27}$$

and Y is the Heaviside's function. Then let f be a microlocal solution in some neighborhood of O of the equation

$$(\hat{y\eta} - h\varepsilon)f = O(h^\infty) \ , \tag{28}$$

f is microlocally outside of 0 a linear combination of $\varphi_\pm$ and $\psi_\pm$; we write:

$$f \sim \sum x_\pm\varphi_\pm + y_\pm\psi_\pm \ . \tag{29}$$

We have the relation (see [7]):

$$\begin{pmatrix} y_+ \\ y_- \end{pmatrix} = T(\varepsilon) \begin{pmatrix} x_+ \\ x_- \end{pmatrix} \tag{30}$$

Using the notations of figure 7, we have then:

$$\begin{pmatrix} x_3 \\ x_4 \end{pmatrix} = T(\varepsilon) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} . \tag{31}$$

Let us put:

$$\chi'(O) = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \text{ avec } a > 0,\ b < 0. \tag{32}$$

where χ is the canonical map of theorem 2.

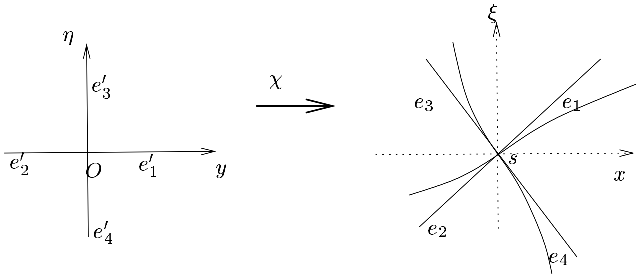

Figure 9: the choices of the e_i's and of χ.

We may assume that $s_j = O$. Let $S(x, y) = S_0(x, y) + O((|x| + |y|)^3)$ be the generating function of χ defined by:

$$\chi(y, -\frac{\partial S}{\partial y}) = (x, \frac{\partial S}{\partial x}) \tag{33}$$

and $S(O) = 0$. We get:

$$S_0(x, y) = \frac{1}{2b}(dx^2 - 2xy + ay^2) . \tag{34}$$

The FIO U is then given by:

$$Uf(x) = \int^\star e^{\frac{i}{h}S(x,y)} C_h(x, y) f(y) dy , \tag{35}$$

where $C_h(x, y) \sim \sum_{j=0}^\infty C_j(x, y) h^j$ and $C_0(O) = 1$.

Let us define $\Phi_\pm = U\varphi_\pm$ and $\Psi_\pm = U\psi_\pm$. We compute the WKB form of these functions for $x_0 \neq 0$, but close to 0. We apply stationary phase method to the integral:

$$\Phi_\pm(x_0) = \int^\star e^{\frac{i}{h}S(x_0,y)} C_h(x_0,y)\phi_\pm(y)g(y)dy \ , \tag{36}$$

where $g(y) \in C_0^\infty(\mathbb{R}\setminus 0)$ is 1 near y_0 and such that $\chi(y_0,0) = (x_0,\xi_0)$. We get:

$$\Phi_\pm(x_0) = Y(\pm x_0) e^{\frac{i}{h}S_1(x_0)} e^{i\varepsilon \ln|\frac{x_0}{a}|} e^{-i\frac{\pi}{2}} |\frac{b}{x_0}|^{\frac{1}{2}} (A_0(x_0) + O(h)) \ , \tag{37}$$

where $A_0(x) = 1 + O(x)$ and $S_1(x)$ is the generating function of the arc $\chi(\mathbb{R}\times 0)$ which vanishes at $x = 0$. In the same way

$$\Psi_\pm(x_0) = Y(\mp x_0) e^{\frac{i}{h}S_2(x_0)} e^{-i\varepsilon \ln|\frac{x_0}{b}|} e^{-i\frac{\pi}{2}} |\frac{b}{x_0}|^{\frac{1}{2}} (B_0(x_0) + O(h)) \ , \tag{38}$$

where $B_0(x) = 1 + O(x)$ and S_2 is the generating function of the arc $\chi(0\times\mathbb{R})$ which vanishes at $x = 0$.

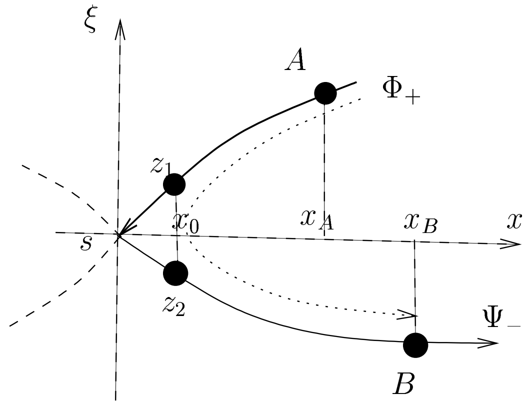

Figure 10: computation of the holonomy.

Let us evaluate $\Phi_+(x_A)$ and $\Psi_-(x_B)$ starting from their values at x_0 in order to calculate their phase shift, using the usual WKB formulae.

Putting $z_j = (x_0, S_j'(x_0))$, we get:

$$\Phi_+(x_A) = -iC_+(x_A) e^{\frac{i}{h}\int_{z_1}^A \xi dx + i\varepsilon \ln\frac{x_0}{a} - i\int_{z_1}^A H_1 dt} (A_0(x_0) + O(h)) \ , \tag{39}$$

where the integrals are computed on Z and $C_+(x_A) > 0$; in the same way:

$$\Psi_-(x_B) = -iC_-(x_B) e^{\frac{i}{h}\int_{z_2}^B \xi dx - i\varepsilon \ln\frac{x_0}{|b|} - i\int_{z_b}^B H_1 dt} (B_0(x_0) + O(h)) \ , \tag{40}$$

where $C_-(x_B) > 0$.

Using the preceding computations, we can find the phase shift $\Psi_-(x_B) = e^{i\Omega}\Phi_+(x_A)$. Going to the limit where $a, b \to s_j$ and using $\omega(s_j\vec{z}_1, s_j\vec{z}_2) \sim \frac{x^2}{a|b|}$, we get:

$$\Omega = \frac{i}{h}\int_A^B \xi dx - i\mathrm{vp}\int_A^B H_1 dt + O(h) \ , \tag{41}$$

In order to check the validity of the formula (24), let us assume that the microlocal solutions Φ_+ and Ψ_- corresponds to the same edge $e \in E(Z \setminus T)$. If A and B have the same limit point, we should have:

$$x_+\Phi_+(x_A) = x_-\Psi_-(x_B)e^{i\frac{\pi}{2}m_\gamma}$$

which gives

$$x_+ = x_- e^{i\Omega + i\frac{\pi}{2}m_\gamma}$$

So that:

$$h_\gamma^{-1} = e^{i\Omega + i\frac{\pi}{2}m_\gamma}$$

7 Summary of quantization conditions

Summarizing, we start with a semi-classical Hamiltonian whose principal symbol H_0 is real and whose sub-principal symbol is denoted by H_1. We first look at the characteristic manifold $Z = H_0^{-1}(0)$, and calculate the invariants ε of the saddle points. They are formal series in h whose first term ε_0 is given by the formula (14). We then choose some maximal tree T of Z and some orientation of the cut edges. It is then possible to calculate the holonomies of the corresponding cycles using formula (24). We then describe any microlocal solution in terms of the trivialisation of $\mathcal{F}_1$ in the following way:

$$u = \sum_e x_e u_e$$

where the sum is on the edges of T. The conditions on the x_e's are then given by the matrices T_ε associated to each saddle point and the holonomies $x_{e_-} = h_\gamma x_{e_+}$ if the cycle γ corresponds to the cut edge $e = e_+ \cup e_-$ following e_- and then e_+. The relative error on these conditions is of order $O(h^\infty)$; it is of order $O(h)$ when we approximate the holonomies using equation (24); in that case, it is also possible to replace ε by ε_0 without changing the relative error.

8 The double well potential.

8.1 Generic study of the double well potential.

In this section, we will apply the previous theory to the situation of [7] and [8] where $X = T^\star\mathbb{R}$ and $V:\ \mathbb{R} \to \mathbb{R}$ is a function with a double well. Without loss of generality, we may suppose that:

$$V(0) = 0,\ V'(0) = 0,\ \mathcal{V} = V''(0) << 0$$

e.g. $V(x) = x^2((x-b)^2 - a^2)$ with $a > b > 0$.

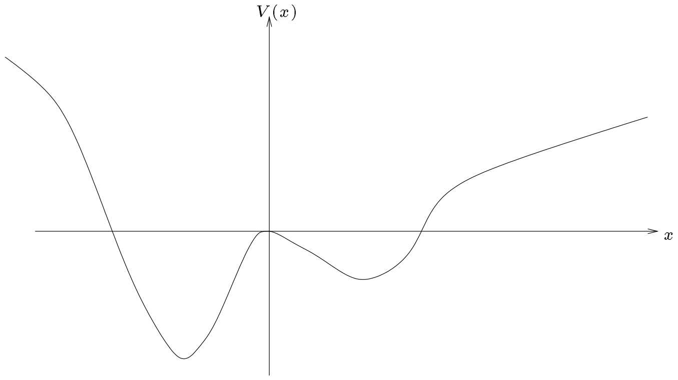

Figure 11: a double-well potential.

Let

$$\hat{H} = -\frac{1}{2}h^2\frac{d^2}{dx^2} + V(x) - \lambda h \tag{42}$$

be the corresponding Schrödinger operator. A normalized solution of $\hat{H}u = O(h^\infty)$ exists if and only if λh is an eigenvalue of $-\frac{1}{2}h^2\frac{d^2}{dx^2} + V(x)$ up to a relative error of order $O(h^\infty)$ (relative to the closest eigenvalue).

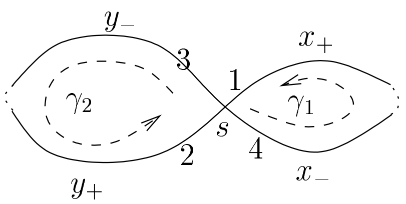

Figure 12: the double well potential in the phase space.

