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To cite this version:
Yves Colin de Verdière. Bohr-Sommerfeld phases for avoided crossings. 2006. hal-00574571

HAL Id: hal-00574571
https://hal.science/hal-00574571
Preprint submitted on 8 Mar 2011

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Bohr-Sommerfeld phases for avoided crossings

Yves Colin de Verdière *†‡

March 8, 2011

Introduction

0.1 Adiabatic limit in quantum mechanics

The problem of adiabatic limit in quantum mechanics with avoided eigenvalues crossings will be the basic example in our paper.

Let us describe it in a precise way. We start with a smooth family of $N \times N$ Hermitian matrices $A(t)$ with $a \leq t \leq b$ and consider the following linear system of differential equations:

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

Solving this equation gives an unitary map $S_h$ defined by $S_h(X(a)) = X(b)$. We call it the scattering matrix of the problem. Adiabatic Theorems describe the asymptotic behaviour of $S_h$ when $h \to 0$.

1. The classical adiabatic theorem [3, 17] concerns the case where the eigenvalues of $A(t)$ satisfy, for all $t$:

$$\lambda_1(t) < \lambda_2(t) < \cdots < \lambda_N(t).$$

In this case, if we start with $X_j(a)$ an eigenvector of $A(a)$ with eigenvalue $\lambda_j(a)$, we have $X_j(b) = \exp(i \int_a^b \lambda_j(s) ds)Y_j(b) + O(h)$ where $Y_j(b)$ is obtained by parallel transporting $X_j(a)$ along $[a, b]$ in the eigenbundle $L_j(t) = \ker(A(t) - \lambda_j(t))$ w.r. to the geometric (or Berry) connection defined by

$$\nabla_{\partial/\partial t} Y(t) = \proj_{L_j(t)} \frac{dY}{dt}$$

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†Key-words: adiabatic limit, semi-classical analysis, Landau-Zener formula, avoided crossings, pseudo-differential operators

‡MSC 2000: 34E05, 35S30, 81Q20, 81Q70
2. Another case which is well known [1, 3, 13, 19], is the case where the eigenvalues of $A(t)$ cross transversally. Then the previous results remains true with a less good remainder term $O(\sqrt{h})$ but we need to label the eigenbundle by following smoothly the eigenvalues at the crossings points. In other words, there is some exchange between $L_j$ and $L_{j\pm 1}$ at each crossing point.

So the scattering matrix remains diagonal but with some relabeling of the indices $j = 1, \cdots, N$.

We want to consider the bifurcation between the 2 situations. For that purpose, we allow $A(t)$ to depend smoothly of a $d-$dimensional parameter $\mu$ close to 0 in $\mathbb{R}^d$. We will assume that $A_0(t)$ admits eigenvalues crossings transversally. For $\mu$ small, $A_\mu$ will have avoided eigenvalue crossings. We will derive in this paper a way to get the asymptotic behaviour of $S_{\mu, h}$ w.r. to both small parameter $\mu$ and $h$.

Basically the result uses 2 parts:

1. The local situation where a suitable Landau-Zener formula can be used describing the local $2 \times 2$ scattering matrix (see [15, 8]).

2. The global problem where we have to take into account interferences given by what we called Bohr-Sommerfeld phases. In the case of several crossings (analytic case), using Stokes lines, they are many works where the interferences effects are exponentially small [16, 18].

0.2 Born-Oppenheimer approximation

Another important example comes from the Born-Oppenheimer approximation. We consider, on the real line a Schrödinger equation with matrix valued potential as follows:

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

where $V$ is an Hermitian matrix depending smoothly on $x \in \mathbb{R}$. We are interested in the eigenvalue equation $(\hat{H} - E)\tilde{u}(x) = 0$ with $\tilde{u} : \mathbb{R} \rightarrow \mathbb{C}^n$. If there is no degenerate eigenvalues of $V(x)$ smaller than $E$, then eigenfunctions can be found using a WKB-Maslov Ansatz in a very similar way to the scalar case. It is the generic situation for a single $V$ [14, 20]. The most precise results are shown in [12]. However, if $V$ depends on some external parameters $\mu$ close to 0 in $\mathbb{R}^d$, it is possible that, in a stable way, $V_{\mu}(x)$ admits degenerate eigenvalues. The problem we adress in this case is the description of Bohr-Sommerfeld rules uniformly w.r. to $\mu$. 

