Bohr-Sommerfeld phases for avoided crossings

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Introduction

We consider in this paper a self-adjoint semi-classical system of N pseudo-differential equations of order 0 with N complex valued unknown functions $\vec{U} = (U_1, \cdots, U_N)$,

$$\widehat{H}\vec{U} = 0(h^\infty) \tag{1}$$

on the real line. Here $\hat{H} = (\hat{H}_{i,j})_{1\leq i,j \leq N}$ is a matrix of semi-classical pseudo-differential operators of order 0 in 1 variable x with $(\hat{H}_{i,j})^\star = \hat{H}_{i,j}$. For applications, it will be important to consider the case where $\hat{H} = \hat{H}_\mu$ depends smoothly on a germ of parameters $\mu \in (\mathbb{R}^d, 0)$. In our previous papers [5, 6], we derived normal forms near the eigenvalues crossings which allow to compute a *local scattering* matrix including the Landau-Zener amplitude. The goal of this paper is to compute *global objects* including *interferences effects.* The general picture is already provided by the study of the scalar case [9] from which we know that we need to define ad'hoc *Bohr-Sommerfeld phases.*

We want to cover the following examples:

- *Adiabatic limit in quantum mechanics with avoided crossings:* in that case, $\mu = 0$ is the case of true crossings. We want to compute the global scattering matrix. Our results extend the adiabatic theorem of quantum mechanics which is usually given with a gap condition. The references [1], [3], [13] and [19] chap. IV have no gap condition, but do not include the case of *avoided crossings.* The case of one avoided crossing and the Landau-Zener formula is now well understood thanks to the works of several people starting with [15], see also [8].

  In the case of several crossings (analytic case), using Stokes lines, they are many works where the interferences effects are exponentially small [16, 18],

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but they do not cover the case of avoided crossings uniformly w.r. to the perturbation parameter.

The main point here is to get results on the formal series expansion in h, i.e. modulo $O(h^\infty)$, of the scattering matrix, *uniformly* w.r. to the deformation parameter.

- *Born-Oppenheimer type operators:* in this case, μ includes the spectral parameter (see also [14] and [20]). We are interested into the asymptotic expansion of the eigenvalues using *singular* Bohr-Sommerfeld quantization rules. There is no previous result of this type except in the non singular case where the most precise results are shown in [12].

The general terminology is the same as in [5] and [6], but in the present paper, our phase space will always be 2 dimensional:

$$H^{\mu}_{\mathrm{class}} : T^\star\mathbb{R} \to \mathrm{Herm}(\mathbb{C}^N) \ ,$$

the (matrix valued) principal symbol, is the *dispersion matrix*, and $C_\mu = p_\mu^{-1}(0)$ with $p_\mu = \det(H^{\mu}_{\mathrm{class}})$ the *dispersion relation.*

We first recall the local normal form as derived in our previous papers [5, 6] and we solve it. After that, we come to the new part which consists in deriving global objects in the spirit of [9].

We will need another piece of information which we call *Bohr-Sommerfeld phase;* let us take any simple cycle c (with singular vertices $z_1, \cdots, z_j, \cdots, z_p$) of the dispersion relation C_0. We will associate to c a real valued symbol $\mathbf{S}_h(\mu) \sim \sum_{j=0}^{\infty} S_j(\mu)h^j$ were the S_j's are formal power series in μ. S_0 is a purely classical object which involves regularized action integrals. $S_1(0)$ is computed using the transport equation which is smooth along the edges $[z_j, z_{j+1}]$ *(Berry phases)* and singular Maslov indices. From the Bohr-Sommerfeld phases we recover the global objects mod $O(h^\infty)$.

1 The local normal form

Let us recall the following result from [11, 5, 6] (see also [8]):

Theorem 1 *Let us assume that the function $p_0(x,\xi) = \det(H_{\mathrm{class},\mu=0})$ admits at the point $z_0 \in T^\star\mathbb{R}$ a non degenerated critical point of Morse index 1 (also called* hyperbolic critical point*, because the Hamiltonian vector field of p_0 is hyperbolic at the singular point z_0) and with critical value $p_0(z_0) = 0$.*

Then, we can find the following objects which depends smoothly on μ close enough to 0:

- *A smooth family of germs of canonical transformations* $\chi_\mu : (T^\star\mathbb{R}, 0) \to (T^\star\mathbb{R}, z_0)$ *such that*

$$p_\mu(\chi_\mu(x,\xi)) = e_\mu(x,\xi)(x\xi - \gamma_0(\mu))$$

  with e_μ *an invertible germ function and* γ_0 *a germ of* ≥ 0 *function of* μ *satisfying* $\gamma_0(0) = 0$*. Moreover, the Taylor expansion of* γ_0 *is unique.*

- *A smooth family of unitary FIO's* U_μ *associated to* χ_μ *and* $N \times N$ *matrix of* ΨDO *'s* A_μ

so that, we have the following normal form (called the Landau-Zener normal form*) near* z_0*:*

$$A_\mu^\star U_\mu^\star \hat{H}_\mu U_\mu A_\mu = \begin{pmatrix} \begin{pmatrix} D & \alpha \\ \bar{\alpha} & x \end{pmatrix} & 0 \\ 0 & Q \end{pmatrix}$$

with $D = \frac{h}{i}\frac{\partial}{\partial x}$, $\alpha(\mu,h) \sim \Sigma_{j=0}^\infty a_j(\mu)h^j$ *a symbol and* Q *is elliptic.*