We have:

$$\det(H''_0) = \mathcal{V}, \quad \varepsilon_0 = \frac{\lambda}{\sqrt{-\mathcal{V}}} \tag{43}$$

The holonomy equations read:

$$x_- = h_{\gamma_1} x_+,\ y_- = h_{\gamma_2} y_+ \ , \tag{44}$$

and the critical point relations are:

$$\begin{pmatrix} y_- \\ x_- \end{pmatrix} = T(\varepsilon) \begin{pmatrix} x_+ \\ y_+ \end{pmatrix} . \tag{45}$$

We get the following quantization relation:

$$\det \left(\begin{pmatrix} 0 & h_{\gamma_2} \\ h_{\gamma_1} & 0 \end{pmatrix} - T(\varepsilon) \right) = 0 \ . \tag{46}$$

or equivalently "1 is an eigenvalue of the matrix":

$$T(\varepsilon) \begin{pmatrix} 0 & h_{\gamma_1}^{-1} \\ h_{\gamma_2}^{-1} & 0 \end{pmatrix}, \quad T(\varepsilon) = \mathcal{E} \begin{pmatrix} 1 & ie^{-\varepsilon\pi} \\ ie^{-\varepsilon\pi} & 1 \end{pmatrix}$$

This matrix is unitary, hence we may apply [8, Appendix] and rewrite the quantization condition as a real equation, like [8, Proposition 3]:

Proposition 1 *The equation $\hat{H}u = O(h^\infty)$ has a normalized eigenfunction if and only if λ satisfies the following condition:*

$$\frac{1}{\sqrt{1+e^{2\pi\varepsilon}}} \cos\left(\frac{\varphi_1 - \varphi_2}{2}\right) = \cos\left(\frac{\varphi_1+\varphi_2}{2} + \frac{\pi}{2} + \varepsilon \ln h + \arg \Gamma(\frac{1}{2} + i\varepsilon)\right) \tag{47}$$

where ε depends on λ (cf. (11) and (43)) and:

$$e^{i\varphi_1} = h_{\gamma_1}^{-1}, \quad e^{i\varphi_2} = h_{\gamma_2}^{-1}$$

We want to calculate more explicitly (47) up to a relative error of order $O(h)$. Hence we replace ε by ε_0, and calculate φ_1 and φ_2 using (24). We observe that the Maslov indices are $+1$ and that the A_{γ_i} values are opposite to the area inside the cycles γ_i (since $d(\xi dx) = -dx \wedge d\xi$). It remains to do the calculation of the regularized integrals I_{γ_i}.

Note that along a trajectory of the Hamiltonian $H = \xi^2/2 + V(x)$ one has:

$$\frac{dx}{dt} = \xi_\pm = \pm\sqrt{-2V(x)}$$

Let γ denotes one of the two cycles, let A be the intersection of γ with the x axis. Let x_A be the x-coordinate of A (e.g. for $V(x) = x^2((x-b)^2 - a^2)$, $x_A = b \pm a$). From definition (8), we get:

$$\begin{aligned} I_\gamma &= \lim_{\tilde{a}\tilde{b} \to s_j} (\int_A^{\tilde{a}} H_1 dt + \int_{\tilde{b}}^{A} H_1 dt + a(0) \ln \int_{R_{\tilde{a},\tilde{b}}} \omega) \\ &= \lambda \lim_{x\to 0} (2 \int_{x_A}^{x} \frac{-dX}{\sqrt{-2V(X)}} + \frac{1}{\sqrt{-\mathcal{V}}} \ln|2x\sqrt{-2V(x)}|) \end{aligned}$$

8.2 Non singular limit.

In this section, we show that the limit of the singular Bohr-Sommerfeld quantization rules as $\varepsilon \to \pm\infty$ are the usual quantization rules.

We apply the Stirling formula:

$$\arg \Gamma(\frac{1}{2} + i\varepsilon) = \varepsilon \ln |\varepsilon| - \varepsilon + o(1),$$

and evaluate the area inside the curve $\frac{\xi^2}{2} + V(x) = \tau$ as τ tends to 0. From Equation (10) (section 2.2), we get:

$$A(\tau) = A(0) + 2\frac{\tau}{\sqrt{|\mathcal{V}|}}(1 - \ln \frac{|\tau|}{\sqrt{|\mathcal{V}|}}) - (I_{\gamma_1} + I_{\gamma_2})\tau + O(\tau^2 \ln |\tau|),$$

where $H_1 = 1$ in the definition of the I_γ integrals.

Here $\tau = \lambda h$ and we must change the sign of $A(\tau)$ since the cycles are oriented using the trigonometric convention:

$$\begin{aligned} \int_{H=\lambda h} \xi\, dx &= \int_{H=0} \xi\, dx + 2\frac{\lambda h}{\sqrt{|\mathcal{V}|}}(\ln \frac{|\lambda h|}{\sqrt{|\mathcal{V}|}} - 1) + (I_{\gamma_1} + I_{\gamma_2})\lambda h + O(\lambda^2 h^2 \ln h) \\ &= \int_{H=0} \xi\, dx + 2\varepsilon_0 h(\ln |h\varepsilon_0| - 1) - h(I_{\gamma_1} + I_{\gamma_2})H_1 + O(\lambda^2 h^2 \ln h) \end{aligned}$$

where $H_1 = -\lambda$.

If λ tends to $+\infty$, Equation (47) is satisfied if the argument of the cosine of the right hand-side is $\pi/2$ modulo π, hence:

$$\frac{\varphi_1 + \varphi_2}{2} + \varepsilon \ln h - \varepsilon + \varepsilon \ln \varepsilon + o_\varepsilon(1) = k\pi \tag{48}$$

On the other hand:

$$\begin{aligned} \frac{\varphi_1 + \varphi_2}{2} &= \frac{\pi}{2} + \frac{1}{2h}\int_{H=0} \xi\, dx - \frac{1}{2}(I_{\gamma_1} + I_{\gamma_2})(H_1) \\ &= \frac{\pi}{2} + \frac{1}{2h}\int_{H=\lambda h} \xi\, dx - \varepsilon_0(\ln |h\varepsilon_0| - 1) + O(h \ln h\ \varepsilon_0^2) \end{aligned}$$

therefore (48) becomes:

$$\frac{1}{2h}A(h\varepsilon) + \frac{\pi}{2} + O(h \ln h\ \varepsilon^2) + o_{\varepsilon \to +\infty}(1) = k\pi$$

which is the usual Bohr-Sommerfeld quantization rule. We leave the same verification as λ tends to $-\infty$ as an exercise for the reader.

8.3 Analytic calculations for polynomial potentials of degree 4.

In this section we examine further the example $V(x) = x^2((x-b)^2 - a^2)$.

8.3.1 Results.

Using our preferred CAS (computer algebra system), we determine analytically the A_{γ_i}'s:

$$\begin{aligned}
A_{\gamma_d} &= \sqrt{2}\left(-\frac{2\sqrt{a^2-b^2}^3}{3} - \sqrt{a^2-b^2}b^2 - ba^2\arcsin(\frac{b}{a}) - \frac{a^2b\pi}{2}\right)\\
A_{\gamma_g} &= \sqrt{2}\left(-\frac{2\sqrt{a^2-b^2}^3}{3} - \sqrt{a^2-b^2}b^2 - ba^2\arcsin(\frac{b}{a}) + \frac{a^2b\pi}{2}\right)
\end{aligned}$$

and I_γ's:

$$I_{\gamma_d} = \varepsilon_0\left(\frac{7}{2}\ln 2(a^2-b^2) - 2\ln a\right) = \varepsilon_0\left(\frac{7}{2}\ln(2(a^2-b^2)) - 2\ln a\right) \tag{49}$$

We observe that $I_{\gamma_g} = I_{\gamma_d}$, this will be explained in Section 8.3.2.

Hence (24) reads, up to a relative error of order $O(h)$:

$$\begin{aligned}
\varphi_1 - \varphi_2 &= \sqrt{2}\frac{a^2b\pi}{h}\\
\varphi_1 + \varphi_2 &= \pi - 2\varepsilon_0(\frac{7}{2}\ln(2(a^2-b^2)) - 2\ln a) +\\
&+ \sqrt{2}\frac{2}{h}\left(-\frac{2\sqrt{a^2-b^2}^3}{3} - \sqrt{a^2-b^2}b^2 - ba^2\arcsin(\frac{b}{a})\right)\ ,
\end{aligned}$$

then we apply (47) and we get:

Proposition 2 *The solutions ε_0 of:*

$$\begin{aligned}
\frac{1}{\sqrt{1+e^{2\pi\varepsilon_0}}}\cos(\frac{a^2b\pi}{2h}) &= \cos\left(\pi - 2\varepsilon_0\left(\frac{7}{2}\ln(2(a^2-b^2)) - 2\ln a\right) +\right. \\
&+ \frac{\sqrt{2}}{h}\left[-\frac{2\sqrt{a^2-b^2}^3}{3} - \sqrt{a^2-b^2}b^2 - ba^2\arcsin(\frac{b}{a})\right] +\\
&+ \left.\varepsilon_0\ln h + \arg\Gamma(\frac{1}{2}+i\varepsilon_0)\right)
\end{aligned} \tag{50}$$

correspond to the eigenvalues $\lambda h = \sqrt{2(a^2-b^2)}\varepsilon_0 h$ of the Schrödinger operator

$$H = -\frac{1}{2}h^2\frac{d^2}{dx^2} + V(x) = x^2((x-b)^2 - a^2)$$

up to a relative error of order $O(h)$ (relative means relative to the closest eigenvalue).

If we want to get the numerical values of the eigenvalues, we are left to solve (50). In appendix A, we will compare the corresponding eigenvalues λh to the eigenvalue that we calculate using purely numerical technics (Runge-Kutta's method here) to show the accuracy of the singular Bohr-Sommerfeld quantization rules. The semi-classical method is very useful for small values of h because the computation time is essentially independent of h, as it growths linearly for the Runge-Kutta method since we have to choose a step of size εh (therefore we must make $1/(\varepsilon h)$ steps)

8.3.2 Equality $I_{\gamma_d} = I_{\gamma_g}$

The equality $I_{\gamma_g} = I_{\gamma_d}$ for polynomial potentials of degree 4 can be shown directly. From (10), we have to show that $A_+(E) - A_-(E) =$ constant, where $A_\pm(E)$, $E < 0$, stand for the areas of the two components of $\{(x,\xi)/\xi^2 + V(x) \leq E\}$. Let $\gamma_\pm$ denote the border of these two domains, one has:

$$\frac{dA_\pm}{dE} = \int_{\gamma_\pm} \frac{dx}{\xi} \ . \tag{51}$$

The 1-form $\frac{dx}{\xi}$ is holomorphic on the smooth holomorphic projective compactification of the curve $\xi^2 + V(x) = E$. This curve is a torus if V is a polynomial of degree 4, hence the curves γ_+ and γ_- are homotopic (for they are non degenerate and they don't intersect), which completes the proof of (51).