2
0.3 The general setting

Both examples can be put together as follows: we consider a self-adjoint semi-classical system of \( N \) (pseudo-)differential equations of order 0 with \( N \) complex valued unknown functions \( \vec{U} = (U_1, \cdots, U_N) \),

\[
\hat{H} \vec{U} = 0(h^{\infty})
\]

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 \( (\hat{H}_{i,j})^* = \hat{H}_{i,j} \). Viewing the previous examples, 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.

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

\[
H^\mu_{\text{class}} : T^* \mathbb{R} \to \text{Herm}(\mathbb{C}^N),
\]

the (matrix valued) principal symbol, is the dispersion matrix, and \( C_\mu = p_\mu^{-1}(0) \) with \( p_\mu = \det(H^\mu_{\text{class}}) \) 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 \( S_0(\mu) \sim \sum_{j=0}^{\infty} S_j(\mu) h^j \) were the \( S_j \)'s are formal power series in \( \mu \). \( S_0 \) 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 [4, 5] (see also [8]):

**Theorem 1** Let us assume that the function \( p_0(x, \xi) = \det(H_{\text{class}, \mu=0}) \) admits at the point \( z_0 \in T^* \mathbb{R} \) 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 \( \mu \) close enough to 0:

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

\[
P_\mu (\chi_\mu (x, \xi)) = e_\mu (x, \xi) (x\xi - \gamma_0 (\mu))
\]

with \( e_\mu \) an invertible germ function and \( \gamma_0 \) a germ of \( \geq 0 \) function of \( \mu \) satisfying \( \gamma_0 (0) = 0 \). Moreover, the Taylor expansion of \( \gamma_0 \) is unique.

- A smooth family of unitary FIO’s \( U_\mu \) associated to \( \chi_\mu \) and \( N \times N \) matrix of \( \Psi DO 's \) \( A_\mu \) so that, we have the following normal form (called the Landau-Zener normal form) near \( z_0 \):

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

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

Moreover, \( a_0 \) is a complex valued function of \( \mu \) which satisfies

\[
|a_0|^2 (\mu) = \gamma_0 (\mu) ,
\]

and we have

\[
\gamma_0 (\mu) = - \frac{p_\mu (z_0)}{\sqrt{|\det p'_0 (z_0)|}} + O (\mu^3) .
\]

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

(\( \star \)) if \( W \subset \text{Herm}(\mathbb{C}^N) \) is the submanifold defined by \( \text{dim} \ker H = 2 \), we assumed there that \( (\mu, z) \rightarrow H_{\text{class, } \mu} (z) \) 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 \( \mu \rightarrow a_0 (\mu) \) 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 \( \mu \) 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 \( \chi \). 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 \( H_{\text{class}} \) from \( m \) to \( m \pm 1 \) while crossing these arcs. The sign of this change is preserved by the gauge transform.
Figure 1: the jumps of the Morse index of the dispersion matrix

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.

**Remark 3** The symbol $\alpha$ is not uniquely defined because a diagonal unitary gauge transform preserves the normal form while changing $\alpha$ 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 (9).

The matrix $A$ is defined up to matrices which will change the phase of $\alpha$. 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 $A_0((\mathbb{C} \oplus 0) \oplus 0) = E_1$ and $A_0((0 \oplus \mathbb{C}) \oplus 0) = E_2$ 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

$$\gamma_0(\mu) = \frac{\text{gap}(\mu)^2}{4(|\lambda_+ - \lambda_-|)} + O(\mu^3)$$

where 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 $2 \times 2$ scattering matrix $T$ for the Landau-Zener normal form :

$$\begin{align*}
(D u + \alpha v) &= 0 \\
(\bar{\alpha} u + x v) &= 0
\end{align*}
$$
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 $C_{\alpha}^{LZ} = \{ x \xi = \gamma \}$ be the characteristic manifold. The set $C_{\alpha}^{LZ} \cap \{ \max(|x|, |\xi|) \geq a \}$ is the union of 4 connected arcs. These arcs are labelled $\Lambda_{\pm}^{in, out}$ as follows:

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

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 $\Lambda_{\pm}^{in, out}$:

\[
\begin{align*}
W_{-}^{out} &: \quad u_{-}^{out}(x) = x^{i\frac{\gamma}{h}}_-, \quad v_{-}^{out}(x) = -\bar{\alpha}x^{i\frac{\gamma}{h}-1}_- \\
W_{+}^{in} &: \quad u_{+}^{in}(x) = x^{i\frac{\gamma}{h}}_+, \quad v_{+}^{in}(x) = \bar{\alpha}x^{i\frac{\gamma}{h}-1}_+ \\
W_{-}^{in} &: \quad \tilde{u}_{-}^{in}(\xi) = -\alpha\xi^{i\frac{\gamma}{h}-1}_-, \quad \tilde{v}_{-}^{in}(\xi) = \xi^{i\frac{\gamma}{h}}_-
\end{align*}
\]

\[
W_{+}^{out} : \quad \tilde{u}_{+}^{out}(\xi) = \alpha\xi^{i\frac{\gamma}{h}-1}_+, \quad \tilde{v}_{+}^{out}(\xi) = \xi^{i\frac{\gamma}{h}}_+ \quad (6)
\]

Figure 2: the 4 arcs of the characteristic manifold and Morse indices
where\(\hat{f}(\xi)\) is the \(h\)-Fourier transform of \(f(x)\) defined by
\[
\hat{f}(\xi) = \frac{1}{\sqrt{2\pi h}} \int_{\mathbb{R}} e^{-\frac{i\xi}{h} x} f(x) dx ,
\]
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 (5) near the origin:

\[
\begin{align*}
W_{\text{out}}(x) &\leftrightarrow h^{\frac{1}{2} + i\frac{\gamma}{h}} \frac{\Gamma(1 + i\frac{\gamma}{h})}{\sqrt{2\pi \alpha}} (i e^{\frac{\pi}{h} x} W_{\text{in}}^{-}(x) + i e^{-\frac{\pi}{h} x} W_{\text{out}}^{+}(x)) \\
W_{\text{in}}^{+}(x) &\leftrightarrow h^{\frac{1}{2} + i\frac{\gamma}{h}} \frac{\Gamma(1 + i\frac{\gamma}{h})}{\sqrt{2\pi \alpha}} (-i e^{-\frac{\pi}{h} x} W_{\text{in}}^{-}(x) - i e^{\frac{\pi}{h} x} W_{\text{out}}^{+}(x))
\end{align*}
\]

If \(W_{\text{in}} := y_{+} W_{\text{in}}^{+} + y_{-} W_{\text{in}}^{-}\) and \(W_{\text{out}} := z_{+} W_{\text{out}}^{+} + z_{-} W_{\text{out}}^{-}\) are WKB-solutions of Equation (4) outside the origin, we get, for any microlocal solution near the origin,
\[
\begin{pmatrix}
y_{+} \\
y_{-}
\end{pmatrix} = T \begin{pmatrix}
z_{-} \\
z_{+}
\end{pmatrix}
\]
where \(T\) is the unitary matrix defined by:
\[
T = \frac{1}{A} \begin{pmatrix}
\frac{1}{B} & 1 \\
B^2 - A^2 & -B
\end{pmatrix}
\]
with
\[
A = i h^{\frac{1}{2} + i\frac{\gamma}{h}} \frac{\Gamma(1 + i\frac{\gamma}{h})}{\sqrt{2\pi \alpha}} e^{\frac{\pi}{h} x}, \quad B = i h^{\frac{1}{2} + i\frac{\gamma}{h}} \frac{\Gamma(1 + i\frac{\gamma}{h})}{\sqrt{2\pi \alpha}} e^{-\frac{\pi}{h} x} .
\]

The matrix \(T\) will be called the local scattering matrix associated to the singular point (and the choice of a normal form). Unitarity of \(T\) is checked using the well-known formula
\[
\Gamma(1 + ix)\Gamma(1 - ix) = \frac{\pi x}{\sinh \pi x}
\]
which implies \(|A|^2 = |B|^2 + 1, \ AB = \bar{A}B\).

The transmission coefficient
\[
\tau = \left| \frac{B}{A} \right| = \exp(-\frac{\pi \gamma}{h})
\]
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

$$S_h(\mu) = S_0(\mu) + hS_1(\mu) + \cdots$$

where the $S_j$’s are smooth w.r. to $\mu$.