Moreover, a_0 *is a complex valued function of* μ *which satisfies*

$$|a_0|^2(\mu) = \gamma_0(\mu) \ ,$$

and we have

$$\gamma_0(\mu) = -\frac{p_\mu(z_0)}{\sqrt{|\mathrm{det} p_0''(z_0)|}} + O(\mu^3) \ .$$

Remark 1 *In [6], Theorem 1 is proved under the following transversality hypothesis:*

($\star$) **if** $W \subset \mathrm{Herm}(\mathbb{C}^N)$ **is the submanifold defined by** $\dim\ker H = 2$**, we assumed there that** $(\mu, z) \to H_{\mathrm{class},\mu}(z)$ **is transversal to** W **at the point** $(0, z_0)$**.**

This hypothesis can be restored using more parameters, so that Theorem 1 is also correct. For simplicity,

we will assume that hypothesis ($\star$) **holds true in what follows.**

It implies that $\mu \to a_0(\mu)$ *is a submersion from* $(\mathbb{R}^d, 0)$ *onto* $(\mathbb{C}, 0)$*. We will denote by* $Z = a_0^{-1}(0)$*.* Z *is a smooth germ of codimension* 2 *manifold of* $(\mathbb{R}^d, 0)$*. Formal expansions w.r. to the parameter* μ *mean formal expansions along* Z*.*

Remark 2 *Contrary to the scalar case, there is no arbitrary choice concerning the images of the half axes* $\{\xi = 0, x > 0\}$*, ... by* χ*. The smooth arcs of the dispersion relation are oriented in the following way: there is a change of the Morse index of the quadratic form associated to* H_{class} *from* m *to* $m \pm 1$ *while crossing these arcs. The sign of this change is preserved by the gauge transform which acts directly on the previous quadratic form by an invertible linear change of variable. We choose to orient the arcs so that the Morse index is bigger on the right than on the left of the path.*

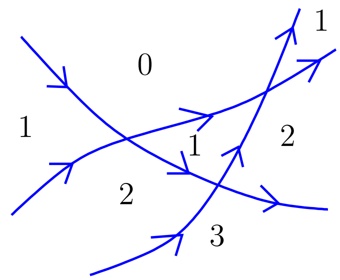

Figure 1: the jumps of the Morse index of the dispersion matrix

Remark 3 *The symbol α is not uniquely defined because a diagonal unitary gauge transform preserves the normal form while changing α by some phase shift $\exp(i\varphi(h))$. Its modulus $\gamma(\mu, h) = |\alpha(\mu, h)|^2$ is uniquely defined from the Landau-Zener coefficient given in Equation (6).*

The matrix A is defined up to matrices which will change the phase of α. More precisely, if A_0 is the principal symbol of A at the crossing point, the only prescription is that A_0 is a map from $\mathbb{C}^N$ to $\mathbb{C}^N$ which sends $\mathbb{C}^2 \oplus 0$ into $\ker H_0(z_0)$ and satisfies $A_0\left((\mathbb{C} \oplus 0) \oplus 0\right) = E_1$ and $A_0\left((0 \oplus \mathbb{C}) \oplus 0\right) = E_2$ where $E_j = \lim_{z \to z_0, z \in \Lambda_j \setminus z_0} \ker H_0$ with $\Lambda_1 = \chi_0(\{\xi = 0\})$ and $\Lambda_2 = \chi_0(\{x = 0\})$. The choice of $(A_0)_{|\mathbb{C}^2 \oplus 0}$ will be important in the computation of $S_1(0)$ in section 5.

The previous result is a microlocal result and the subject of the present paper is to get a global result.

In the *adiabatic case* (see Section 6.1), we get

$$\gamma_0(\mu) = \frac{\mathrm{gap}(\mu)^2}{4(|\lambda'_+ - \lambda'_-|)} + O(\mu^3)$$

where $\mathrm{gap}(\mu)$ is the minimal gap of the avoided crossing and $\lambda'_\pm$ are the slopes of the unperturbed eigenvalues at the crossing point.

2 The local scattering matrix for the Landau-Zener normal form

The goal of this section is to compute in a very explicit way the local 2×2 scattering matrix $\mathcal{T}$ for the Landau-Zener normal form :

$$(\mathrm{LZ}) \begin{cases} Du + \alpha v &= 0 \\ \bar{\alpha} u + xv &= 0 \end{cases} \tag{2}$$

with $D = \frac{h}{i}\frac{\partial}{\partial x}$.