9 The triple well potential.

Same context as in section 8, but V is a potential with three wells so that the corresponding saddle points are at the same height.

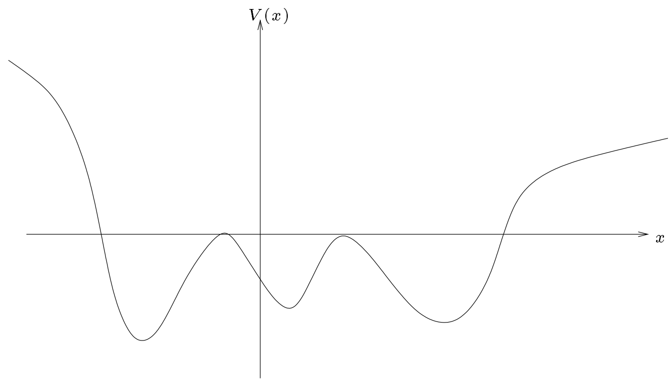

Figure 13: a triple well potential.

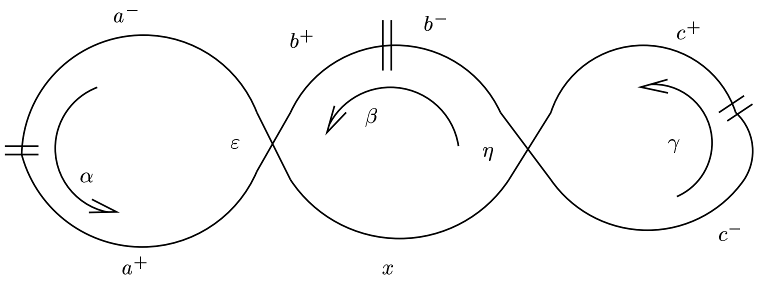

Figure 14: the triple well potential in the phase space.

We construct a maximal tree (see figure 14) with 7 edges denoted by $a^\pm$, $b^\pm$, $c^\pm$ and x. The holonomy equations corresponding to the three cycles α, β and γ are:

$$a^+ = a^-/h_\alpha, \quad b^+ = b^-/h_\beta, \quad c^+ = c^-/h_\gamma$$

Let ε and η denote the semi-classical invariants of the two vertices, the following relations hold:

$$\begin{pmatrix} a^- \\ x \end{pmatrix} = T(\varepsilon) \begin{pmatrix} b^+ \\ a^+ \end{pmatrix}, \quad \begin{pmatrix} b^- \\ c^- \end{pmatrix} = T(\eta) \begin{pmatrix} c^+ \\ x \end{pmatrix}$$

Hence:

$$\begin{pmatrix} T(\varepsilon) & 0 \\ 0 & T(\eta) \end{pmatrix} \begin{pmatrix} b^+ \\ a^+ \\ c^+ \\ x \end{pmatrix} - \begin{pmatrix} a^- \\ x \\ b^- \\ c^- \end{pmatrix} = 0$$

Since:

$$\begin{pmatrix} a^- \\ x \\ b^- \\ c^- \end{pmatrix} = \begin{pmatrix} 0 & h_\alpha & 0 & 0 \\ 0 & 0 & 0 & 1 \\ h_\beta & 0 & 0 & 0 \\ 0 & 0 & h_\gamma & 0 \end{pmatrix} \begin{pmatrix} b^+ \\ a^+ \\ c^+ \\ x \end{pmatrix}$$

the system has a non-trivial solution if and only if:

$$\det \left(\begin{pmatrix} T(\varepsilon) & 0 \\ 0 & T(\eta) \end{pmatrix} - \begin{pmatrix} 0 & h_\alpha & 0 & 0 \\ 0 & 0 & 0 & 1 \\ h_\beta & 0 & 0 & 0 \\ 0 & 0 & h_\gamma & 0 \end{pmatrix} \right) = 0$$

Let $\mathcal{E}$ and $\mathcal{N}$ denote the common factors of the coefficients of the matrices $T(\varepsilon)$ and $T(\eta)$ defined by (19) for $\mathcal{E}$ and a similar formula for $\mathcal{N}$. Dividing the first two lines of the determinant by $\mathcal{E}$ and the last two lines by $\mathcal{N}$, we get:

$$\begin{vmatrix} 1 & ie^{-\varepsilon\pi} - \frac{h_\alpha}{\mathcal{E}} & 0 & 0 \\ ie^{-\varepsilon\pi} & 1 & 0 & \frac{-1}{\mathcal{E}} \\ \frac{-h_\beta}{\mathcal{N}} & 0 & 1 & ie^{-\eta\pi} \\ 0 & 0 & ie^{-\eta\pi} - \frac{h_\gamma}{\mathcal{N}} & 1 \end{vmatrix} = 0$$

Now we expand the determinant with respect to the first column:

$$(1 - ie^{-\eta\pi}(ie^{-\eta\pi} - \frac{h_\gamma}{\mathcal{N}}))(1 - ie^{-\varepsilon\pi}(ie^{-\varepsilon\pi} - \frac{h_\alpha}{\mathcal{E}})) + \frac{h_\beta}{\mathcal{N}}(ie^{-\varepsilon\pi} - \frac{h_\alpha}{\mathcal{E}})\frac{-1}{\mathcal{E}}(ie^{-\eta\pi} - \frac{h_\gamma}{\mathcal{N}}) = 0$$

Defining:

$$A = e^{-\varepsilon\pi} + i\frac{h_\alpha}{\mathcal{E}}, \quad C = e^{-\eta\pi} + i\frac{h_\gamma}{\mathcal{N}} \tag{52}$$

we rewrite the previous equation as:

$$(1 + e^{-\eta\pi}C)(1 + e^{-\varepsilon\pi}A) = \frac{-h_\beta}{\mathcal{N}\mathcal{E}}AC \tag{53}$$

We want to show that this complex equation reduces to a real equation for real values of E. For this we will prove that the modulus of both sides are equal. Let us introduce the following notations:

$$\tilde{\alpha} = \arg h_\alpha - \arg \mathcal{E}, \quad \tilde{\gamma} = \arg h_\gamma - \arg \mathcal{N} \tag{54}$$

Using this notation we may rewrite:

$$A = e^{-\varepsilon\pi} + \sqrt{1 + e^{-2\varepsilon\pi}}e^{i\tilde{\alpha}}, \quad C = e^{-\eta\pi} + \sqrt{1 + e^{-2\eta\pi}}e^{i\tilde{\gamma}}$$

since $|\mathcal{E}| = 1/\sqrt{1 + e^{-2\varepsilon\pi}}$. Hence:

$$\begin{aligned} 1 + e^{-\varepsilon\pi}A &= 1 + e^{-2\varepsilon\pi} + e^{-\pi\varepsilon}\sqrt{1 + e^{-2\pi\varepsilon}}e^{i\tilde{\alpha}} \\ &= \sqrt{1 + e^{-2\varepsilon\pi}}e^{i\tilde{\alpha}}\overline{A} \end{aligned}$$

and Equation (53) becomes:

$$e^{i\tilde{\alpha}+i\tilde{\gamma}}\sqrt{1 + e^{-2\varepsilon\pi}}\sqrt{1 + e^{-2\eta\pi}}\,\overline{AC} = \frac{-h_\beta}{\mathcal{E}\mathcal{N}}AC$$

It is now clear that both sides have the same modulus, therefore this equation reduces to:

$$\tilde{\gamma} + \tilde{\alpha} = \pi + \arg h_\beta - \arg \mathcal{E} - \arg \mathcal{N} + 2\arg A + 2\arg C \quad (2\pi)$$

Eventually we get the:

Proposition 3 *The eigenvalues of the triple well potential Schrödinger operator correspond to the solutions λ of:*

$$\arg(h_\alpha) + \arg(h_\gamma) = \arg(h_\beta) + \pi + 2\arg A + 2\arg C \quad (2\pi) \tag{55}$$

up to a relative error of order $O(h^\infty)$. Here h_α, h_β and h_γ denote the holonomies of the 3 cycles and A, C as defined in (52), (19).

Exercise:
Let $a > 0$, $b > 0$ and define:

$$V(x) = a(x^2-1)^3 - b(x^2-1)^2 = (x^2-1)^2(ax^2 - a - b)$$

Calculate the singular Bohr-Sommerfeld quantization rules and compare with purely numerical technics, as for the quadratic potential of section 8.3.

Hints:
We have:

$$V'(x) = 2x(3a(x^2-1)^2 - 2b(x^2-1)) = 2x(x^2-1)(3ax^2 - 3a - 2b)$$

hence this potential has five critical points: 0, ± 1, $\pm\sqrt{1 + 2b/(3a)}$. The corresponding critical values are: $-a-b<0$, 0, $-4b^3/(27a^2) < 0$ and the corresponding Hessians are: $6a + 4b > 0$, $-8b < 0$ and $24b + 16b^2/(3a) > 0$. Hence V has two local maxima at ± 1 with $V(\pm 1) = 0$. It is possible to calculate analytically the action integrals since for $x \in [-1, 1]$:

$$W(x) = \sqrt{-V(x)} = (1-x^2)\sqrt{b + a - ax^2}$$

and $1/W$ both admit an explicit anti-derivative.

10 The Hill Equation.

In this section we are concerned with the Schrödinger operator

$$\hat{H} = -\frac{h^2}{2}\frac{d^2}{dx^2} + V(x)$$

where $V : \mathbb{R} \to \mathbb{R}$ is a C^∞ periodic potential of period $T > 0$ such that $\sup_{x\in\mathbb{R}} V(x) = 0$.

10.1 Hill's Equation spectrum, discrimant

Let us recall some well known facts about the spectrum of the Hill equation and its discriminant.

The operator $\hat{H}$ is essentially self-adjoint and has a continuous spectrum made of the union of intervals called *bands* separed by *gaps*.

In order to get quantitative informations on these bands, let us introduce the *discriminant* function $\Delta(E)$. Let $P_E : \mathbb{C}^2 \to \mathbb{C}^2$ be the linear map defined by $P_E(u(0), u'(0)) = (u(T), u'(T))$ where u is the unique solution of $(\hat{H} - E)u = 0$. It is easy to prove that P_E has determinant 1.

Definition 4 *The* discriminant *of the Hill equation is defined by:*

$$\Delta(E) = \mathrm{trace}(P_E) \ .$$

The graph of $\Delta(E)$ looks like figure 15.

