# THE LEVEL CROSSING PROBLEM IN SEMI-CLASSICAL ANALYSIS II. The Hermitian case

Yves Colin de Verdière

March 21, 2003

Prépublication de l'Institut Fourier n<sup>0</sup> 603 (2003) http://www-fourier.ujf-grenoble.fr/prepublications.html

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 http://www-fourier.ujf-grenoble.fr/~ycolver/

# Introduction

This paper  $\begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$  is the second part of [2]. We want to study microlocally the solutions of a self-adjoint system of semi-classical pseudo-differential operators using normal forms. In our paper [2], we studied the case where the principal symbol (called the dispersion matrix) is a real symmetric matrix. We will consider here the case where the dispersion matrix  $H_{\text{class}}$  is complex Hermitian. There are several cases to consider depending on the rank of the restriction of the symplectic form to the codimension 4 singular manifold  $\Sigma$ :

- 1. The *symplectic* case
- 2. The *elliptic* corank 2 case
- 3. The hyperbolic corank 2 case
- 4. The case of one degree of freedom with some parameters (avoided crossings)

<sup>&</sup>lt;sup>1</sup>Keywords: Mode conversion, polarization, Born-Oppenheimer approximation, eigenvalues crossing, pseudo-differential systems, semi-classical analysis, normal form

<sup>&</sup>lt;sup>2</sup>Mathematics Subject Classification 2000: 35C20, 35Q40, 35S30, 53D05

 $<sup>^{3}</sup>Acknowledgments:$  many thanks to Clotilde Fermanian-Kammerer and Alain Joye for their comments on a preliminary version

Our goal is to get local normal forms for these systems both for the principal symbol (classical normal form) and for the pseudo-differential system (semi-classical normal form). The classical normal form uses canonical transformations and gauge transforms while the semi-classical normal form uses quantized version of the previous (Fourier integral operators and pseudo-differential gauge transforms). The semi-classical normal form can be used in order to describe the solutions of the system near the singular manifold (Landau-Zener type formulae, propagation of localized states, semi-classical measures). The reader is supposed to have already a knowledge of [2]. Some arguments work the same way and are only sketched.

# 1 The geometric setting

We will consider a  $d \times d$  Hermitian system of pseudo-differential equations

 $\widehat{H}\vec{U}=0$ 

in  $\mathbb{R}^n$  near some point  $z_0 \in T^*\mathbb{R}^n$  (with the symplectic form  $\Omega = \sum_{j=1}^n d\xi_j \wedge dx_j$ ) where the kernel of the principal symbol  $H_{\text{class}}$  is of dimension 2. We will denote by  $p = \det(H_{\text{class}})$ ; the manifold  $\{p = 0\}$  (more precisely the principal ideal  $C^{\infty}.p$ ) is the *dispersion relation*. We can reduce the system near the point  $z_0$  to a  $2 \times 2$ system for which the principal symbol vanishes at the point  $z_0$ . We will assume that

(\*) the mapping  $z \to H_{\text{class}}(z)$  is transversal at  $z_0$  to  $W_2 = \{A | \dim \ker A = 2\} \subset \text{Herm}(\mathbb{C}^d)$ .

The inverse image  $H^{-1}_{\text{class}}(W_2)$  is then a codimension 4 manifold  $\Sigma$  of the phase space  $T^*\mathbb{R}^n$ , the singular locus; we have

$$\Sigma = \{ z \in T^* \mathbb{R}^n \mid \dim \ker H_{\text{class}}(z) = 2 \} .$$

We will study 4 cases:

- 1. The symplectic case where  $\Sigma$  is a symplectic submanifold of  $T^*\mathbb{R}^n$ . It implies (see Lemma 1) that the linearization M of  $\mathcal{X}_p$  at  $z_0$  admits 2 pairs of non vanishing eigenvalues  $\pm \lambda$ ,  $\pm i\omega$  with  $\lambda > 0$ ,  $\omega > 0$ .
- 2. The hyperbolic corank 2 case where  $\Omega_{|\Sigma}$  is of corank 2 and M admits 1 pair of real nonzero eigenvalues  $\pm \lambda$  with  $\lambda > 0$ .
- 3. The elliptic corank 2 case where  $\Omega_{|\Sigma|}$  is of corank 2 and M admits 1 pair of imaginary nonzero eigenvalues  $\pm i\omega$  with  $\omega > 0$ .
- 4. The case of one degree of freedom with parameters: in that case, it is needed to have parameters in order to get the transversality assumption  $(\star)$ .

The following result, used in 1., is easy to check:

**Lemma 1** Let Q be a quadratic form on  $T^*\mathbb{R}^2$  with signature (+, -, -, -). The Hamiltonian linear vector field  $\mathcal{X}_Q$  associated to Q admits  $(\pm \lambda, \pm i\omega)$  with  $\lambda > 0$ ,  $\omega > 0$  as eigenvalues.