Let us put $\gamma = |\alpha|^2$ and let us choose some small $a > 0$ and assume $\gamma < a^2$. Let $C_\alpha^{\rm LZ} = \{x\xi = \gamma\}$ be the characteristic manifold. The set $C_\alpha^{\rm LZ} \cap \{\max(|x|, |\xi|) \geq a\}$ is the union of 4 connected arcs. These arcs are labelled $\Lambda_\pm^{\rm in, out}$ as follows:

- $\Lambda_+^{\rm in} = \{(x,\xi) \in C_\alpha^{\rm LZ} \mid x \leq -a\}$
- $\Lambda_+^{\rm out} = \{(x,\xi) \in C_\alpha^{\rm LZ} \mid \xi \leq -a\}$
- $\Lambda_-^{\rm in} = \{(x,\xi) \in C_\alpha^{\rm LZ} \mid \xi \geq a\}$
- $\Lambda_-^{\rm out} = \{(x,\xi) \in C_\alpha^{\rm LZ} \mid x \geq a\}$.

The meaning of the labels is as follows:

- "in" (resp. "out") means that the arc oriented according to remark 2 is incoming (resp. outgoing).
- "+" (resp. "$-$") means that the vanishing eigenvalue of the dispersion matrix is the largest (resp. smallest) one.

We start defining 4 WKB (exact) solutions of the previous system associated to the 4 Lagrangian arcs $\Lambda_\pm^{\rm in, out}$:

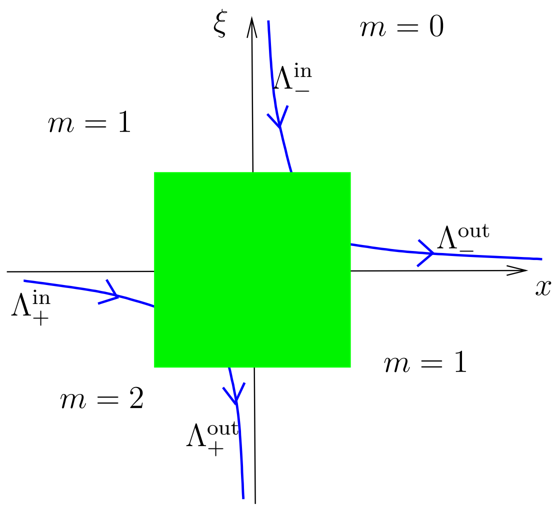

Figure 2: the 4 arcs of the characteristic manifold and Morse indices

$$\begin{cases} W_-^{\rm out} & : \quad u_-^{\rm out}(x) = x_+^{i\frac{\gamma}{h}}, \ v_-^{\rm out}(x) = -\bar{\alpha} x_+^{i\frac{\gamma}{h}-1} \\ W_+^{\rm in} & : \quad u_+^{\rm in}(x) = x_-^{i\frac{\gamma}{h}}, \ v_+^{\rm in}(x) = \bar{\alpha} x_-^{i\frac{\gamma}{h}-1} \\ W_-^{\rm in} & : \quad \widehat{u_-^{\rm in}}(\xi) = -\alpha \xi_+^{-i\frac{\gamma}{h}-1}, \ \widehat{v_-^{\rm in}(\xi)} = \xi_+^{-i\frac{\gamma}{h}} \\ W_+^{\rm out} & : \quad \widehat{u_+^{\rm out}}(\xi) = \alpha \xi_-^{-i\frac{\gamma}{h}-1}, \ \widehat{v_+^{\rm out}}(\xi) = \xi_-^{-i\frac{\gamma}{h}} \end{cases} \tag{3}$$

where $\widehat{f}(\xi)$ is the $h-$Fourier transform of $f(x)$ defined by

$$\widehat{f}(\xi) = \frac{1}{\sqrt{2\pi h}} \int_{\mathbb{R}} e^{-i\frac{x\xi}{h}} f(x)|dx| \ ,$$

and $x_\pm = Y(\pm x)|x|$ with Y the Heaviside function.

Computing the Fourier transforms of $u_\pm$ and $v_\pm$, we get the following compatibility conditions in order to get microlocal solutions of (2) near the origin:

$$\begin{cases} W_-^{\mathrm{out}}(x) \leftrightarrow & h^{\frac{1}{2}+i\frac{\gamma}{h}} \frac{\Gamma(1+i\frac{\gamma}{h})}{\sqrt{2\pi}\alpha} \left(i e^{\pi\frac{\gamma}{2h}} W_-^{\mathrm{in}}(x) + i e^{-\pi\frac{\gamma}{2h}} W_+^{\mathrm{out}}(x) \right) \\ W_+^{\mathrm{in}}(x) \leftrightarrow & h^{\frac{1}{2}+i\frac{\gamma}{h}} \frac{\Gamma(1+i\frac{\gamma}{h})}{\sqrt{2\pi}\alpha} \left(-i e^{-\pi\frac{\gamma}{2h}} W_-^{\mathrm{in}}(x) - i e^{\pi\frac{\gamma}{2h}} W_+^{\mathrm{out}}(x) \right) \end{cases}$$