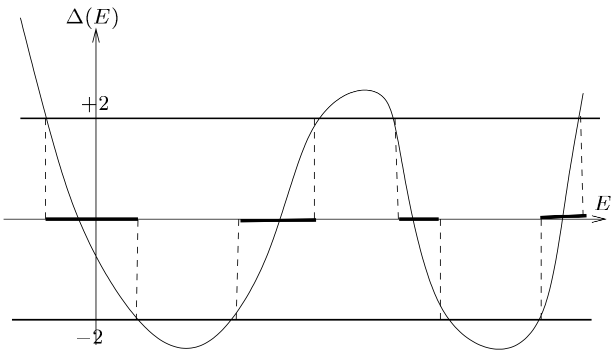

Figure 15: the discriminant $\Delta(E)$.

We define the periodic spectrum $E_1^+ < \cdots \le E_k^+ \le \cdots$ as the spectrum of the operator $\hat{H}$ restricted to the periodic functions. The E_k^+'s are precisely the solutions of $\Delta(E^+) = 2$. We have a similar definition for the anti-periodic spectrum $E_1^- \le \cdots \le E_k^- \le \cdots$, this is the spectrum of $\hat{H}$ restricted to anti-periodic functions. The E_k^-'s are the solutions of $\Delta(E^-) = -2$. The following inequalities hold:

$$E_1^+ < E_1^- \le E_2^- < E_2^+ \le E_3^+ < E_3^- \le \cdots$$

and the bands are given by:

$$B_{2j-1} = [E_{2j-1}^+, E_{2j-1}^-], \ j = 1, 2, \cdots$$

$$B_{2j} = [E_{2j}^-, E_{2j}^+], \ j = 1, 2, \cdots \ .$$

More generally, the spectrum of $\hat{H}$ over kT-periodic functions is the union of the solutions of: $\Delta(E) = 2\cos\frac{2\pi j}{k}$.

The sizes of the bands are exponentially small for $E < 0$ as $h \to 0^+$ and the sizes of the gaps are exponentially small for $E > 0$. We want to describe the transition between this two regions, for this we will compute the asymptotic expansion series of $\Delta_1(\lambda) = \Delta(h\lambda)$. Moreover, we will use this asymptotic to describe the spectrum of H restricted to kT-periodic functions.

10.2 Semi-classical asymptotic of the discriminant if the potential has a unique maximum per period.

In this section, we assume that $V^{-1}(0) = 2\pi\mathbb{Z}$ and $V"(0) < 0$, e.g. $V(x) = \cos x - 1$. Let $\gamma_\pm$ denote the 2 cycles of $T^\star(\frac{\mathbb{R}}{2\pi\mathbb{Z}})$ defined by $\gamma_+(s) = (s, \sqrt{-2V(s)}),\ 0 \leq s \leq 2\pi$ and $\gamma_-(s) = (2\pi - s, -\sqrt{-2V(2\pi - s)}),\ 0 \leq s \leq 2\pi$.

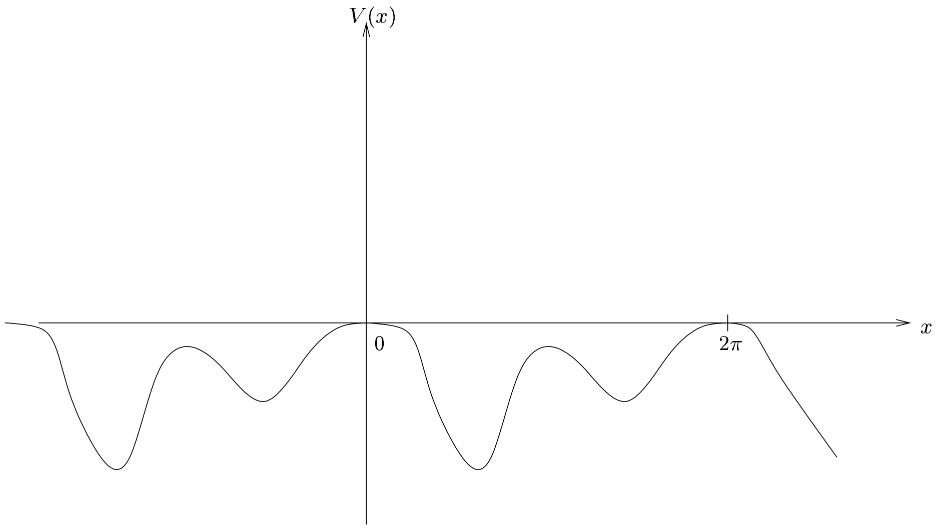

Figure 16: an example of periodic potential.

Theorem 5 *The holonomy of γ_+ and γ_- are equal. Let α be this common value:*

$$\alpha = e^{\frac{i\Omega}{h} - i\lambda J} + O(h) \tag{56}$$

where $\Omega = \int_{\gamma_+} \xi dx$ and $J = \mathrm{vp} \int_{\gamma_+} dt$.

Let ε be the semi-classical invariant of the critical point $(0,0)$:

$$\varepsilon = \sum_{j=0}^{\infty} \varepsilon_j(\lambda) h^j, \quad \varepsilon_0 = \frac{\lambda}{|V"(0)|^{\frac{1}{2}}}.$$

The following relation holds for $|\lambda| \leq M$:

$$\Delta_1(\lambda) = 2\sqrt{1 + e^{-2\pi\varepsilon}} \cos\left(\arg\alpha + \varepsilon \ln h + \arg\Gamma(\frac{1}{2} + i\varepsilon)\right) + O(h^\infty) \ , \tag{57}$$

hence

$$\Delta_1(\lambda) = 2\sqrt{1 + e^{-2\pi\varepsilon_0}} \cos\left(-\frac{\Omega}{h} - \lambda J + \varepsilon_0 \ln h + \arg\Gamma(\frac{1}{2} + i\varepsilon_0)\right) + O(h \ln h) \ . \tag{58}$$

This result extends to the C^∞ case the result of März ([14]) which was valid under analyticity assumptions.

Corollary 1 *It follows immediately that in the region where $\lambda \to 0$, we have:*

$$\Delta_1(\lambda) = 2\sqrt{2}\cos\left(\frac{\Omega}{h} + \frac{\lambda \ln h}{|V"(0)|^{\frac{1}{2}}}\right) + O(\lambda) + O(h\ln h) \ . \tag{59}$$

Hence the gaps and bands have asymptotically the same length l:

$$l = \frac{\pi h |V"(0)|^{\frac{1}{2}}}{2|\ln h|} \ .$$

Proof.–

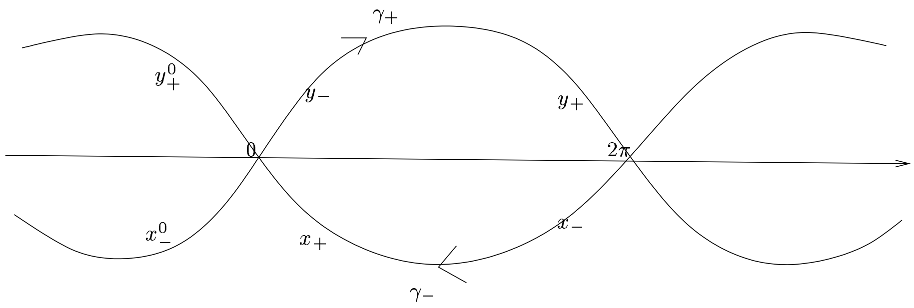

Figure 17: the phase portrait for the Hill's equation

Near $x = 0^+$, a solution of the Schrödinger equation is characterized by its coordinates (y_+^0, x_-^0) in the basis (e_3, e_2) of microlocal solutions. Let (y_-, x_+) [respectively (y_+, x_-)] denote the coordinates of the same solution near $x = 2\pi$ with respect to the basis (e_1, e_4) [resp. (e_3, e_2)]. The P_E matrix is the matrix defined by $(y_+, x_-) = P_E(y_+^0, x_-^0)$. Its expression is easily deduced from the T matrix and the holonomies:

$$y_+ = h_{\gamma^+}^{-1} y_-, \ x_+ = h_{\gamma^-}^{-1} x_-, \quad \begin{pmatrix} y_+^0 \\ x_+ \end{pmatrix} = T(\varepsilon) \begin{pmatrix} y_- \\ x_-^0 \end{pmatrix} \tag{60}$$

Factoring $\mathcal{E}$ in the $T(\varepsilon)$ matrix (cf. (19)), we get:

$$P_E = \begin{pmatrix} 1/\alpha\mathcal{E} & -ie^{-\pi\varepsilon}/\alpha \\ \alpha i e^{-\pi\varepsilon} & \alpha\mathcal{E}(1 + e^{-2\pi\varepsilon}) \end{pmatrix}$$

Hence $\det(P_E) = 1$ as it should be and:

$$\mathrm{tr}\ (P_E) = 2\sqrt{1 + e^{-2\pi\varepsilon}} \cos\left(\arg(\alpha) + \varepsilon \ln(h) + \arg \Gamma(\frac{1}{2} + i\varepsilon)\right) \ . \tag{61}$$

□

10.3 The periodic spectrum

The periodic spectrum is easily deduced from the equation $\Delta_1(\lambda) = 2$. We will now determine it by a direct method. We will also describe these two methods in section 11 in the more complicated case of the spectrum of the Hill's equation on $2T$ and $3T$ periodic functions. The situation is similar to the double well

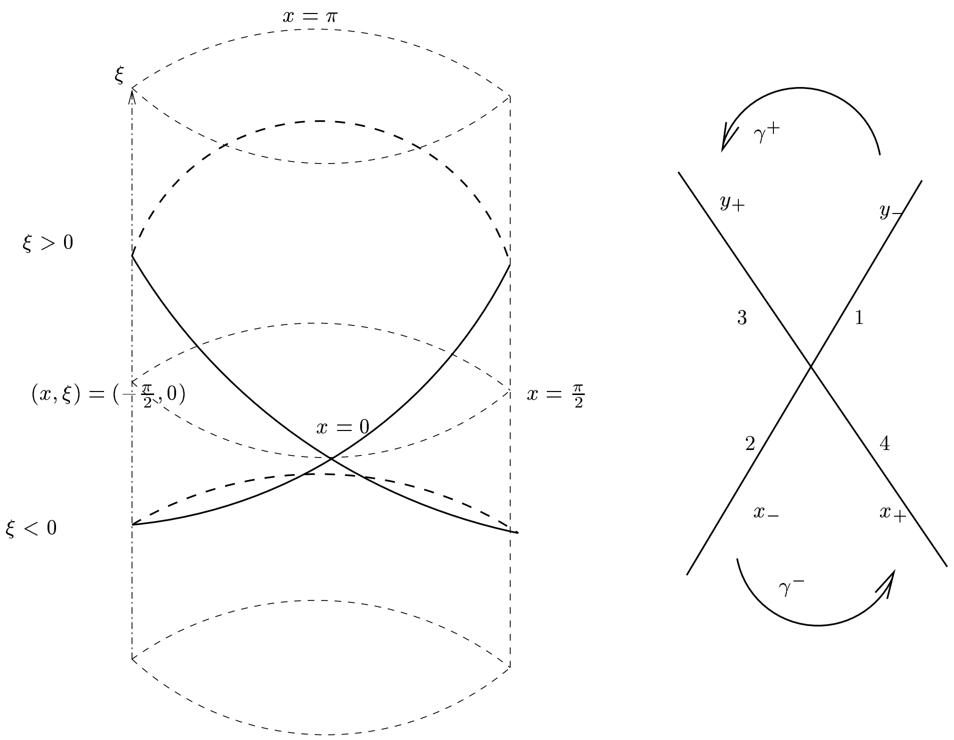

Figure 18: the 0 energy trajectory in the phase space for the pendulum

potential, but here the pairs of exponentially close eigenvalues occurs for energy value that are *greater* (instead of smaller) than the critical energy, these pairs comes from the microlocal effect between the two classical symmetric trajectories.