If d = 2 and

$$H_{\rm class} = \begin{pmatrix} p_1 + p_2 & p_3 + ip_4 \\ p_3 - ip_4 & p_1 - p_2 \end{pmatrix} ,$$

we define:

$$\omega_{i,j} = \{p_i, p_j\} ,$$
  

$$\Pi = \omega_{1,2}\omega_{3,4} - \omega_{1,3}\omega_{2,4} + \omega_{1,4}\omega_{2,3}$$
(1)

( $\Pi$  is the Pfaffian of the antisymmetric matrix  $(\omega_{i,j})$ ) and

$$\delta = \frac{1}{8} \text{Tr}(M^2) = \omega_{1,2}^2 + \omega_{1,3}^2 + \omega_{1,4}^2 - \omega_{2,3}^2 - \omega_{2,4}^2 - \omega_{3,4}^2 .$$

**Proposition 1** We get the following classification:

- 1. The symplectic case corresponds to  $\Pi(z_0) \neq 0$
- 2. The hyperbolic corank 2 case corresponds to the vanishing of  $\Pi$  on  $\Sigma$  near  $z_0$  and  $\delta(z_0) > 0$
- 3. The elliptic corank 2 case corresponds to the vanishing of  $\Pi$  on  $\Sigma$  near  $z_0$ and  $\delta(z_0) < 0$ .

Proof.-

A basis of the image of M is the set of Hamiltonian vector fields  $\mathcal{X}_{p_j}$ ,  $j = 1, \dots, 4$ . The restriction of  $\Omega$  to ImM admits the matrix  $(\omega_{i,j})$  in this basis. We have  $\det(\omega_{i,j}) = \Pi^2$ . This gives the first condition. The map M is given by

$$M = 2(dp_1 \otimes \mathcal{X}_{p_1} - \sum_{j=2}^4 dp_j \otimes \mathcal{X}_{p_j})$$

so that the matrix of the restriction of M to ImM is  $2(\varepsilon_{i,j}\omega_{i,j})$  with  $\varepsilon_{1,j} = 1$  and  $\varepsilon_{i,j} = -1$  if  $i \ge 2$ . In the corank 2 case, the square of any of the nonzero eigenvalues of M is then  $4\delta(z_0)$ .

*Examples* of these cases have been studied in various papers:

1. The symplectic case in [7]: it is the case where  $E.B \neq 0$  with the notations of that paper.

- 2. The hyperbolic corank 2 in Born-Oppenheimer approximation, [11], [9] and [8]. In [7], it is the case where E.B = 0 and |E| > |B|.
- 3. The case of one degree of freedom with parameters is studied in [3] (adiabatic limit, hyperbolic case) (see also [12] and [15]) and in [5] and [6] (elliptic case: band crossings).

# 2 The general strategy

We will proceed for each case along the same lines:

- 1. Reduction to a  $2 \times 2$  system. This part is always the same and is recalled in section 3
- 2. Finding a normal form for the dispersion relation: this part works by
  - Finding a "Birkhoff normal form" along the singular manifold  $\Sigma$
  - Using Sternberg's Theorem in order to get a normal form for the hyperbolic part
- 3. Using a general result stated in section 4 , we pass, using a gauge transform J, from a normal for the dispersion relation to a normal form for the dispersion matrix
- 4. In order to get the semi-classical normal form, we need to solve the following type of homological equation

$$\{S, H_0\} + C^* H_0 + H_0 C = R$$

where  $H_0$  is the classical normal form, R is given, S is an unknown real valued function and C an unknown matrix valued function. Fortunately, this equation is the linearization of the classical normal form, so that we can solve it for free!

The realization of this program is more difficult than in [2], especially in the corank 2 case which is not structurally stable.

# **3** Reduction to a $2 \times 2$ system

It is well known (see [1] or [2]) that near a point  $z_0 \in T^*\mathbb{R}^n$  such that

$$\dim \ker H_{\text{class}}(z_0) = 2 ,$$

we can split microlocally the system into a direct sum of a  $(d-2) \times (d-2)$  elliptic block and a  $2 \times 2$  block whose principal symbol vanishes at  $z_0$ .

The dispersion relations of the initial system and the small one are the same. In what follows, we will always assume that this splitting has been done and therefore we have a  $2 \times 2$  system to study.

For convenience, the transversality hypothesis  $(\star)$  has been formulated in section 1 for the big system.