If $W^{\mathrm{in}} := y_+ W_+^{\mathrm{in}} + y_- W_-^{\mathrm{in}}$ and $W^{\mathrm{out}} := z_+ W_+^{\mathrm{out}} + z_- W_-^{\mathrm{out}}$ are WKB-solutions of Equation (2) outside the origin, we get, for any microlocal solution near the origin,

$$\begin{pmatrix} z_- \\ z_+ \end{pmatrix} = \mathcal{T} \begin{pmatrix} y_+ \\ y_- \end{pmatrix}$$

where $\mathcal{T}$ is the *unitary matrix* defined by:

$$\mathcal{T} = \frac{1}{A} \begin{pmatrix} -B & 1 \\ B^2 - A^2 & -B \end{pmatrix} \tag{4}$$

with

$$A = i h^{\frac{1}{2}+i\frac{\gamma}{h}} \frac{\Gamma(1+i\frac{\gamma}{h})}{\sqrt{2\pi}\alpha} e^{\pi\frac{\gamma}{2h}}, \ B = i h^{\frac{1}{2}+i\frac{\gamma}{h}} \frac{\Gamma(1+i\frac{\gamma}{h})}{\sqrt{2\pi}\alpha} e^{-\pi\frac{\gamma}{2h}} \ . \tag{5}$$

The matrix $\mathcal{T}$ will be called the *local scattering matrix* associated to the singular point (and the choice of a normal form). Unitarity of $\mathcal{T}$ is checked using the well known formula

$$\Gamma(1+ix)\Gamma(1-ix) = \frac{\pi x}{\sinh \pi x}$$

which implies $|A|^2 = |B|^2 + 1, \ A\bar{B} = \bar{A}B$.

The transmission coefficient

$$\tau = \left| \frac{B}{A} \right| = \exp(-\pi \frac{\gamma}{h}) \tag{6}$$

gives the *Landau-Zener formula*. The previous explicit expression for the scattering matrix will allow to define in the next section the Bohr-Sommerfeld phases and to take into account interferences patterns due to several (avoided) crossings.

3 Singular Bohr-Sommerfeld phases

3.1 Outline

To each cycle c of the dispersion relation C_0, we can associate, using the recipe of [9], a singular phase of the form

$$\mathbf{S}_h(\mu) = S_0(\mu) + hS_1(\mu) + \cdots$$

where the S_j's are smooth w.r. to μ.

In this section, we will define precisely these phases. We show that they are uniquely defined as formal power series w.r. to (μ, h). More precisely, each $S_j(\mu)$ is well defined modulo flat functions on Z (see Remark 1). We will give more precise properties of S_0 in section 4 and S_1 in section 5: $S_0(\mu)$ is, as a formal power series, a purely classical object derived from the dispersion relation, while $S_1(0)$ is a semi-classical object associated to phases given by the transport equation which in the adiabatic case are *Berry phases*.

3.2 Bohr-Sommerfeld phases: a definition

Let us take a simple oriented cycle c of the dispersion relation C_0 (boundary of a bounded component of $T^\star\mathbb{R} \setminus C_0$). Let $z_1,\ z_2, \cdots, z_n$ be the singular points of c ordered cyclically around c. For each singular point z_j, let us build a FIO U_j and a ΨDO gauge transform A_j (all depending smoothly on μ) which give the normal form of Theorem 1 with $\alpha_j = \alpha_j(\mu, h)$ a full symbol.

We will define $\mathcal{H}_\mu(c) = \exp(i\mathcal{S}_h(\mu)/h)$ as follows: we will denote by $W_{\pm,j}^{\text{in, out}}$ the images of $W_\pm^{\text{in, out}}$ by the operators $U_j^\mu A_j^\mu$. These functions are WKB solutions of equation (1) associated to arcs of C_μ near z_j. We introduce also WKB solutions u_j of (1) along arcs of C_μ close to $]z_j, z_{j+1}[$. From those objects we get a global holonomy $\mathcal{H}_\mu(c)$ of the cycle c defined as follows: we have (by uniqueness, modulo multiplication by a full symbol, of WKB solutions) for example near z_j:

$$u_j = x_j W_{-,j}^{\text{in}},\ u_{j-1} = y_j W_{+,j}^{\text{in}}\ .$$

We define $\mathcal{H}_\mu(c) = \Pi_{j=1}^n y_j x_j^{-1}$. In other words, $\mathcal{H}_\mu(c)$ is the holonomy of a sheaf on c given by the WKB solutions on the smooth part of the cycle and whose jumps of section are given from the normal forms. In our previous example $W_{+,j}^{\text{in}} \to W_{-,j}^{\text{in}}$.

Lemma 1 *We have $|\mathcal{H}_\mu(c)| = 1 + O(h^\infty)$.*

Proof.–

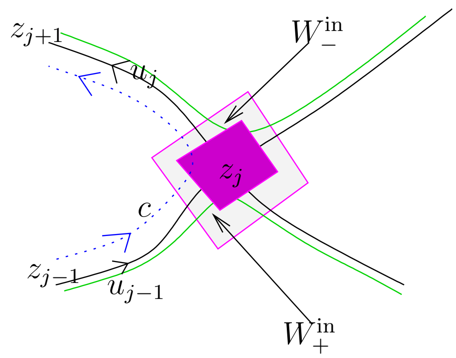

Figure 3: defining $\mathcal{H}_\mu(c)$

Following [7] section 11.2.1. and Figure 4, we associate to the cycle c an unitary scattering matrix $\mathcal{S}_c$ which is computable from the local unitary scattering matrices associated to the singular points and the holonomy $\mathcal{H}_\mu(c)$. If this holonomy does not satisfy $|\mathcal{H}_\mu(c)| = 1 + O(h^\infty)$, the global scattering matrix would not be unitary: the previous matrix is the product of (unitary) local scattering matrices and a diagonal matrix whose unique nonzero entry is $\mathcal{H}_\mu(c)$.