In the transition energy interval, one has (cf. figure 18):

$$y_+ = h_{\gamma^+}^{-1} y_-, x_+ = h_{\gamma^-}^{-1} x_-, \quad \begin{pmatrix} y_+ \\ x^+ \end{pmatrix} = T(\varepsilon) \begin{pmatrix} y_- \\ x_- \end{pmatrix} \tag{62}$$

Hence 1 is eigenvalue of the unitary matrix:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = T(\varepsilon) \begin{pmatrix} h_{\gamma^+} & 0 \\ 0 & h_{\gamma^-} \end{pmatrix}$$

As for the double-well potential, we apply the following Equation from [8, appendix]:

$$|a| \cos\left(\frac{\arg ad}{2} - \arg a\right) = \cos\left(\frac{\arg ad}{2}\right)$$

and we get the singular Bohr-Sommerfeld quantization rules:

$$\frac{1}{\sqrt{1+e^{-2\pi\varepsilon}}} = \cos\left(\arg\alpha + \varepsilon\ln h + \arg\Gamma(\frac{1}{2}+i\varepsilon)\right) \tag{63}$$

This equation may be deduced from (57) and $\Delta_1(\lambda) = 2$ as well. Let us remark the minus sign in front of ε in the exponential of the left hand-side of (63), it confirms the existence of pairs of eigenvalues for $E > 0$ instead of $E < 0$ (as obtained for the symmetric double-well potential). A more precise study of the solutions of (63) could be done, and would show the same universal transition of the eigenvalue ladders.

Example: For the Mathieu Equation $V(x) = \cos x - 1$, we find $\Omega = 8$ and $J = -5\ln 2$. We have done a numerical comparison of the eigenvalues obtained by applying the singular Bohr-Sommerfeld rules and by using direct numerical methods, see section A.2.

10.4 The semi-classical asymptotic of the discriminant for two maxima per period

In this section, we study the Hill's equation assuming that the potential has two maxima per period. With the notations of figure 19, it suffices to calculate (B^+, Y) as a function of (b^+, y). The holonomy equations read:

$$a^+ = a^-\frac{\beta}{\alpha}, \quad b^+ = b^-\frac{1}{\beta^2}, \quad x^+ = x^-\alpha\beta$$

and the critical invariant equations are:

$$\begin{pmatrix} b^- \\ x^+ \end{pmatrix} = T(\eta)\begin{pmatrix} a^+ \\ y \end{pmatrix}, \quad \begin{pmatrix} a^- \\ Y \end{pmatrix} = T(\varepsilon)\begin{pmatrix} B^+ \\ x^- \end{pmatrix}$$

Using again our preferred CAS, we determine the function $(b^+, y) \to (B^+, Y)$. We check that the corresponding matrix has determinant 1, and its trace is given by:

$$\begin{aligned}\Delta &= 2\sqrt{1+e^{-2\pi\varepsilon}}\sqrt{1+e^{-2\pi\eta}}\cos(\arg\alpha + \arg\beta - \arg\mathcal{E} - \arg\mathcal{N}) + \\ &\quad +2e^{-\pi(\varepsilon+\eta)}\cos(\arg\beta - \arg\alpha).\end{aligned}$$

It is now easy to get informations about the lengths of the bands and gaps as λ tends to 0. Modulo a relative error of order $1/|\ln(h)|$, we get:

$$\Delta = 4\cos(\arg\alpha + \arg\beta - (\varepsilon+\eta)\ln(h)) + 2\cos(\arg\beta - \arg\alpha)$$

and we rewrite this Equation as:

$$\Delta = 2 + 4\left[\cos(\arg\alpha + \arg\beta - (\varepsilon+\eta)\ln(h)) - \sin\left(\frac{\arg\beta - \arg\alpha}{2}\right)^2\right]$$

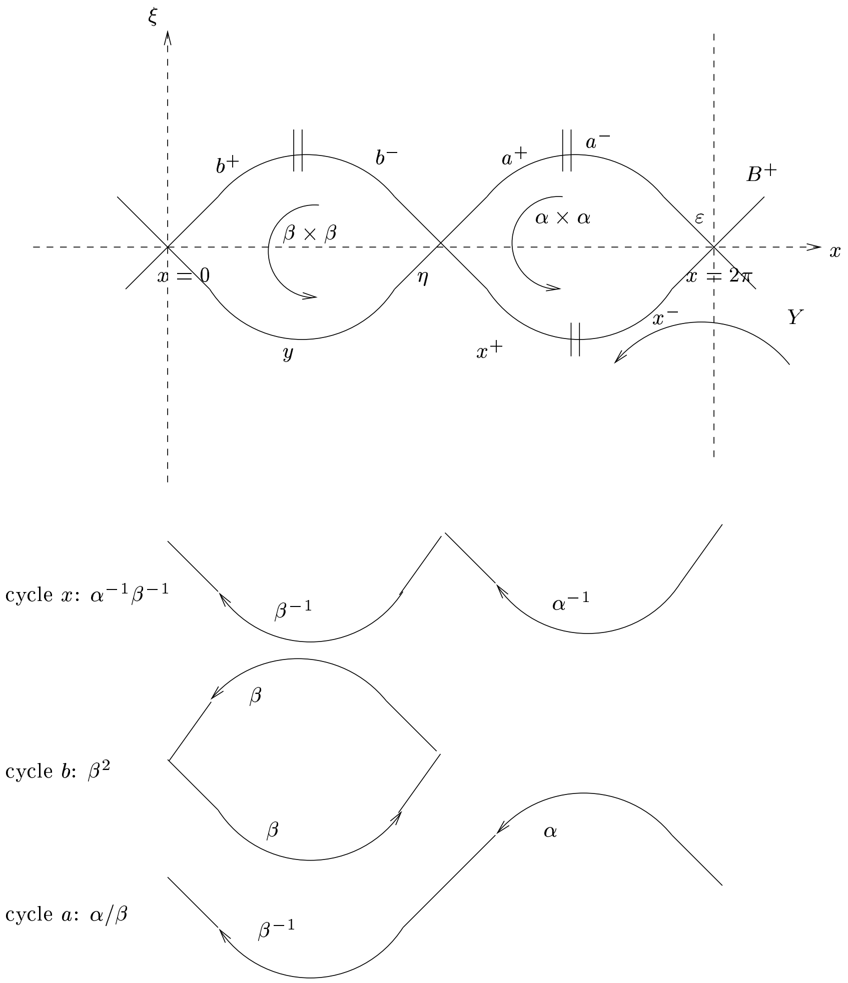

Figure 19: the double well for the pendulum

Therefore the inequality $\Delta > 2$ is equivalent to:

$$\cos(\arg\alpha + \arg\beta - (\varepsilon + \eta)\ln(h)) > \sin\left(\frac{\arg\beta - \arg\alpha}{2}\right)^2 \tag{64}$$

up to a $1/|\ln(h)|$ relative error. Hence, the bands and gaps do not have generically the same length near the 0 energy, except if $\beta = \alpha$. These lengths depend on the value of $\arg\beta - \arg\alpha$. For example it is possible to have gaps of asymptotically small length or, conversely, bands of asymptotically small length.

11 The periodic spectrum over $2T$ and $3T$ periodic functions

We proved in the previous section that the pendulum showed the same universal transition as the double well potential. It is natural to explore the situation of the double and triple translation-symmetric well over $M = \mathbb{R}/(2\pi\mathbb{Z})$. The reference models are $V(x) = 1 - \cos(2x)$ and $1 - \cos(3x)$.

11.1 The translation-symmetric double well.

11.1.1 Direct method

In this situation, we will have pairs of exponentially close eigenvalues in both energy domains ($E > 0$ and $E < 0$), but the tunneling trajectories that explain these couplings are different.