# 4 A lemma about gauge transforms

The following Lemma will be used several times:

**Lemma 2** Let  $H : \mathbb{R}^4_X \times \mathbb{R}^N_\lambda \to \text{Herm}(2)$  be a smooth map such that

$$\det(H(X,\lambda)) = X_1 X_2 - (X_3^2 + X_4^2) .$$

There exist uniquely defined  $\varepsilon = \pm 1$ ,  $\alpha = \pm 1$  and a smooth germ of map  $J : \mathbb{R}^4 \times \mathbb{R}^N \to GL(2, \mathbb{C})$  such that

$$J^{\star}H(X,\lambda)J = \begin{pmatrix} \alpha X_1 & X_3 + i\varepsilon X_4 \\ X_3 - i\varepsilon X_4 & \alpha X_2 \end{pmatrix}$$

The proof follows exactly the same lines as the proof of Lemma 5 in [2].

# 5 The symplectic case

### 5.1 The normal form for the dispersion relation

**Proposition 2** Assuming (\*) and (1.) (we are in the symplectic case and both pairs of eigenvalues do not vanish), near any point  $z_0$  of the singular set  $\Sigma$ , there exists a canonical transformation  $\chi$  and two invertible positive (> 0) germs e(z) and  $b(\tau, z')$  so that:

$$\det(H_{\text{class}}) \circ \chi = e(z) \left( x_1 \xi_1 - b^2 (x_2^2 + \xi_2^2, z') (x_2^2 + \xi_2^2) \right) + O_Y(\infty)$$

where  $Y = \{x_2 = \xi_2 = 0\}, z = (x_1, \xi_1, x_2, \xi_2, z' = (x', \xi'))$  are canonical coordinates near  $0 \in T^* \mathbb{R}^n$ .

Proof.-

We start using the same kind of arguments as in the proof of Theorem 2 in [2]. We get then a (formal) Birkhoff normal form along the singular set  $\Sigma$  of the form:

$$A(x_1\xi_1, x_2^2 + \xi_2^2, z') + O_{\Sigma}(\infty)$$
,

with A a smooth function which satisfies

$$A(\tau_1, \tau_2, z') = \lambda(z')\tau_1 - \frac{\omega(z')}{2}\tau_2 + O(\tau_1^2 + \tau_2^2) .$$

There is a minus sign in front of the  $\tau_2$  term because it is the only way to get the appropriate signature (+, -, -, -) for p'' along  $\Sigma$ . Using Taylor formula, we can rewrite A as follows

$$A(\tau_1, \tau_2, z') = F(\tau_1, \tau_2, z')(\tau_1 - \tau_2 b^2(\tau_2, z')) .$$

Using Sternberg's linearization as in [2], we get the result. We use the following version of Sternberg's Theorem whose proof can be given using the same arguments as in Nelson's book [14]:

**Theorem (Sternberg)** Let X be a smooth vector field on  $T^*\mathbb{R}^n$  and  $\Sigma = \{x_1 = \xi_1 = x_2 = \xi_2 = 0\}$ . Let us assume that  $X = X_0 + X_1$  with  $X_1$  is compactly supported and  $X_1 = O_{\Sigma}(\infty)$ . We assume

$$X_0 = x_1 \partial_{x_1} - \xi_1 \partial_{\xi_1} + Y_0(x_2, \xi_2, z') ,$$

with  $Y_0$  tangent to all codimension 2 subspaces  $x_1 = a$ ,  $\xi_1 = b$ . There exists a diffeomorphism  $\chi$  which is tangent of order  $\infty$  to the identity along  $\Sigma$  such that

$$\chi^{\star}(X_0 + X_1) = X_0 + O_Y(\infty)$$
.

Moreover, if X and  $X_0$  are Hamiltonian vector fields,  $\chi$  can be choosen to be symplectic.

**Remark 1** The normal form is convergent in the case of 2 degrees of freedom and analytic data. This is implied by a result of Moser [13].

### 5.2 The gauge transform

Using Lemma 2 with  $X_1 = x_1$ ,  $X_2 = \xi_1$ ,  $X_3 = bx_2$ ,  $X_4 = b\xi_2$ , we get a gauge transform. The value of  $\alpha$  can be changed to +1 using the canonical transformation  $(x_1, \xi_1) \rightarrow (-x_1, -\xi_1)$ .

Both signs of  $\varepsilon$  in the classical normal form give non equivalent Hamiltonians. Using the notations of Equation (1) in Section 1, we have:

$$\varepsilon = \operatorname{sign}(\Pi(z_0))$$
.

So  $\varepsilon = 1$  if the orientations of the normal bundle to  $\Sigma$  given by  $dp_1 \wedge \cdots \wedge dp_4$ and  $\Omega \wedge \Omega$  are the same and  $\varepsilon = -1$  if they are not the same. It is clear that  $\varepsilon$ is invariant by gauge transform, the group  $GL(2, \mathbb{C})$  being connected. **Remark 2** We can see that in a more topological way: let us denote by  $\lambda_{-} \leq \lambda_{+}$ the eigenvalues close to 0 of the dispersion matrix. The open cones  $C_{\pm} \subset p^{-1}(0)$ which correspond respectively to  $\lambda_{-} = 0 < \lambda_{+}$  ( $\lambda_{-} < \lambda_{+} = 0$ ) are well defined near  $\Sigma$ : Morse indices differs by 1 on those cones. Moreover, both cones are oriented by p > 0. The spaces  $\{z' = \text{constant}\}$  are co-oriented by the z' symplectic structure, hence oriented. It follows that the basis of the cone  $C_{+} \cap \{z' = \text{constant}\}$  (a 2sphere) is a well defined homology class of the germ of  $C_{+}$ . Hence the polarization bundle have a well defined first Chern class on  $C_{+}$  and both signes in the normal form gives both signes in the Chern class.