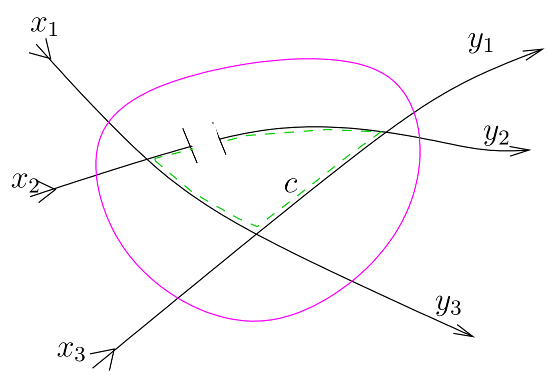

Figure 4: the scattering matrix associated to a cycle

□

Taking the Logarithms, we get the phase $\mathbf{S}_h(\mu)/h = \sum_{j=0}^{\infty} S_j(\mu)h^{j-1}$ which is well defined modulo a multiple of 2π.

Lemma 2 *Given the gauge transforms used in the normal form of Theorem 1, the Taylor expansions of the S_j's at $\mu = 0$ are uniquely defined.*

Proof.–

We will use the fact that the local scattering matrix computed in Section 2 is *irreducible* in the domain $h^N \leq |\alpha(\mu)| \leq \sqrt{h}$, meaning that none of the entries are $O(h^\infty)$ in this domain. It implies that, for each j, the $W_{\pm,j}^{\text{in, out}}$'s can be, up to a global multiplication by a symbol, defined as sets of WKB solutions for which the scattering matrix is given by Equations (4) and (5) with the value of α given by the normal form at the point z_j.

□

4 The classical part S_0

4.1 S_0 is classical

We have the following:

Theorem 2 *For any simple cycle c of C_0, the function $S_0(\mu)$ depends only on the dispersion relation C_μ.*

Proof.–

From the definition, S_0 depends only on the terms in $1/h$ in the phases of the images by our normal form transformations of the explicit solutions of the normal form. Those terms depends only on the canonical transformations used in the normal form and the associated generating functions via stationnary phases (the Lagrangian manifolds).

□

4.2 S_0 as a regularized action integral

Let us denote by $|\mu| = d(\mu, Z)$. As in [9], it would be nice to get $S_0(\mu)$ as a regularisation of an usual action integral. A basic fact in [9] was that any simple cycle c is a limit of a cycle of C_μ as $\mu \to 0_\pm$. This is no longer the case here because $\gamma_0 \geq 0$; one can see an example in section 4.4. The idea is now to forget the initial problem and to work only with the dispersion relation C_μ which can be embedded into a larger family $C_{t,\mu}$ for which we can define action integral in some suitable sectors of the (t, μ) space. We can then restrict to $t = 0$ and get our actions S_0.

We will calculate S_0 by first computing the same object $\Sigma_0(t, \mu)$ for $C_{t,\mu} = \{p(x, \xi, \mu) - t = 0\}$ and taking $S_0(\mu) = \Sigma_0(0, \mu)$.

The cycle c is a limit of a cycle $c(t, \mu)$ of $C_{t,\mu}$ as $(t, \mu) \to 0$ in some sector $\Omega_\pm := \{(t, \mu) | \pm t > 0, |\mu| << |t|\}$.

We have, for $(t, \mu) \in \Omega$,

$$\Sigma_0(t, \mu) = \int_{c_{t,\mu}} \xi dx + \sum_{j=1}^{p} \pm\gamma_{0,j}(t, \mu)(\ln|\gamma_{0,j}(t, \mu)| - 1) \ ,$$

where the $\pm$ signs depends on orientation and can be determined from the Logarithmic singularities of the action integrals. The contributions $\pm\gamma_{0,j}(t, \mu)(\ln|\gamma_{0,j}(t, \mu)| - 1)$ come from the phase shift between $x_+^{i\gamma/h}$ and $\xi_+^{-i\gamma/h}$ expressed as a WKB function of the single variable x.

Knowing that Σ_0 is smooth, the previous formula defines the Taylor expansion of Σ_0 w.r. to (t, μ) and hence the Taylor expansion of S_0 w.r. to μ.

4.3 The analytic case

In the analytic case, we could also consider the Riemann surfaces $X_\mu = \{p_\mu = 0\}$ and look at some complex cycles c_μ on X_μ whose limit is c. Those cycles are not unique, but the real part of their action integrals are well defined and we can then take directly the previous regularisation.

4.4 An example

Let us consider the adiabatic equation:

$$\frac{h}{i}\frac{dX}{dt} = A_\mu(t)X$$

with

$$A_\mu(t) = \begin{pmatrix} t^2 & \mu \\ \mu & 2 - t^2 \end{pmatrix}$$

and the only cycle c_0 of C_0 passing by the singular points $(\pm 1, \pm 1)$. It is clear that c_0 is not a limit of real cycle c_μ of C_μ, because the matrix $A_\mu(t)$ has real eigenvalues for each t and so C_μ is the union of 2 disjoint graphs and has no real cycle.