There is a little cycle of holonomy α^2, and two big cycles of holonomies α^{-2} and 1. The two critical points have the same semi-classical invariant ε. With the notations of figure 20, p. 34, we get:

$$\begin{pmatrix} a^- \\ y \\ b^- \\ x^+ \end{pmatrix} = \begin{pmatrix} T(\varepsilon) & 0_2 \\ 0_2 & T(\varepsilon) \end{pmatrix} \begin{pmatrix} b^+ \\ x^- \\ a^+ \\ y \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \alpha^2 & 0 & 0 & 0 \\ 0 & \alpha^2 & 0 & 0 \end{pmatrix} \begin{pmatrix} b^+ \\ x^- \\ a^+ \\ y \end{pmatrix}$$

This homogeneous system has a non trivial solution (b^+, x^-, a^+, y) if and only if its determinant is 0. Factoring $\mathcal{E}$ in each line (cf. (19)) gives:

$$\begin{vmatrix} 1 & ie^{-\varepsilon\pi} & -1/\mathcal{E} & 0 \\ ie^{-\varepsilon\pi} & 1 & 0 & -1/\mathcal{E} \\ -\alpha^2/\mathcal{E} & 0 & 1 & ie^{-\varepsilon\pi} \\ 0 & -\alpha^2/\mathcal{E} & ie^{-\varepsilon\pi} & 1 \end{vmatrix} = 0,$$

and eventually:

$$\mathcal{E}(1 - ie^{-\varepsilon\pi}) = \pm\alpha \quad \text{where} \quad \mathcal{E}(1 + ie^{-\varepsilon\pi}) = \pm\alpha \tag{65}$$

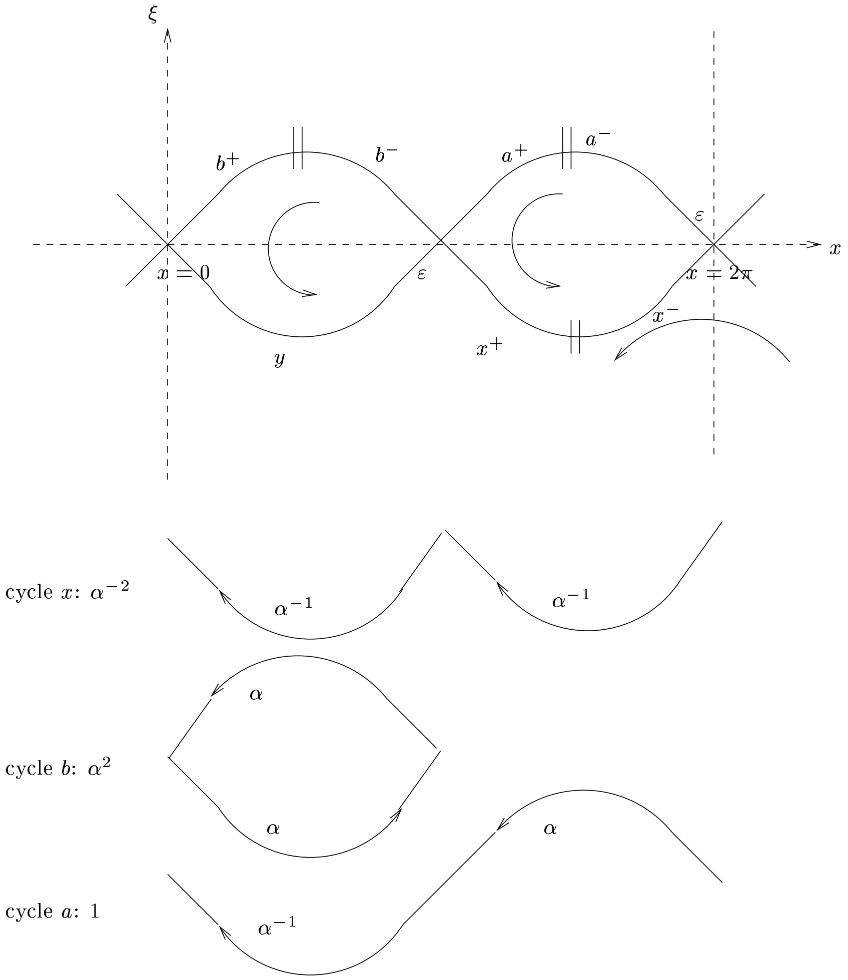

Figure 20: the symmetric double-well for the pendulum

As a consequence, we obtain the equidistribution of the eigenvalues near energy 0 in the semi-classical limit (here “near” means after a zoom-out of factor $1/h$).

11.1.2 The trace method.

The eigenvalues may be distinguished by parity properties: the periodic [respectively anti-periodic] eigenvalues correspond to eigenfunctions that satisfy $f(x+\pi) = f(x)$ [resp. $f(x+\pi) = -f(x)$]. Hence we have to check if 1 and -1 are eigenvalues of the translation matrix over a half period, or, since the determinant of this matrix is 1, to check that the trace is 2 (periodic eigenvalue) or -2 (anti-periodic). Therefore we are lead to the equation:

$$\cos\left(\arg(\alpha) + \varepsilon\ln(h) + \arg\Gamma(\frac{1}{2} + i\varepsilon)\right) = \pm\frac{1}{\sqrt{1+e^{-2\pi\varepsilon}}} \tag{66}$$

For $\varepsilon = 0$, we find again the equidistribution of the eigenvalues with the following parity: periodic, anti-periodic, anti-periodic, periodic.

We can compare (66) and (65): since all members of (65) have modulus 1, these 4 equations are equivalent to the equations obtained by taking the arguments. Getting (66) is now easy.

Let us apply equation (64) with $\alpha = \beta$ and $\varepsilon = \eta$. Observing that $\cos(2x) = 2\cos^2 x - 1$ and that the orientation convention of the cycles are reversed to those of (56) (hence holonomies are inverses), we eventually get (66).

11.2 The translation-symmetric triple well.

11.2.1 Direct method.

The critical energy area makes here a transition between triplets ($E < 0$) and pairs ($E > 0$) of exponentially close eigenvalues.

The semi-classical invariants of this situation are:

- two “small” cycles having the same holonomy denoted by α^2
- two “big” cycles, their holonomies are α^{-1} and $\alpha^{-3} = a^3$.
- three vertices having the same invariant ε

With the notations of figure 21, we get:

$$\begin{pmatrix} a^- \\ z \\ b^- \\ x^+ \\ c^- \\ y \end{pmatrix} = \begin{pmatrix} T(\varepsilon) & 0 & 0 \\ 0 & T(\varepsilon) & 0 \\ 0 & 0 & T(\varepsilon) \end{pmatrix} \begin{pmatrix} c^+ \\ x^- \\ a^+ \\ y \\ b^+ \\ z \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1/\alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & \alpha^2 & 0 \\ 0 & \alpha^3 & 0 & 0 & 0 & 0 \\ \alpha^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} c^+ \\ x^- \\ a^+ \\ y \\ b^+ \\ z \end{pmatrix}$$

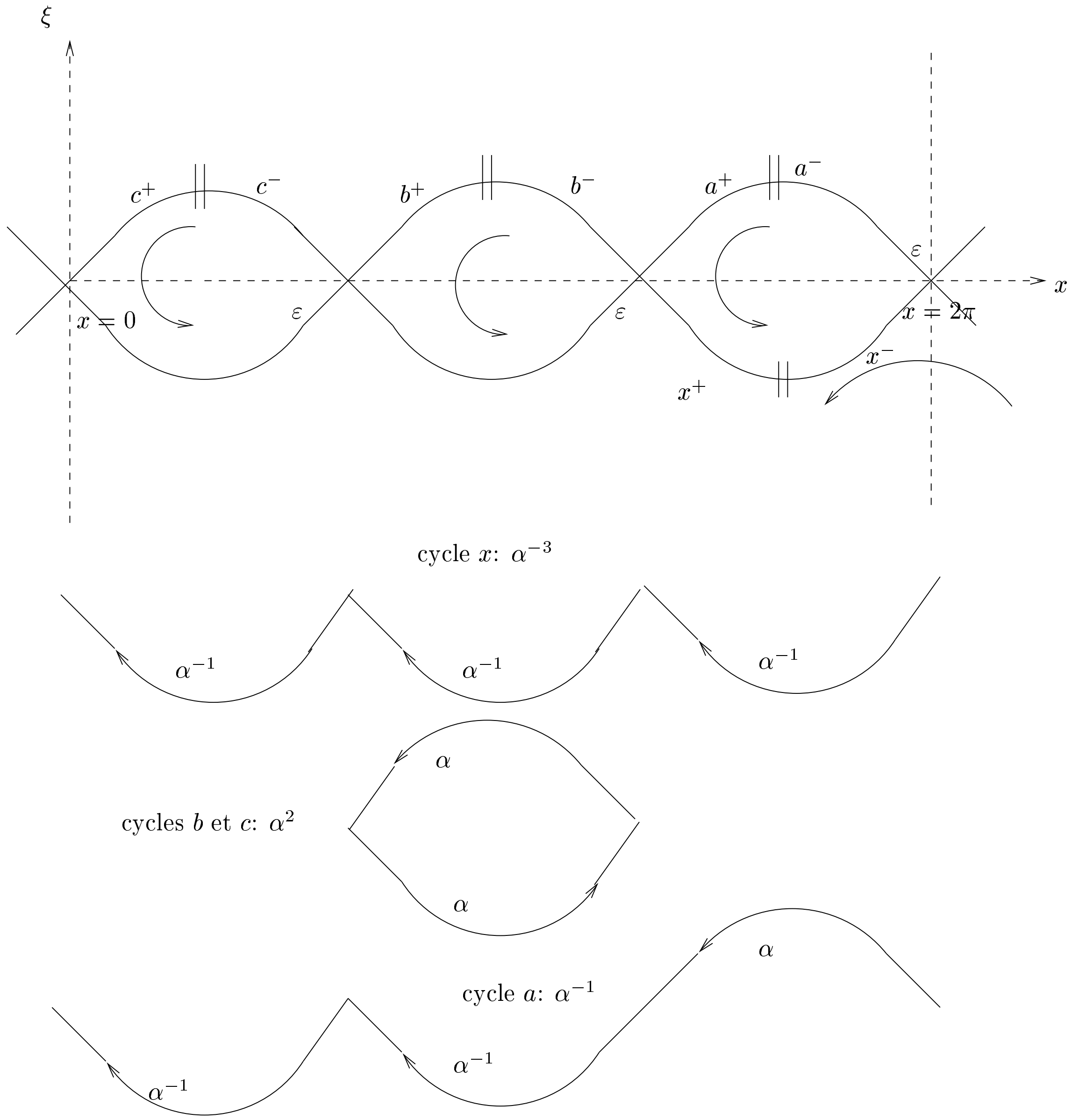

Figure 21: the translation-symmetric triple well potential

Factoring $\mathcal{E}$ in the $T(\varepsilon)$ matrix (see (19)), we get the quantization rule as the nullity of the determinant of a 6×6 matrix:

$$\begin{vmatrix} 1 & ie^{-\pi\varepsilon} & -1/(\alpha\mathcal{E}) & 0 & 0 & 0 \\ ie^{-\pi\varepsilon} & 1 & 0 & 0 & 0 & -1/\mathcal{E} \\ 0 & 0 & 1 & ie^{-\pi\varepsilon} & -\alpha^2/\mathcal{E} & 0 \\ 0 & -\alpha^3/\mathcal{E} & ie^{-\pi\varepsilon} & 1 & 0 & 0 \\ -\alpha^2/\mathcal{E} & 0 & 0 & 0 & 1 & ie^{-\pi\varepsilon} \\ 0 & 0 & 0 & -1/\mathcal{E} & ie^{-\pi\varepsilon} & 1 \end{vmatrix} = 0.$$