### 5.3 The classical normal form

Using the previous results, we get:

**Theorem 1** We assume that  $H_{\text{class}}$  satisfies  $(\star)$  and 1. (the symplectic case). Then there exists a canonical transformation  $\chi$  and a gauge transform  $J \in GL(2, \mathbb{C})$  such that:

$$J^{\star}(H_{\text{class}} \circ \chi) J := H_{\text{symp}} + O_Y(\infty)$$

where

$$H_{\text{symp}} = \begin{pmatrix} \xi_1 & b(x_2^2 + \xi_2^2, z')(x_2 \pm i\xi_2) \\ b(x_2^2 + \xi_2^2, z')(x_2 \mp i\xi_2) & x_1 \end{pmatrix}$$

and  $b = b(x_2^2 + \xi_2^2, z') > 0$  is smooth.

## 5.4 The semi-classical normal form

**Theorem 2** We assume that  $H_{\text{class}}$  satisfies ( $\star$ ) and 1. (the symplectic case). Using FIO and gauge transform, we get the following microlocal normal form:

$$\widehat{H} = \begin{pmatrix} \widehat{\xi}_1 & \widehat{B}a \\ a^* \widehat{B}^* & x_1 \end{pmatrix} + R$$

where

- *B* is an elliptic ΨDO whose total symbol is > 0 and depends only on x<sup>2</sup><sub>2</sub>+ξ<sup>2</sup><sub>2</sub>
   and z'
- $a = x_2 \pm i\xi_2$
- The full symbol of R is flat on Y

Proof.-

Using the same method as in the proof of Theorem 3 in [2] (Lemma 4), we need to solve the following homological equation:

$$\{S, H_{\text{symp}}\} + C^{\star}H_{\text{symp}} + H_{\text{symp}}C = R$$

where R is given and S (real valued) and C (matrix valued) are unknown functions. This can be done directly by solving the normal form problem for  $H_{\text{symp}} + \varepsilon R$  which satisfy our basic hypothesis (( $\star$ ) and 2.) for all small  $\varepsilon$  (this case is *structurally stable*) and taking the first order term in  $\varepsilon$ .

### 5.5 Microlocal solutions

We will study the + case of the normal form. The - case is similar. We will see how to extend the method of [7] in order to solve the local model. We define

$$u = \sum_{j=0}^{\infty} a_j(x_1, x')\varphi_j(x_2), \ v = \sum_{j=0}^{\infty} b_j(x_1, x')\varphi_j(x_2)$$

where  $\varphi_j$  is the usual  $L^2(\mathbb{R}, dx_2)$  orthonormal basis such that  $\varphi_j = c_j \alpha^j \varphi_0$  with  $c_j > 0$ ,  $\varphi_0 = c_0 \exp(-x_2^2/2h)$  and  $\alpha = -h\partial_{x_2} + x_2$  is the creation operator.

We get the following systems, where B(j) is the pseudo-differential operator in the x' variable obtained by Weyl-quantizing the (> 0) symbol of B at the value  $x_2^2 + \xi_2^2 = (2j + 1)h$ :

$$\left(\begin{array}{cc}\frac{h}{i}\partial_{x_1}&\sqrt{2(j+1)h\widehat{B(j)}}\\\sqrt{2(j+1)h\widehat{B(j)}}&x_1\end{array}\right)\left(\begin{array}{c}a_j\\b_{j+1}\end{array}\right)=0$$

and  $b_0 = 0$ .

# 6 The corank 2 case

### 6.1 Singular perturbations and homological equations

#### 6.1.1 Introduction

The corank 2 case is more difficult, because it is not *structurally stable*: a generic perturbation of the dispersion matrix will be in the symplectic case. In the subsection 6.1.3, we will find the space of infinitesimal deformations of the corank 2 case. In the subsection 6.1.4, we will look at a Birkhoff normal form for the Taylor expansion along  $\Sigma$  of the dispersion relation. In the subsection 6.1.5 we will look at the homological equation needed for finding the semi-classical normal form.