5 The subprincipal action

We know that the Landau-Zener coefficient given by Equation (6) is $0(h^\infty)$ if $|\mu| >> \sqrt{h}$. It implies that in order to solve our problem up to $O(\sqrt{h})$ terms it is enough to know S_0 mod $O(|\mu|^3)$ and S_1 for $\mu \in Z$. Let us assume that we have local coordinates so that $0 \in Z$. We will describe below the calculus of $S_1(0)$.

Lemma 3 *Assuming $|\mu| = 0$, the principal part $\vec{a}(x)\exp(iS(x)/h)$ of the WKB solutions of Equation (1) associated to arcs $]z_j, z_{j+1}[$ of C_0 can be smoothly extended beyond the singular vertices as WKB functions.*

Proof.–

> The property is invariant by FIO and it is enough to prove it for the solutions of the normal form given in Equation (3). The point is that $a_0(0) = 0$, hence $\gamma = O(h^2)$.

□

The previous result is related to the fact that the adiabatic theorem is still valid in case of eigenvalue crossings (see [1, 3]).

We will define on c a piecewise smooth Hermitian line bundle L with a connection as follows:

- On each arc $[z_j, z_{j+1}]$, $L_z = \ker H_{\text{class}}(z)$ with the connection given by the transport equation as in [12] (in the case of the adiabatic limit, it is the so called *geometric connection* or *Berry phase* [2]).
- At each singular point, there are 2 limit fibers $L_{\pm,j}$ and from A_0 (defined in Remark 3) we have an isomorphism between both limits given by transporting the isomorphism $(1,0) \to (0,1)$ of $\mathbb{C} \oplus 0$ on $0 \oplus \mathbb{C}$ by $(A_0)_{|\mathbb{C}^2 \oplus 0}$.

Definition 1 *The phase* $\exp(iS_1^{\nabla}(0))$ *is the holonomy of the discontinuous line bundle* L*.*

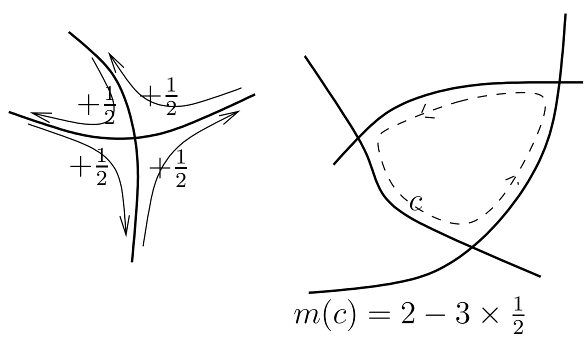

Figure 5: the singular Maslov indices

Using the calculus of [10] (page 20) (we alert the reader that the previous convention for Maslov indices are not the same in the paper [9]), we can also put the:

Definition 2 *The (singular) Maslov index* $m(c) \in \mathbb{Z}/2$ *of a simple cycle* c *which is the boundary of a bounded connected component of* $T^\star\mathbb{R} \setminus C_0$ *is given by:* $m(c) = m_{\text{smooth}}(c) + m_{\text{sing}}(c)$ *where* $m_{\text{smooth}}(c)$ *is the usual Maslov index of a smooth deformation of* c *while* $m_{\text{sing}}(c)$ *is a sum of* $\pm\frac{1}{2}$ *associated to the singular points according to the rules of Figure 5.*

The Maslov index of any cycle is defined by linearity from the previous Maslov indices, so it gives a cocycle. For example, the Maslov index of a smooth cycle (even if not simple) is the usual one, namely ± 2.

Theorem 3 *Using the previous definitions, we have:*

$$S_1(0) = S_1^{\nabla}(0) + m(c)\frac{\pi}{2} \ .$$

Proof.–

The proof follows essentially the lines of [9] p. 474-476.

Let us give some details. A priori, there are several cases to check depending on the position of the cycle c at the singular points w.r. to the verticals. We will assume that the matrix

$$\chi'(O) = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

of the canonical transformation $\chi = \chi_0$ satisfies $a \neq 0$ and $b \neq 0$, this is the *generic case.* We define

$$\varepsilon = \begin{cases} +1 \text{ if } ab > 0 \\ -1 \text{ if } ab < 0 \end{cases} .$$

The generating function $\varphi(x, y) = \varphi_2(x, y) + O(|x|^3 + |y|^3)$ of χ, defined by $\chi(y, -\partial_y \varphi) = (x, \partial_x \varphi)$, satisfies $\varphi_2(x, y) = \frac{1}{2b}(dx^2 - 2xy + ay^2)$. We need to compute mod $o_h(1)$ the values for x close to 0 of the images by the normal form transform of

$$W_-^{\rm out}(y) = \begin{pmatrix} Y(y) \\ 0 \end{pmatrix}$$

and

$$\widehat{W_-^{\rm in}}(\eta) = \begin{pmatrix} 0 \\ Y(\eta) \end{pmatrix} .$$

Let us assume that the principal symbol of the ΨDO gauge transform is the $N \times N$ matrix

$$\sigma(A)(y, \eta) = \begin{pmatrix} \vec{\alpha}_1(y, \eta) & \vec{\alpha}_2(y, \eta) & \cdots \end{pmatrix} .$$