In this section, we will define precisely these phases. We show that they are uniquely defined as formal power series w.r. to $(\mu, h)$. 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 $T^*\mathbb{R} \setminus C_0$). Let $z_1$, $z_2$, $\ldots$, $z_n$ 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 $\Psi DO$ gauge transform $A_j$ (all depending smoothly on $\mu$) which give the normal form of Theorem 1 with $\alpha_j = \alpha_j(\mu, h)$ a full symbol.

We will define $H_\mu(c) = \exp(iS_h(\mu)/h)$ as follows: we will denote by $W_{\pm,j}^{\text{in, out}}$ the images of $W_{\mp,j}^{\text{in, out}}$ by the operators $U_j^\mu A_j^\mu$. These functions are WKB solutions of equation (4) associated to arcs of $C_\mu$ near $z_j$. We introduce also WKB solutions $u_j$ of (4) along arcs of $C_\mu$ close to $[z_j, z_{j+1}]$. From those objects we get a global holonomy $H_\mu(c)$ of the cycle $c$ defined as follows: we have (by uniqueness, modulo multiplication by a full symbol, of WKB solutions) for example near $z_j$:

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

We define $H_\mu(c) = \prod_{j=1}^n y_j x_j^{-1}$. In other words, $H_\mu(c)$ 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 $W_{+j}^{\text{in}} \rightarrow W_{-j}^{\text{in}}$.

\textbf{Lemma 1} We have $|H_\mu(c)| = 1 + O(h^\infty)$.

\textit{Proof}.–
Following [7] section 11.2.1. and Figure 4, we associate to the cycle $c$ an unitary scattering matrix $S_c$ which is computable from the local unitary scattering matrices associated to the singular points and the holonomy $H_\mu(c)$. If this holonomy does not satisfy $|H_\mu(c)| = 1 + O(h^\infty)$, 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 $H_\mu(c)$.

Figure 3: defining $H_\mu(c)$

Following [7] section 11.2.1. and Figure 4, we associate to the cycle $c$ an unitary scattering matrix $S_c$ which is computable from the local unitary scattering matrices associated to the singular points and the holonomy $H_\mu(c)$. If this holonomy does not satisfy $|H_\mu(c)| = 1 + O(h^\infty)$, 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 $H_\mu(c)$.

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

**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 $W_{\text{in, out}}^{\pm,j}$'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 (7) and (8) with the value of $\alpha$ given by the normal form at the point $z_j$.

\[ \Box \]

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 $C_\mu$.

**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).

\[ \Box \]

4.2 $S_0$ as a regularized action integral

Let us denote by $|\mu| = d(\mu, Z)$. As in [3], it would be nice to get $S_0(\mu)$ as a regularisation of an usual action integral. A basic fact in [3] was that any simple cycle $c$ is a limit of a cycle of $C_\mu$ 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 $C_\mu$ which can be embedded into a larger family $C_{t,\mu}$ for which we can define action integral in some suitable sectors of the $(t, \mu)$ 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 $x_{+}^{i\gamma/\hbar}$ and $\xi_{+}^{-i\gamma/\hbar}$ expressed as a WKB function of the single variable $x$.

Knowing that $\Sigma_0$ is smooth, the previous formula defines the Taylor expansion of $\Sigma_0$ w.r. to $(t, \mu)$ and hence the Taylor expansion of $S_0$ w.r. to $\mu$.

### 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 $c_\mu$ on $X_\mu$ 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 $c_\mu$ of $C_\mu$, because the matrix $A_\mu(t)$ has real eigenvalues for each $t$ and so $C_\mu$ 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 (9) is $0(\hbar^\infty)$ if $|\mu| \gg \sqrt{\hbar}$. It implies that in order to solve our problem up to $O(\sqrt{\hbar})$ terms it is enough to know $S_0$ mod $O(|\mu|^3)$ and $S_1$ for $\mu \in \mathbb{Z}$. Let us assume that we have local coordinates so that $0 \in \mathbb{Z}$. We will describe below the calculus of $S_1(0)$.

**Lemma 3** Assuming $|\mu| = 0$, the principal part $\bar{a}(x)\exp(iS(x)/\hbar)$ of the WKB solutions of Equation (4) 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 (6). 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 \((1, 0) \rightarrow (0, 1)\) 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](image)

\[
m(c) = 2 - 3 \times \frac{1}{2}
\]

**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 \( T^* \mathbb{R} \setminus C_0 \) 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 4.
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 $\pm 2$.