#### **6.1.2** Singular deformations of $\Sigma$

**Definition 1** Let  $\Sigma = \{x_1 = \xi_1 = x_2 = x_3 = 0\} \subset (T^* \mathbb{R}^n, \Omega)$ . A smooth deformation  $\Sigma_{\varepsilon}$  of  $\Sigma$  is called singular if the corank of  $\Omega_{|\Sigma_{\varepsilon}}$  is constant ( $\equiv 2$ ). A deformation (F, G, A, B) given by

$$\Sigma_{\varepsilon} = \{ x_1 = \varepsilon F(\sigma), \ \xi_1 = \varepsilon G(\sigma), \ x_2 = \varepsilon A(\sigma), \ x_3 = \varepsilon B(\sigma) \mid \sigma \in \Sigma \}$$

is called infinitesimally singular if it can be modified by  $O(\varepsilon^2)$  terms so that the new deformation is singular.

Lemma 3 The space of infinitesimally singular deformations is the space

$$(F, G, \frac{\partial T}{\partial \xi_2}, \frac{\partial T}{\partial \xi_3})$$

where F, G, T are arbitrary functions on  $\Sigma$ .

Proof.-

Let us start with a singular deformation whose infinitesimal deformation is given by (F, G, A, B). We see that the pull-back of  $\Omega_{|\Sigma_{\varepsilon}}$  on  $\Sigma$  is given by:

$$\Omega_{\varepsilon} = d\xi' \wedge dx' - \varepsilon (dA \wedge d\xi_2 + dB \wedge d\xi_3) + O(\varepsilon^2)$$

We have

$$\Omega_{\varepsilon}^{n-1} = -(n-1)\varepsilon(d\xi' \wedge dx')^{n-2} \wedge (dA \wedge d\xi_2 + dB \wedge d\xi_3) + O(\varepsilon^2)$$

whose vanishing implies there exists T such that

$$A = \frac{\partial T}{\partial \xi_2}, \ B = \frac{\partial T}{\partial \xi_3}.$$

Conversely, let us start with the infinitesimal deformation given by (F, G, T). Let  $S = T + \xi_1 F - x_1 G$ . Let  $\chi_{\varepsilon}$  the flow at time  $\varepsilon$ of the Hamiltonian vector field  $\mathcal{X}_S$  generated by S. The deformation  $\Sigma_{\varepsilon} = \chi_{\varepsilon}(\Sigma)$  is singular. It is easy to check that the infinitesimal deformation associated to  $\Sigma_{\varepsilon}$  is  $(F, G, \frac{\partial T}{\partial \xi_2}, \frac{\partial T}{\partial \xi_3})$ .

#### 6.1.3 Singular perturbations of the dispersion matrix

Let us denote by  $H_{\rm hyp}$  (resp.  $H_{\rm ell}$ ) some dispersion matrices given by

$$H_{\rm hyp} = \begin{pmatrix} \xi_1 & x_2 + ix_3 \\ x_2 - ix_3 & x_1 \end{pmatrix} + O_{\Sigma}(2)$$
  
(resp.  $H_{\rm ell} = \begin{pmatrix} x_2 & x_1 + i\xi_1 \\ x_1 - i\xi_1 & x_3 \end{pmatrix} + O_{\Sigma}(2)$ ).

**Definition 2** • We say that a smooth deformation

$$H_{\varepsilon} = H_{\text{hyp}} (\text{resp. } H_{\text{ell}}) + \varepsilon K_0 + O(\varepsilon^2)$$
 (2)

is singular if it satisfies the hypothesis 2 (resp. 3) of section 1 for  $\varepsilon$  small enough.

- An infinitesimal deformation  $K_0$  is singular if it can be embedded into a smooth singular deformation
- **Lemma 4** An infinitesimal deformation  $K_0$  is singular if and only if there exists  $T: \Sigma \to \mathbb{R}$  so that

$$\left((K_0)_{1,2}\right)_{|\Sigma} = \frac{\partial T}{\partial \xi_2} + i \frac{\partial T}{\partial \xi_3}$$

• The same result holds in the elliptic case by replacing the previous condition by:

$$\begin{cases} ((K_0)_{1,1})_{|\Sigma} = \frac{\partial T}{\partial \xi_2} \\ ((K_0)_{2,2})_{|\Sigma} = \frac{\partial T}{\partial \xi_3} \end{cases}$$

Proof.-

Lemma 4 is an easy consequence of Lemma 3.

#### 6.1.4 Homological equation to high order

We will give a Lemma in the hyperbolic case, the elliptic case works similarly:

**Lemma 5** Let  $H_N$  be the space of function homogeneous of degree N w.r. to  $(x_1, \xi_1, x_2, x_3)$  and  $p_0 = x_1\xi_1 - (x_2^2 + x_3^2)$ . We can solve the following equation:

$$\{U+W, p_0\} + Vp_0 + x_3^N \tau(\sigma) = \rho + O_{\Sigma}(N+1)$$
(3)

where  $\rho \in H_N$  is given. The unknowns functions are:

- $U \in H_N$
- $W \in H_{N-1}$  an homogeneous polynomial of degree N-1 w.r. to the variables  $(x_2, x_3)$  with coefficients in  $C^{\infty}(\Sigma)$
- $V \in H_{N-2}$
- $\tau \in C^{\infty}(\Sigma)$ .