We get for the components of both WKB solutions for x small but nonzero:

$$W_{-,j}^{\rm out}(x) = (2\pi h)^{-3/2} \int_{y' \geq O} e^{\frac{i}{h}(\varphi(x,y) + (y-y')\eta)} C(x, y) \vec{\alpha}_1(y, \eta) dy dy' d\eta \ ,$$

with $C(0,0)=|b|^{-\frac{1}{2}}$, and

$$W^{\rm in}_{-,j}(x)=(2\pi h)^{-1}\int_{\eta\geq O} e^{\frac{i}{h}(\varphi(x,y)+y\eta)}C(x,y)\vec{\alpha}_2(y,\eta)dyd\eta\ .$$

If we evaluate the integrals by stationnary phase, the dominant contributions come from the critical points and not from the boundary. The determinant of both Hessians are the same, while the signature differs by 1. The final result follows then by

- Looking at the value of the stationnary phase calculations as x is close to 0: the limits are respectively

  $$C(0,0)e^{i\varepsilon\pi/4}\vec{\alpha}_1(0,0)$$

  and

  $$C(0,0)\vec{\alpha}_2(0,0)$$

- if $\varepsilon>0$, one should add a contribution of the smoothed c, while if $\varepsilon<0$ there is no such contribution.
- Remembering that

  $$A_{0|\mathbb{C}^2\oplus 0}=\left(\begin{array}{cc}\vec{\alpha}_1(0,0) & \vec{\alpha}_2(0,0)\end{array}\right)\ .$$

□

6 Application 1: adiabatic limit with avoided crossings

6.1 Adiabatic limit

We consider the following equation:

$$\frac{1}{i}\frac{dX}{d\tau}=A_\mu(h\tau)X \tag{7}$$

where $A_\mu(t),\ 0\leq t\leq a$, is a self-adjoint matrix which is smooth w.r. to (t,μ) and we consider $0\leq\tau\leq a/h$. The limit $h\to 0$ of this equation is called the *adiabatic limit.*

We can rewrite Equation (7) in a standard *semi-classical* form by puting $t=h\tau$:

$$\frac{h}{i}\frac{dX}{dt}=A_\mu(t)X \tag{8}$$

where $0\leq t\leq a$.

We will assume that the eigenvalues of $A_\mu(0)$ and $A_\mu(a)$ are all non degenerate. The scattering matrix $\mathcal{S}(\mu,h):\mathbb{C}^N\to\mathbb{C}^N$ is defined by $X(0)\to X(a)$ where X is a solution of Equation (8).

6.2 Outside eigenvalues crossings

Let $\lambda(t)$ be an eigenvalue of multiplicity 1 of $A_0(t)$ for t in some open intervall I. Then Equation (8) admits a unique (up to multiplication by some function of h) formal *WKB solution* given by

$$X(t) = e^{i\Lambda(t)/h}\left(\sum_{j=0}^{\infty} a_j(t)h^j\right)$$

where $\Lambda'(t) = \lambda(t)$ and $a_0(t)$ satifies:

- $a_0(t) \in \ker\left(A_0(t) - \lambda(t)\right)$
- $\nabla a_0(t) = 0$ where ∇ is the *geometric* or *Berry* connection.

Let us recall that $\nabla_{\partial/\partial t} a(t) = \Pi_t a'(t)$ where Π_t is the orthogonal projection of $\mathbb{C}^N$ onto the eigenspace $\ker(A_0(t) - \lambda(t))$.

The previous statement is the content of the so called *quantum adiabatic theorem* and goes back to [3].

6.3 Avoided crossings

What happens when eigenvalues become degenerate at some values of t?

Let us try to understand the *generic situation.* It is well known that eigenvalue crossings for a real symmetric (resp. complex Hermitian) matrix is a codimension 2 (resp. 3) property. It is the content of the well known Wigner-Von Neumann theorem [21].

Physically, eigenvalues crossings can still occur for symmetry reasons. But, if we break the symmetry by a small perturbation of size μ, we will get the so-called *avoided crossings.* We have now two small parameters: the semi-classical (adiabatic) parameter h and the perturbation parameter μ. The previous results allow to discuss the uniform expansion of the scattering matrix w.r. to both small parameters.

6.4 Precise assumptions

We will assume that the eigenvalues of $A_0(t)$ cross transversally only by pairs on $]0, a[$. The dispersion relation $C_\mu \subset T^\star[O, a]$ is defined by $p_\mu(t, \tau) = \det(\tau \mathrm{Id} - A_\mu(t))$. So that C_μ is exactly the union of the graphs of the eigenvalues of $A_\mu(t)$.

6.5 Calculation of the scattering matrix

Let us describe how to compute the global scattering matrix in the case of Figure 7. Let us start with the 4 local scattering matrices $\mathcal{S}_j,\ j = 1, \cdots, 4$ and the 2 holonomies $\mathcal{H}_\mu(c_k),\ k = 1, 2$.