This determinant can be factored as:

$$(\alpha - \mathcal{E}(1 - ie^{-\pi\varepsilon}))(\alpha - \mathcal{E}(1 + ie^{-\pi\varepsilon}))\left(\alpha^2 + \alpha\mathcal{E} + \mathcal{E}^2(1 + e^{-2\pi\varepsilon})\right)^2 = 0$$

Hence we find two simple eigenvalues, solutions of:

$$\mathcal{E}(1 - ie^{-\pi\varepsilon}) = \pm\alpha$$

and two eigenvalues of multiplicity 2, solutions of:

$$\mathcal{E} = \alpha\frac{-1 \pm i\sqrt{4(1 + e^{-2\pi\varepsilon}) - 1}}{2(1 + e^{-2\pi\varepsilon})}$$

If we make a zoom-out of the eigenvalues near 0, their repartition will be asymptotically the same as the repartition of the following complexes on the unit circle:

$$\frac{-1 \pm i}{\sqrt{2}}(\text{simple}), \quad \frac{-1 \pm i\sqrt{7}}{2\sqrt{2}}(\text{double})$$

Therefore the transition area looks like figure 22 where we have used a bold level for double eigenvalues on the ladder

11.2.2 The trace method.

We study the trace of the translation matrix on one third of a period. The periodicity/anti-periodicity of eigenfunctions is replaced by the relation:

$$f(x + \frac{2\pi}{3}) = e^{2ik\pi/3}f(x)$$

Remark that $k = 1$ and $k = 2$ correspond to eigenfunctions that are conjugated, this explains the fact that eigenvalues of multiplicity 2 correspond to a trace of $2\cos(2\pi/3)$. The non degenerate eigenvalues correspond to eigenfunctions that are $2\pi/3$ periodic, the transition of these eigenvalues will therefore be similar to the transition of the eigenvalues of the single pendulum. For multiplicity 2 eigenvalues, we get:

$$\cos\left(\arg(\alpha) + \varepsilon\ln(h) + \arg\Gamma(\frac{1}{2} + i\varepsilon)\right) = \pm\frac{1}{2\sqrt{1 + e^{-2\pi\varepsilon}}}$$

As an easy consequence, we obtain for $\varepsilon = 0$ the same description as in figure (22).

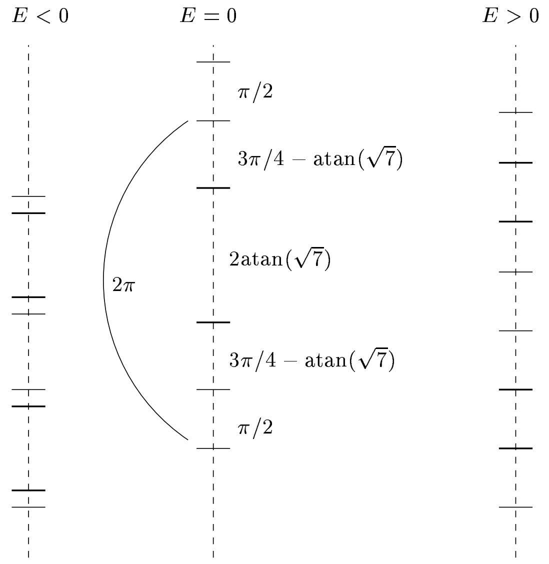

Figure 22: universal transition for the triple well

12 Scattering matrices

12.1 One channel scattering.

We are interested in an example studied by Rouleux ([17]). Let $V(x)$ be a C^∞ potential such that (see figure 23):

- $V(x) = 0$ for $x \geq x_1 > 0$
- $V(0) = V_0 > 0$, $V'(0) = 0$ and $V''(0) < 0$.
- $V^{-1}(V_0) = \{x_0, 0\}$ for an $x_0 < 0$ such that $V'(x_0) < 0$.

Hence $V^{-1}((-\infty, V_0]) = [x_0, +\infty($.

Let $k > 0$. The Schrödinger equation

$$-\frac{h^2}{2}\varphi'' + V(x)\varphi = k^2\varphi$$

has a unique solution $\varphi \in L^2(\mathbb{R}^-)$, such that:

$$\varphi = r(k)e^{i\sqrt{2}kx/h} + e^{-i\sqrt{2}kx/h}, \quad x \geq x_1$$

It is well know that $r(k)$ has modulus 1, $r(k)$ is called the *reflection coefficient*. Using the previous methods, we will calculate $r(k)$ up to an error of order $O(h)$ for $k = \sqrt{V_0} + O(h)$.

Let $W_o = \sqrt{V_0}$. We may write $k = W_0 + h\omega$ with $\omega = O(1)$. Hence, $H_0 = \frac{1}{2}\xi^2 + V(x) - V_0$ and $H_1 = -W_0\omega$.

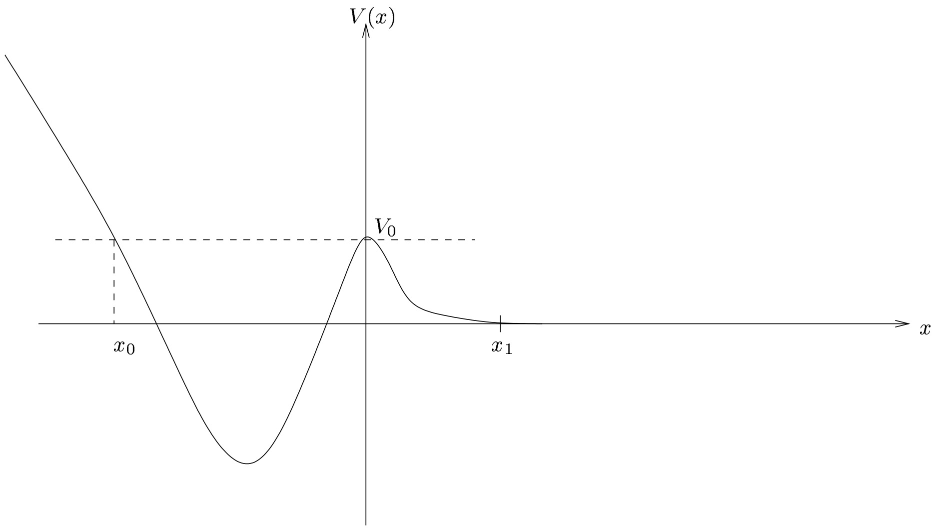

Figure 23: 1 channel scattering potential.

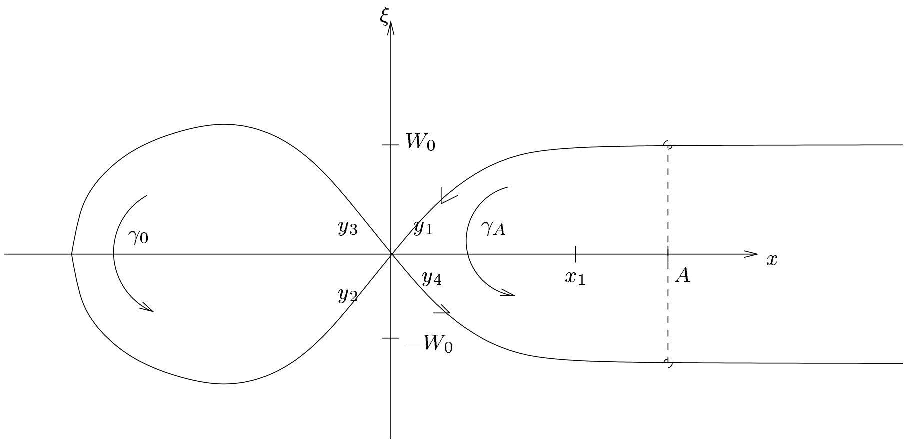

Figure 24: 1 channel scattering in the phase space.

Fix $A > x_1$ and let γ_A be the single path of the phase space joining (A, W_0) to $(A, -W_0)$ in the characteristic manifold $\xi^2 + V(x) = V_0$. The phase shift of a standard solution along γ_A is given (see (41)) by:

$$\alpha = e^{\frac{i}{h}\int_{\gamma_A}\xi dx - \mathrm{iv.p.}\int_{\gamma_A} H_1 dt}(1 + O(h)) \ .$$

Using the same notations as for the double well potential, we get:

$$y_2 = \frac{y_3}{\beta}, \quad y_1 = \alpha r(k) e^{2ikA} y_4$$

and

$$\begin{pmatrix} y_3 \\ y_4 \end{pmatrix} = T(\varepsilon) \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \ . \tag{67}$$

Hence:

$$r(k) = e^{-2ikA}\frac{1}{\alpha\beta}\exp\left(2i\arg\left(\sqrt{1+e^{-2\pi\varepsilon}}\frac{\beta}{\gamma} - ie^{-\varepsilon\pi}\right)\right)(1 + O(h)) \ , \tag{68}$$

where $\gamma = e^{i\arg\mathcal{E}}$. Since α and β have modulus 1, we get the classical result $|r(k)| = 1$. Let us remark that $r(k)$ does not depend of the choice of $A > x_1$ (e^{-2ikA} cancels with the part of α depending on A).

12.2 Two channels scattering.

Let us consider the volcano-top example. This is a Schrödinger equation on $\mathbb{R}$ like (42) with the following assumptions:

- $V(x) \to -a, \ a > 0$ as $x \to +\infty$,
- $V(x) \to -b, \ b > 0$ as $x \to -\infty$,
- $\sup V = 0$,
- $V^{-1}(0) = \{x_1, x_2\}$ with $x_1 < x_2$ and $V''(x_i) < 0$.

This example has been studied by Fujiie and Ramond ([10]) in the analytic case.