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

$$S_1(0) = S^V_1(0) + m(c)\frac{\pi}{2}.$$  

**Proof.**–

The proof follows essentially the lines of [8] 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 $\chi$, defined by $\chi(y, -\partial_y \varphi) = (x, \partial_x \varphi)$, satisfies $\varphi_2(x, y) = \frac{1}{2\pi}(dx^2 - 2xy + ay^2)$. We need to compute mod $o_h(1)$ the values for $x$ close to 0 of the images by the normal form transform of

$$W^\text{out}_-(y) = \begin{pmatrix} Y(y) \\ 0 \end{pmatrix}$$

and

$$\widehat{W}^\text{in}_-(\eta) = \begin{pmatrix} 0 \\ Y(\eta) \end{pmatrix}.$$  

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

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

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

$$W_{-j}^\text{out}(x) = (2\pi h)^{-3/2} \int_{y' \geq 0} e^{i\chi(x, y) + (y - y')\eta} C(x, y)\tilde{\alpha}_1(y, \eta)dydy'd\eta,$$  

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with $C(0, 0) = |b|^{-\frac{1}{2}}$, and
\[ W_{-j}^{in}(x) = (2\pi h)^{-1} \int_{\eta \geq 0} e^{\frac{i}{\hbar}(\varphi(x,y) + y\eta)} C(x, y)\tilde{\alpha}_2(y, \eta) dy d\eta. \]

If we evaluate the integrals by stationary 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 stationary phase calculations as $x$ is close to 0: the limits are respectively
  \[ C(0, 0)e^{ie\pi/4}\tilde{\alpha}_1(0, 0) \]
  and
  \[ C(0, 0)\tilde{\alpha}_2(0, 0) \]
- if $\varepsilon > 0$, one should add a contribution of the smoothed $c$, while if $\varepsilon < 0$ there is no such contribution.
- Remembering that
  \[ A_0|_{C^2=0} = (\tilde{\alpha}_1(0, 0) \quad \tilde{\alpha}_2(0, 0)) \]

\[ \square \]

6 Application 1: adiabatic limit with avoided crossings

6.1 Adiabatic limit

We consider the following equation:
\[ \frac{1}{i} \frac{dX}{d\tau} = A_\mu(h\tau)X \]  \hspace{1cm} (10)
where $A_\mu(t)$, $0 \leq t \leq a$, is a self-adjoint matrix which is smooth w.r. to $(t, \mu)$ and we consider $0 \leq \tau \leq a/h$. The limit $\hbar \to 0$ of this equation is called the adiabatic limit.

We can rewrite Equation (10) in a standard semi-classical form by putting $t = h\tau$:
\[ \frac{h}{i} \frac{dX}{dt} = A_\mu(t)X \]  \hspace{1cm} (11)
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 $S(\mu, h) : \mathbb{C}^N \to \mathbb{C}^N$ is defined by $X(0) \to X(a)$ where $X$ is a solution of Equation (11).
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 (11) 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:

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

Let us recall that $\nabla_{\partial/\partial t} a(t) = \Pi_t a'(t)$ where $\Pi_t$ 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 $\mu$, we will get the so-called avoided crossings. We have now two small parameters: the semi-classical (adiabatic) parameter $h$ and the perturbation parameter $\mu$. 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 $C_\mu \subset T^*[O, a]$ is defined by $p_\mu(t, \tau) = \det(\tau Id - A_\mu(t))$. So that $C_\mu$ 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 $S_j$, $j = 1, \cdots, 4$ and the 2 holonomies $H_\mu(c_k)$, $k = 1, 2$. 

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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 \( \vec{x} \).

\[
\begin{align*}
  w_- &= \mathcal{H}_\mu(c_1)w_+ \\
  v_- &= \mathcal{H}_\mu(c_2)v_+ \\
  z &= S_1 \begin{pmatrix} x_3 \\ x_2 \end{pmatrix} \\
  y_3 &= S_2 \begin{pmatrix} w_+ \\ p \end{pmatrix} \\
  y_1 &= S_3 \begin{pmatrix} v_+ \\ u \end{pmatrix} \\
  y_2 &= S_4 \begin{pmatrix} z \\ x_1 \end{pmatrix}
\end{align*}
\]