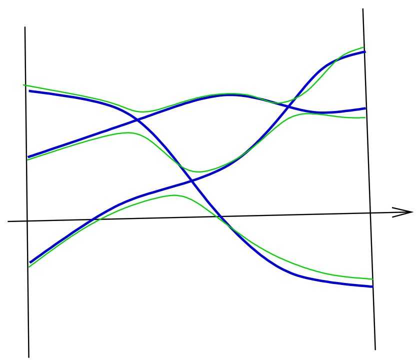

Figure 6: the dispersion relation for the adiabatic limit

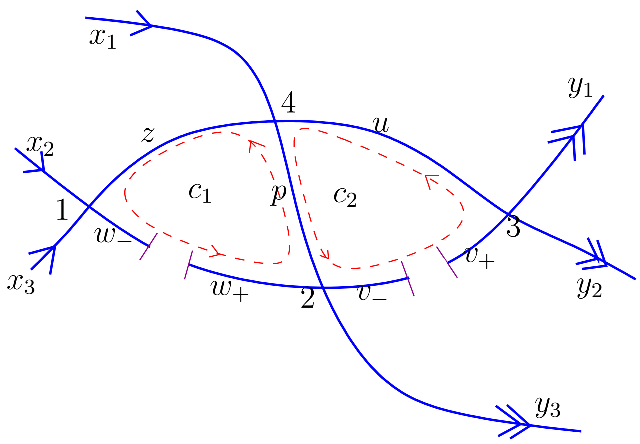

Figure 7: recipe for the global scattering matrix

We try to describe a global solution of our system which is given from WKB solutions associated to each arc of a maximal tree of C_0. We have 10 equations with 13 unknowns which allow to compute $\vec{y}$ from $\vec{x}$.

$$\begin{cases} w_- = \mathcal{H}_\mu(c_1)w_+ \\ v_- = \mathcal{H}_\mu(c_2)v_+ \\ \begin{pmatrix} z \\ w_- \end{pmatrix} = \mathcal{S}_1 \begin{pmatrix} x_3 \\ x_2 \end{pmatrix} \\ \begin{pmatrix} v_- \\ y_3 \end{pmatrix} = \mathcal{S}_2 \begin{pmatrix} w_+ \\ p \end{pmatrix} \\ \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \mathcal{S}_3 \begin{pmatrix} v_+ \\ u \end{pmatrix} \\ \begin{pmatrix} u \\ p \end{pmatrix} = \mathcal{S}_4 \begin{pmatrix} z \\ x_1 \end{pmatrix} \end{cases}$$

It turns out that the global scattering matrix is the product of 5 unitary matrices as follows :

$$\vec{x} \to \begin{pmatrix} x_1 \\ z \\ w_- \end{pmatrix} \to \begin{pmatrix} u \\ p \\ w_+ \end{pmatrix} \to \begin{pmatrix} u \\ v_- \\ y_3 \end{pmatrix} \to \begin{pmatrix} u \\ v_+ \\ y_3 \end{pmatrix} \to \vec{y} \ .$$

7 Application 2: EBK quantization rules

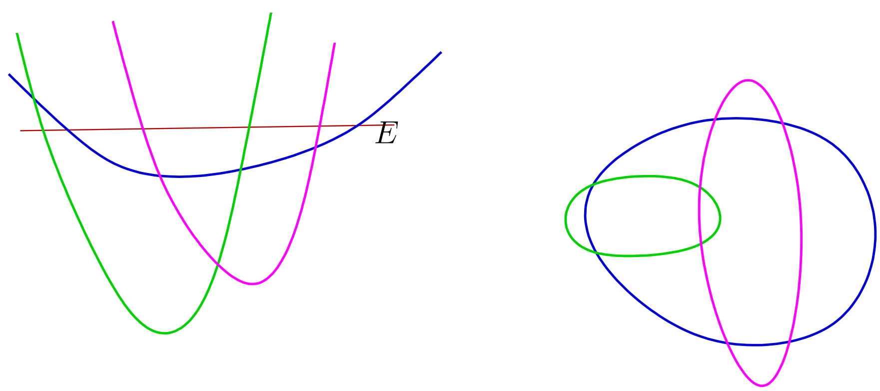

Figure 8: the dispersion relation for the Born-Oppenheimer Hamiltonian

We consider a Born-Oppenheimer Hamiltonian of the following form:

$$\widehat{K_\nu} = -h^2 \frac{d^2}{dx^2} \otimes \mathrm{Id} + V_\nu(x)$$

where $V_\nu : \mathbb{R} \to \mathrm{Herm}(\mathbb{C}^N)$ is smooth w.r. to (x, ν). We assume:

- The eigenvalues of $V_0(x)$ are of multiplicities at most 2 and cross transversally.
- The following properness condition:

$$V_\nu(x) \geq p(x)\mathrm{Id}$$

where $\lim_{|x|\to\infty} p(x) = +\infty$.

- We choose E so that, for any $x \in \mathbb{R}$, E is not a degenerate eigenvalue of $V_0(x)$.
- If the eigenvalue $\lambda_j(x)$ of $V_0(x)$ satisfies $\lambda_j(x_0) = E$, then $\lambda_j'(x_0) \neq 0$.

We can apply the previous method in order to compute EBK quantization rules for the equation $(\widehat{K_\nu} - E)\vec{U} = O(h^\infty)$.

EBK quantization can be solved following the same path; but is this case we have the same number of equations than of unknowns and EBK rule is given by the vanishing of a suitable determinant as in [9].

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