The energy shell in phase space looks like figure 25. Let β be the holonomy of the cycle, and $\mathcal{E}_j, \ j = 1, 2$ be the scalar coefficients factored in the matrices $T(\varepsilon_j)$ (cf. (19)). Then the following equations hold:

$$b^+ = \frac{b}{\beta}, \quad \begin{pmatrix} a^{in} \\ x \end{pmatrix} = T(\varepsilon_1)\begin{pmatrix} b^+ \\ a^{out} \end{pmatrix}, \quad \begin{pmatrix} b \\ c^{in} \end{pmatrix} = T(\varepsilon_2)\begin{pmatrix} c^{out} \\ x \end{pmatrix}$$

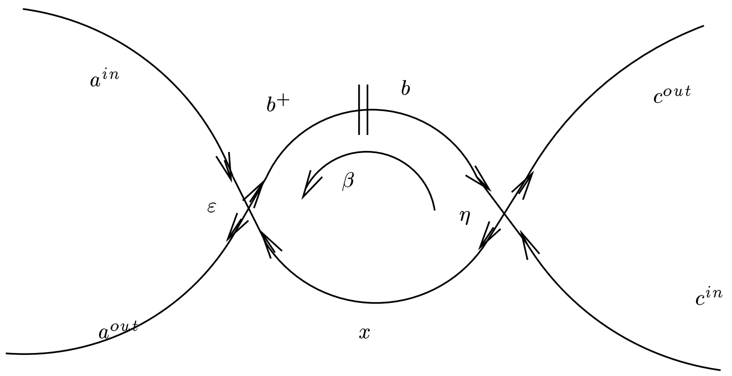

Figure 25: the volcano-top

By Gaussian elimination of b and x, we get:

$$a^{in} = \frac{\mathcal{E}_1}{D}\left[i\left(\frac{\mathcal{E}_1\mathcal{E}_2}{\beta}e^{-\varepsilon_2\pi}(1+e^{-2\varepsilon_1\pi})+e^{-\varepsilon_1\pi}\right)a^{out}+\frac{\mathcal{E}_2}{\beta}c^{out}\right] \tag{69}$$

$$c^{in} = \frac{\mathcal{E}_2}{D}\left[\mathcal{E}_1 a^{out}+i\left(\frac{\mathcal{E}_1\mathcal{E}_2}{\beta}e^{-\varepsilon_1\pi}(1+e^{-2\varepsilon_2\pi})+e^{-\varepsilon_2\pi}\right)c^{out}\right] \tag{70}$$

$$D = 1+e^{-\varepsilon_1\pi}e^{-\varepsilon_2\pi}\frac{\mathcal{E}_1\mathcal{E}_2}{\beta} \tag{71}$$

Note that the denominator D is never 0 for real energies since $|\mathcal{E}_j| = (1+e^{-2\varepsilon_j\pi})^{-1/2}$. The complex zeroes of the analytic continuation of D are named quasi-resonances. Remark that the S matrix such that $S(a^{out}, c^{out}) = (a^{in}, c^{in})$ is unitary as it should.

We will now calculate the modulus of the transmission and reflection coefficients (it is of course possible to calculate the phase shifts in the spirit of the previous section). Let us consider a solution which is micro-locally supported on one of the two incoming branches, e.g. a^{in}. Hence $a^{in} = 1$, $c^{in} = 0$ and $|c^{out}| = |t|$, $|a^{out}| = |r| = \sqrt{1-|t|^2}$. Since S is unitary, we have:

$$|t| = \left|\frac{\mathcal{E}_2\mathcal{E}_1}{D}\right|$$

For example, if we are interested in energies E such that E/h tends to 0, then $\varepsilon_1 = \varepsilon_2 = 0$ and we find the same result as Fujiie and Ramond:

$$|t| = \frac{1}{\sqrt{5+4\cos\beta}}$$

A Numerical results.

A.1 The symmetric double well potential.

Let $V(x) = x^4 - x^2$. In this section, we calculate the eigenvalues of the corresponding Schrödinger operator for different values of h by solving (50) or by applying the Runge-Kutta method to the first order differential system:

$$\frac{d}{dx}\begin{pmatrix} \varphi \\ \varphi' \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \frac{2(V(x)-E)}{h^2} & 0 \end{pmatrix} \cdot \begin{pmatrix} \varphi \\ \varphi' \end{pmatrix} \tag{72}$$

More precisely, we calculate two solutions of (72), starting from two points in the classically forbidden region, the first one is chosen in the connected component of $-\infty$ and the second in the component of $+\infty$. We take $\varphi = 1$ and $\varphi' = 0$ as initial conditions at these points. And we compute the Wronskian $W(E)$ of these 2 solutions at $x = 0$. Since we start from the classically forbidden region, the numerical solution that we obtain in the classically allowed region will behave like a solution which decreases exponentially fast in the component of the starting point region. Therefore, the Wronskian $W(E)$ will vanish if and only if E is eigenvalue. To find these values, we detect sign changes of $W(E)$ first by dichotomy, then by interpolation of the curve $E \to W(E)$ for better accuracy (this is the best method when Newton's method can not be applied. The convergence law of the sequence of E is given by $|E_n - E| \leq |E_0 - E|^{F_n}$ where F_n are the Fibonacci numbers).

On the other hand, rewriting equation (50) for the potential $V(x) = x^4 - x^2$ ($a = 1$ and $b = 0$) gives:

$$\frac{1}{\sqrt{1+e^{2\pi\varepsilon}}} + \cos\left(\varepsilon\ln(h) + \arg\Gamma(\frac{1}{2} + i\varepsilon) - \frac{7}{2}\varepsilon\ln(2) - \frac{2\sqrt{2}}{3h}\right)$$

where $\varepsilon = \frac{E}{\sqrt{2}h}$.

All these functions are standard, except the argument of the Γ function. We have used the `PARI` library from the number theory laboratory of Bordeaux to calculate it. Implementation has been done in `C/C++`, programs are available at: `http://www-fourier.ujf-grenoble.fr/~parisse/bs.tgz`

For $h = 10^{-6}$, we get the following eigenvalues in the interval $[-2.10^{-6}, 3.10^{-6}]$:

Index	Runge-Kutta	Bohr-Sommerfeld
1	-1.68092e-06	-1.68100e-06
2	-1.67670e-06	-1.67678e-06
3	-1.14072e-06	-1.14080e-06
4	-1.12697e-06	-1.12706e-06
5	-0.62743e-06	-0.62751e-06
6	-0.58579e-06	-0.58587e-06
7	-0.15515e-06	-0.15522e-06
8	-0.05032e-06	-0.05041e-06
9	0.29793e-06	0.29786e-06
10	0.48460e-06	0.48451e-06
11	0.78346e-06	0.78339e-06
12	1.02441e-06	1.02432e-06
13	1.30685e-06	1.30677e-06
14	1.57243e-06	1.57234e-06
15	1.85275e-06	1.85266e-06
16	2.12953e-06	2.12944e-06
17	2.41218e-06	2.41208e-06
18	2.69515e-06	2.69506e-06
19	2.98110e-06	2.98101e-06
20	3.26833e-06	3.26824e-06

Note the accuracy of the singular Bohr-Sommerfeld rules. This method is far cheaper than the Runge-Kutta method (about 100× faster).

Comparison 2: for $h = 0.1$, we get the following eigenvalues in the interval $[-0.3, 0.3]$:

Index	Runge-Kutta	Bohr-Sommerfeld
0	-0.156568	-0.16038
1	-0.155061	-0.15861
2	-0.014654	-0.01358
3	0.021032	0.02162
4	0.116728	0.11546
5	0.212051	0.20839

Even for this relatively large h value, the singular quantization rules give an accurate approximation of the eigenvalues. Note however that for this value of h, the Runge-Kutta method is faster! Remark that the mean gap between two consecutives eigenvalues is about $1 \times h$ in this example and about $4 \times h$ for $h = 10^{-6}$. Theoretically, we should find a ratio of 6 instead of 4. This would require to calculate eigenvalues for energies that are much closer to $E = 0$.

Let us now compare the two methods (singular quantization rules and numerical integration) in terms of the position of the ladders of even and odd eigenvalues near the critical energy. We introduce the form factor:

$$R = \frac{E_{2n+1} - E_{2n}}{E_{2n+2} - E_{2n}}$$

where the eigenvalues are indexed starting from $n = 0$ (hence even eigenvalues correspond to even eigenfunctions). For $E_{2n+1} >> h$, eigenvalues are equidistributed hence R tends to $1/2$; for $-E_{2n+1} >> h$, eigenvalues are coupled hence R tends to 0. If $E_{2n+1}/(h\sqrt{|V''(0)|})$ tends to a limit ε_0 as h tends to 0, it is possible to calculate the limit of R:

$$\lim_{h\to 0} R = \frac{\arccos\left((1+e^{2\pi\varepsilon_0})^{-1/2}\right)}{\pi}$$

Hence $R \to 1/4$ for $\varepsilon_0 = 0$. Coming back to the second example above ($h = 0.1$), we get $(E_3 - E_2)/(E_4 - E_2) = 0.27$, a value which is close to the theoretical value of R (since $E_3/(\sqrt{2}h) = 0.15$ is close to 0).

A.2 The pendulum

We make the same kind of comparison for the pendulum (the periodic Schrödinger equation), where we take $V(x) = \cos(x) - 1$ as potential. The singular Bohr-Sommerfeld quantization rules read (see (63)):

$$\frac{1}{\sqrt{1+e^{-2\pi\varepsilon}}} = \cos\left(-\frac{8}{h} - 5\ln(2)\varepsilon + \varepsilon\ln h + \arg\Gamma(\frac{1}{2} + i\varepsilon)\right)$$

with $\varepsilon = E/h$.

We use a numerical method which is slightly different than of the previous section: here we will study the monodromy matrix M. Let $(\varphi, \varphi') = (1, 0)$ and $(\varphi, \varphi') = (0, 1)$ be a couple of (linearly independent) initial conditions at $x = 0$. Using the Runge-Kutta method, we integrate the Schrödinger equation from $x = 0$ to $x = 2\pi$ and determine the matrix M. Energy E is an eigenvalue if and only if 1 is eigenvalue of M. We have now to find the zeroes of $\det(M - I)$.

Let p be the length of a step of the Runge-Kutta method. Then the relative error is of order p^3/h^4 in the $E \geq 0$ energy area. The error is much bigger in the $E < 0$ area because starting and ending in the classically forbidden region multiplies the relative error by an exponential coefficient which is proportional to $e^{-CE/h}$. Hence we can not apply this numerical method if $E < -Dh$ (and if we choose a big value for D, we have to choose a correspondingly small value for p).

The comparison shows that the two methods give close results. In the following example, we take $h = 10^{-3}$, and we obtain:

Index	Runge-Kutta	Bohr-Sommerfeld
0	-0.00339886	-0.00339946
1	-0.00305773	-0.00305821
2	-0.00272065	-0.0027210
3	-0.00238812	-0.00238841
4	-0.00206018	-0.002060396
5	-0.00173847	-0.001738624
6	-0.00142077	-0.0014208684
7	-0.00111594	-0.001116004
8	-0.000805647	-0.000805677
9	-0.000541145	-0.000541155
10	-0.000212948	-0.000212945
11	-5.18091e-05	-5.18018e-05
12	0.000371877	0.0003718748
13	0.000420734	0.000420730
14	0.000978865	0.000978818
15	0.000978865	0.000978818

We note a better accuracy for $E > 0$, as we could expect from the above remark about the instability of the numerical method for $E < 0$.

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