Proof.-

The proof is very close to the proof of Lemma 2 in [2]. We decompose everything into sums of monomial terms in  $(x_2, x_3)$ . At the last step, we fail to be able to solve unless we add a term  $x_3^N \tau(\sigma)$  to  $\rho$ . A bit more specifically, we decompose every function F into monomial w.r. to  $(x_2, x_3)$ :

$$F(x_1,\xi_1,x_2,\xi_2,x_3,\xi_3,z') = \sum F_{i,j}(x_1,\xi_1,\xi_2,\xi_3,z')x_2^i x_3^j$$

We then decompose equation (3) according to the powers of  $x_2^i x_3^j$  into a system of equations  $(E_{i,j})$ ,  $i + j \leq N$ . We first solve equations  $(E_{i,j})$ ,  $i + j \leq N - 1$  recursively by increasing the values of i + j:

$$(E_{i,j}) \{ U_{i,j}, x_1 \xi_1 \} = -V_{i,j} x_1 \xi_1 + \rho_{i,j} + V_{i-2,j} + V_{i,j-2}$$

by choosing  $V_{i,j}$  so that there is no resonant term (powers of  $x_1\xi_1$ ) in the righthandside.

Then we are left with the following system:

$$\begin{cases} (E_{0,N}) & -2\frac{\partial W_{0,N-1}}{\partial \xi_3} + \tau = \rho_{0,N} + V_{0,N-2} \\ (E_{1,N-1}) & -2\frac{\partial W_{0,N-1}}{\partial \xi_2} - 2\frac{\partial W_{1,N-2}}{\partial \xi_3} = \rho_{1,N-1} + V_{1,N-3} \\ \cdots & \cdots = \cdots \\ (E_{N,0}) & -2\frac{\partial W_{N-1,0}}{\partial \xi_2} = \rho_{N,0} + V_{N-2,0} \end{cases}$$

All equations involve only functions on  $\Sigma$ . We solve them recursively from the last. The first one defines  $\tau$ .

#### 6.1.5 Matrix homological equation

Lemma 6 Let us consider the homological equation

$$\{S, H_0\} + C^* H_0 + H_0 C = R + T \tag{4}$$

where R (self-adjoint) is given and S (real-valued), B, T are the unknowns.

• In the hyperbolic case  $H_0 = H_{hyp}$ , equation (4) can be solved with

$$T = i \left( \begin{array}{cc} 0 & t(x_3, \xi_2, \xi_3, z') \\ -t(x_3, \xi_2, \xi_3, z') & 0 \end{array} \right)$$

with t real valued.

• In the elliptic case  $H_0 = H_{ell}$ , equation (4) can be solved with

$$T = \left(\begin{array}{cc} 0 & 0\\ 0 & t(x_3, \xi_2, \xi_3, z') \end{array}\right)$$

with t real valued.

Proof.-

It is enough to choose T so that R + T is an infinitesimal singular deformation and to take the term in  $\varepsilon^1$  in the classical normal form result for a singular deformation  $H_{\text{hyp}} + \varepsilon(R + T) + O(\varepsilon^2)$ .

# 6.2 The normal form for the dispersion relation

**Proposition 3** Assuming ( $\star$ ) and (2.) or (3.) (we are in the case where one pair of eigenvalues does not vanish), near any point  $z_0$  of the singular set  $\Sigma$ , there exists a canonical transformation  $\chi$ , a smooth function  $a(x_3, \sigma)$  and an invertible positive germ e so that:

• In the hyperbolic case (2.):

$$\det(H_{\text{class}}) \circ \chi = e(z) \left( x_1 \xi_1 - \left( x_2^2 + x_3^2 (1 + x_3 a(x_3, \sigma))^2 \right) \right)$$

where  $z = (x_1, \xi_1, x_2, \xi_2, x_3, \xi_3, z' = (x', \xi'))$  are canonical coordinates near  $0 \in T^* \mathbb{R}^n$  and  $\sigma \in \Sigma$ .

• In the elliptic case (3.) :

$$\det(H_{\text{class}}) \circ \chi = e(z) \left( x_2 x_3 \left( 1 + x_3 a(x_3, \sigma) \right) - \left( x_1^2 + \xi_1^2 \right) \right) + O_{\Sigma}(\infty) \ .$$

The proof follows exactly the same lines as in [2].