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

\[
\vec{x} \rightarrow \begin{pmatrix} x_1 \\ z \\ w_- \end{pmatrix} \rightarrow \begin{pmatrix} u \\ p \\ w_+ \end{pmatrix} \rightarrow \begin{pmatrix} u \\ v_- \\ y_3 \end{pmatrix} \rightarrow \begin{pmatrix} u \\ v_+ \\ y_3 \end{pmatrix} \rightarrow \vec{y}.
\]

7 Application 2: EBK quantization rules

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

\[
\hat{K}_\nu = -\hbar^2 \frac{d^2}{dx^2} \otimes \text{Id} + V_\nu(x)
\]

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

Figure 8: the dispersion relation for the Born-Oppenheimer Hamiltonian
• The eigenvalues of $V_0(x)$ are of multiplicities at most 2 and cross transversally.

• The following properness condition:

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

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 $(\tilde{K}_\nu - E)\tilde{U} = O(h^\infty)$.

EBK quantization can be solved following the same path; but in 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 $[9]$.

References

[1] J.E. Avron & A. Elgart, An Adiabatic Theorem without a gap condition. **Commun. Math. Phys.**, 203:445-463, 1999.

[2] M. Berry, Quantal phase factors accompanying adiabatic changes. **Proc. Roy. Soc. Lond.**, A392:45-57, 1984.

[3] M. Born & V. Fock, Beweis des Adiabatensatzes. **Z. Phys.**, 51:165-169, 1928.

[4] F. Bornemann, Homogenization in Time of Singly Perturbed Mechanical Systems. **Lecture Notes in Math. (Springer)**, 1687, (1998).

[5] Y. Colin de Verdière, The level crossing problem in semi-classical analysis I. The symmetric case. **Ann. Inst. Fourier (Actes du colloque en l’honneur de Frédéric Pham)**, 53:1023-1054, 2003.

[6] Y. Colin de Verdière, The level crossing problem in semi-classical analysis II. The Hermitian case. **Prépublication IF no 603 (March 2003)**, to appear in **Ann. Inst. Fourier**, volume in honor of Louis Boutet de Monvel.

[7] Y. Colin de Verdière, Singular Lagrangian manifolds and semi-classical analysis. **Duke Math. J.**, 116:263-298, 2003.

[8] Y. Colin de Verdière, M. Lombardi & J. Pollet, The microlocal Landau-Zener formula. **Annales de l’IHP (Physique théorique)**, 71:95-127, 1999.
[9] Y. Colin de Verdière & B. Parisse, Singular Bohr-Sommerfeld rules. Commun. Math. Phys., 205:459–500, 1999.

[10] Y. Colin de Verdière & San Vũ Ngọc, Singular Bohr-Sommerfeld rules for 2D integrable systems. Ann. Scient. ENS, 36:1-55, 2003.

[11] Y. Colin de Verdière & J. Vey, Le lemme de Morse isochore. Topology, 18:283-293, 1979.

[12] C. Emmrich & A. Weinstein, Geometry of the Transport Equation in Multicomponent WKB Approximation. Commun. Math. Phys., 176:701-711, 1996.

[13] G. Hagedorn, Adiabatic Expansions near Eigenvalue Crossings. Annals of Physics, 196:278-295, 1989.

[14] G. Hagedorn & J. Toloza, A time-Independent Born-Oppenheimer Approximation with Exponentially Accurate Error Estimates. Preprint mparc 04-16, 2003.

[15] A. Joye, Proof of the Landau-Zener formula, Asymptotic Anal., 9:209-258, 1994.

[16] A. Joye, Exponential asymptotics in a singular limit for $n$-level scattering systems. SIAM J. Math., 28:669–703, 1997.

[17] T. Kato, On the adiabatic theorem of quantum mechanics. Phys. Soc. Japan, 5:435-439, 1958.

[18] P. Martin & G. Nenciu, Semi-classical inelastic $S$-matrix for one dimensional $N$-states systems. Reviews in Mathematical Physics, 7:193–242, 1995.

[19] V. Rousse, Landau-Zener transitions for eigenvalue avoided crossings in the adiabatic and Born-Oppenheimer approximations. Asymptotic Analysis, 37:293-328, 2004.

[20] V. Rousse, PhD thesis, Institut Fourier, June 2004.

[21] J. von Neuman & E. Wigner, Über das Verhalten von Eigenwerten bei adiabatischen Prozessen. Phys. Zeit., 30:467–470, 1929.