### 6.3 The classical normal form

Using the same tools as before and [2], we get

**Theorem 3** Assuming  $(\star)$  and (2.) or (3.) (we are in the case where one pair of eigenvalues does not vanish), near any point  $z_0$  of the singular set  $\Sigma$ , there exists a canonical transformation  $\chi$ , a  $GL(2, \mathbb{C})$  valued gauge transform J(z) and a smooth real valued function  $a(x_3, \sigma)$  so that:

• In the hyperbolic case (2.):

$$J^{\star}(H_{\text{class}} \circ \chi) J = \begin{pmatrix} \xi_1 & x_2 + ix_3(1 + x_3a(x_3, \sigma)) \\ x_2 - ix_3(1 + x_3a(x_3, \sigma)) & x_1 \end{pmatrix} (= H_{\text{hyp}})$$

where  $z = (x_1, \xi_1, x_2, \xi_2, x_3, \xi_3, z' = (x', \xi'))$  are canonical coordinates near  $0 \in T^* \mathbb{R}^n$ .

• In the elliptic case (3.) :

$$J^{\star}(H_{\text{class}} \circ \chi) J = \begin{pmatrix} x_2 & x_1 + i\xi_1 \\ x_1 - i\xi_1 & x_3(1 + x_3a(x_3, \sigma)) \end{pmatrix} + O_{\Sigma}(\infty) \ (= H_{\text{ell}}) \ .$$

# 6.4 The semi-classical normal form

From the previous subsections, we deduce the following semi-classical normal forms

**Theorem 4** • In the hyperbolic case (2.):

$$\left(\begin{array}{cc}\frac{h}{i}\partial_{x_1} & x_2 + ix_3(1 + x_3a(x_3, \sigma)) + ih\gamma\\ x_2 - ix_3(1 + x_3a(x_3, \sigma)) - ih\gamma & x_1\end{array}\right)$$

where  $\gamma$  is a self-adjoint pseudo-differential operator of order 0 whose Weylsymbol is independent of  $(x_1, \xi_1, x_2)$ .

• In the elliptic case (3.) :

•

$$\begin{pmatrix} x_2 & x_1 + h\partial_{x_1} \\ x_1 - h\partial_{x_1} & x_3(1 + x_3a(x_3, \sigma)) + h\gamma \end{pmatrix} + O_{\Sigma}(\infty)$$

where  $\gamma$  is a self-adjoint pseudo-differential operator of order 0 whose Weylsymbol is independent of  $(x_1, \xi_1, x_2)$ .

The microlocal solutions of the previous models can be studied following the same lines as in [2]. The main property is that they look like:

$$\begin{pmatrix} \frac{h}{i}\frac{\partial}{\partial x_1} & Q\\ Q^{\star} & x_1 \end{pmatrix} \begin{pmatrix} u\\ v \end{pmatrix} = 0$$

where Q commutes with  $x_1$  and  $\frac{\partial}{\partial x_1}$  in the hyperbolic case

$$\begin{pmatrix} Q & x_1 + h\frac{\partial}{\partial x_1} \\ x_1 - h\frac{\partial}{\partial x_1} & R \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0$$

where Q and R commute with  $x_1$  and  $\frac{\partial}{\partial x_1}$  in the elliptic case.

# 7 One dimensional systems with parameters

## 7.1 Normal forms

In this section we will consider the case of a system

$$\widehat{H(\lambda)}\vec{U} = 0$$

where  $\widehat{H}(\lambda)$  is a  $d \times d$  self-adjoint system in one variable  $x_1$  and depending smoothly of an external parameter  $\lambda \in \mathbb{R}^N$ ,  $N \geq 2$ . Usually  $\lambda$  contains some spectral parameter.

We will assume that

- $(x_1, \xi_1, \lambda) \to H_{\text{class}}(x_1, \xi_1, \lambda)$  satisfies the transversality hypothesis (\*) of section 1 at  $(0, 0, \lambda_0)$ .
- $(x_1, \xi_1) \rightarrow \det(H_{\text{class}}(x_1, \xi_1, \lambda_0))$  admits at the origine a non degenerate critical point. We have two cases the *elliptic* one and the *hyperbolic* one.

The hyperbolic case is strongly related to [3] (see also [15]) while the elliptic normal form has been introduced as a *model* in [5] and [6]. Using the previous methods, one can show the following

**Theorem 5** • Elliptic case: near  $(0, 0, \lambda_0)$ , one can reduce the system using a  $\lambda$ -dependent gauge transform and FIO's to

$$\begin{pmatrix} a_h(\lambda) & x_1 + i\widehat{\xi}_1 \\ x_1 - i\widehat{\xi}_1 & b_h(\lambda) \end{pmatrix} \vec{U} = 0$$

 Hyperbolic case: near (0, 0, λ<sub>0</sub>), one can reduce the system using λ-dependent gauge transform and FIO's to

$$\begin{pmatrix} \widehat{\xi_1} & a_h(\lambda) \\ \overline{a_h}(\lambda) & x_1 \end{pmatrix} \vec{U} = 0$$

The proof is as follows: first apply the isochoric Morse lemma [4] to the dispersion relation. The gauge transform is obtained from Lemma 2. We can then solve the homological equation by linearization of the classical normal from.

### 7.2 Solutions of the elliptic normal form

For completness, we reproduce here the solution of the normal form in the elliptic case which is studied in [5] and [6].

We want to solve near  $(0,0) \in T^*\mathbb{R}$  the following system:

$$\begin{cases} a_h u + (x_1 + h\partial_{x_1})v = 0\\ (x_1 - h\partial_{x_1})u + b_h v = 0 \end{cases}$$

We get, using the notations of subsection 5.5:

- If  $a_h = 0$ ,  $b_h \neq 0$ , no admissible solution
- If  $b_h = 0, \ u = 0, \ v = c\varphi_0$
- If  $a_h b_h \neq 0$ ,
  - If  $a_h b_h \neq 2(n+1)h$ ,  $n \ge 0$ ,  $n \in \mathbb{N}$ , no admissible solution
  - If  $a_h b_h = 2(n+1)h$ ,  $n \ge 0$ ,  $n \in \mathbb{N}$ ,

$$u = c\varphi_n, \ v = -\frac{c\sqrt{2(n+1)h}}{b_h}\varphi_{n+1}$$

Let us assume that N = 2 and  $\lambda = (E, t)$  where E is a spectral parameter and  $\lambda_0 = (E_0, t_0)$ . We have  $a_h = f_h(E, t)$ ,  $b_h = g_h(E, t)$  where  $(E, t) \to (a_h, b_h)$ is a diffeomorphism. We assume  $\frac{\partial f_h}{\partial E} \frac{\partial g_h}{\partial E} > 0$ . Then we have a *macroscopic* (*h*independent) gap in the spectrum for  $t < t_0$  as well as for  $t > t_0$ , but we get that one eigenvalue is moving from one band to the next one as t passes through  $t_0$ (see Figure 1).

# 7.3 Hyperbolic normal form and avoided crossings

The hyperbolic case allows to recover the results of [3] (see also [12] and [15]) on the adiabatic limit. We consider a system:

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

where  $A(\lambda, t)$  is an Hermitian matrix and  $A(\lambda_0, t_0)$  admits an eigenvalue  $\lambda_0$  of multiplicity 2. The previous results apply near the point  $(t_0, \lambda_0)$  of the phase space. We can recover that way a Landau-Zener formula.



Figure 1: one eigenvalue is moving from the upper band to the lower one

# References

- P. Braam and H. Duistermaat, Normal forms of real symmetric systems with multiplicity. *Indag. Math.*, N.S., 4(4):407-421, 1993.
- [2] Y. Colin de Verdière, The level crossing problem in semi-classical analysis I. The symmetric case. Ann. Inst. Fourier (to appear), 2003.
- [3] Y. Colin de Verdière, M. Lombardi and J. Pollet, The microlocal Landau-Zener formula. Annales de l'IHP (Physique théorique), 71:95-127, 1999.
- [4] Y. Colin de Verdière and J. Vey, Le lemme de Morse isochore. Topology, 18:283-293, 1979.
- [5] F. Faure and B. Zhilinskii, Topological Chern Indices in Molecular Spectra. *Phys. Rev. Letters*, 85:960-963, 2000.
- [6] F. Faure and B. Zhilinskii, Topological properties of the Born-Oppenheimer approximation and implications for the exact spectrum. *Lett. Math. Phys.*, 55:219-239, 2001.
- [7] C. Fermanian-Kammerer, A non-commutative Landau-Zener formula. Prépublication Université de Cergy-Pontoise, 01/02:1-34, 2002.

- [8] C. Fermanian-Kammerer, Wigner measures and molecular propagation through generic energy level crossings. *Prépublication Université de Cergy-Pontoise*, 16/02:1-32, 2002.
- [9] C. Fermanian-Kammerer and P. Gérard, A Landau-Zener formula for nondegenerated involutive codimension 3 crossings, *Prépublication Université* de Cergy-Pontoise, 11/02:1-38, 2002.
- [10] W. Flynn and R. Littlejohn, Semi-classical theory of spin-orbit coupling, *Phys. Rev. A*, 45:7697-7717, 1992.
- [11] G. Hagedorn, Molecular Propagation through Electron Energy Level Crossings. *Memoirs of the AMS*, 536 (1994).
- [12] A. Joye, Proof of the Landau-Zener Formula, Asymptotic Analysis, 9:209-258, 1994.
- [13] J. Moser, On the generalization of a theorem of Liapounoff. Comm. Pure Appl. Math., 11:257-271, 1958.
- [14] E. Nelson, Topics in dynamics, I: Flows. Princeton Univ. Press (1969).
- [15] V. Rousse, Landau-Zener Transitions for Eigenvalue Avoided Crossings in the Adiabatic and Born-Oppenheimer Approximations. Archiv mp\_arc, 03-14:1-35, 2003