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THE LEVEL CROSSING PROBLEM IN SEMI-CLASSICAL ANALYSIS
I. The symmetric case

by Yves COLIN DE VERDIÈRE

Introduction.

Let us consider a $d \times d$ self-adjoint system of semi-classical pseudo-differential operators $\widehat{H}\vec{U} = 0$ in $\mathbb{R}^n$. Many examples occur in physics: let us mention the *Born-Oppenheimer approximation* in molecular physics (see [5], [14], [15], [40] and [31]), the *Maxwell equations* for electromagnetic waves in a non homogeneous and anisotropic medium (see [41]), the *propagation of elastic waves in anisotropic media* (see [36]), the *propagation of waves in oceans* (see [35] and [49]), the *spin-orbit interaction* (see [25] and, for a global and geometrical point of view, [19] and [20]). The principal symbol H_{class} of $\widehat{H}$ is a matrix valued function on the phase space $T^\star\mathbb{R}^n$, often called the *dispersion matrix* by physicists. The ideal generated by $\det(H_{\mathrm{class}})$ is called the *dispersion relation.*

Near a *generic point* of the phase space where the principal symbol H_{class} is not invertible, the associated eigenspace $\ker(H_{\mathrm{class}})$ (the *polarization bundle*) is one dimensional and the system reduces mod $O(h^\infty)$ to a scalar one. The principal part of the solution is polarized meaning that it takes values into the polarization bundle. For a precise description of the WKB states in this case, see the nice paper [18].

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An interesting problem, often called the *Mode Conversion* problem (see [24]), is to describe what happens at points where the dimension of $\ker H_{\rm class}$ jumps due to eigenvalues crossings of the dispersion matrix. For the Maxwell equations, the fibers of the zero set of the dispersion relation $\{\xi \in \mathbb{R}^3 \mid \det(H_{\rm class})(x_0, \xi) = 0\}$ are called the *Fresnel surfaces* which in the generic case turn out to have 4 singular points (x_0, ξ_j) where the kernel of $H_{\rm class}(x_0, \xi_j)$ is of dimension 2 (see [41]) and hence the polarization bundle is no more a bundle there. For the elastic waves, the singular set is called *acoustic axis* in [36].

Of course the general situation is very complicated to describe, so that people try to understand the *generic* case. One expect that two zero eigenvalues cross along a submanifold Σ of the phase space of codimension 3 (resp. 4) in the real symmetric (resp. complex Hermitian) case after [50] (see also [9]). But not all submanifolds of a given codimension are equivalent in a symplectic manifold, even locally: restricted to a generic manifold of codimension 3 a symplectic form admits a kernel of dimension 1, while a generic manifold of codimension 4 is symplectic. Near a point where $\dim(\ker H_{\rm class}) = 2$, the system splits into a direct sum of a 2×2 system and a $(d-2) \times (d-2)$ elliptic system. So we need only to study 2×2 systems near points where the dispersion matrix $H_{\rm class}$ vanishes in a generic way.

G. Hagedorn studied this problem for the Born-Oppenheimer approximation in several papers starting with [30] (see also [33] and [34]) by the so-called *matching method* which consists in giving an Ansatz for the states near Σ and to match this Ansatz with the WKB Ansatz in some h-dependent small domain around Σ. The matching method is very difficult to implement and for that reason it is tempting to find another method based on normal forms where we allow both canonical diffeomorphisms in the phase space and gauge transforms in $\mathbb{C}^d$.

In the paper [7], Peter Braam and Hans Duistermaat found a *formal normal form* for the principal symbol of a 2×2 symmetric system near a generic crossing of the eigenvalues. In this normal form, the dispersion matrix is linear w.r.t. to phase space coordinates and is in fact closely related to the model introduced first by Landau [42], [43], p. 381–390 and Zener [52].

In the present paper, we will derive, in the hyperbolic case, a *local normal form* for the principal symbol. Our method, which is quite different from that of [7], is to derive first a normal form for the determinant of the system (the *dispersion relation*), which gives the classical dynamics, up to time reparametrization, using the tool of *wave operators* introduced by E. Nelson [47] in his proof of Sternberg's linearization theorem. This is closely related to Arnold's result [3]. We can then proceed by choosing the gauge transform. After that, the semi-classical microlocal normal form is easy to derive.

From this normal form, we can easily study the microlocal solutions of our system following the same kind of argument as in [11]: the solutions of the normal form are explicit functions. Performing a gauge transform and a Fourier integral operator gives the Mode Conversion rules. This way we derive geometric constructions of the principal symbols of generic Lagrangian solutions and Hagedorn's results [30] for the propagation of coherent states. We give an explicit description of the transmission rules for the principal symbols. These rules give the "Mode Conversion". We describe in particular the following solutions:

- If the incoming state is a WKB-Lagrangian state associated to one eigenvalue and a *generic Lagrangian manifold*, the outgoing state corresponding to the other eigenvalue is a *Gaussian coherent state.*

- If the incoming state is a *Gaussian coherent state* associated to one eigenvalue, the outgoing state splits into 2 parts: the part corresponding to the same eigenvalue is a *non Gaussian coherent state*, while the part corresponding to the other eigenvalue is a *Gaussian coherent state.* This case allows to recover Hagedorn's results [30].

We give precise geometrical rules for the computation of the principal symbols.

An Appendix on *semi-classical coherent states* has been written, because there are several definitions in the literature and we have here an example of coexistence of Gaussian and non Gaussian coherent states. Moreover, we wanted to clarify the behaviour of Gaussian coherent states w.r. to Fourier Integral Operators. The starting point will be the paper [29] by V. Guillemin (see also [6]): we give a short description of the construction of the "semi-classical" symplectic spinors which are easily guessed from Guillemin's "homogeneous" symplectic spinors or Boutet's "Hermite operators" (see [6]).

It seems also to be possible to extend to this case the results of P. Gérard, C. Fermanian-Kammerer and C. Lasser (see [27], [21], [22] and [23]) on the propagation of the associated semi-classical measures: their results mainly depend on a normal form, for more particular Hamiltonians, which is very close to ours.

More general type of crossings could be studied using the same tools: the main hypothesis is the hyperbolicity of the transversal dynamics. We describe also the elliptic case where only a formal normal form is found which allows to describe the coherent states remaining close to the singular part of the characteristic manifold.

Finally, we describe briefly the case of a complex Hermitian principal symbol. This case will be the subject of another publication [10]. Many authors have recently studied this problem: a (non complete) list is [4], [18], [24], [27], [28], [23], [37], [30], [33], [34], [17], [38] and [48].

1. The general setting.

Let $\widehat{H}\vec{U} = O(h^\infty)$ be a $d \times d$ self-adjoint system of (semi-classical) pseudo-differential equations of order 0 on $\mathbb{R}^n$. Our study will be microlocal in $T^\star\mathbb{R}^n$, so we will always reduce to some neighbourhood of $z_0 \in T^\star\mathbb{R}^n$. H_{class}, the principal symbol of $\widehat{H}$, is assumed to be *real valued* and hence symmetric. We will reformulate Braam-Duistermaat's analysis in [7] in the semi-classical context.

Our basic assumptions are:

(H1) *If* $E_0 = \ker H_{\text{class}}(z_0)$, *we have* $\dim E_0 = 2$.

(H2) *Topological hypothesis*: *the mapping* $z \mapsto H_{\text{class}}(z)$ *is transversal at the point* z_0 *to the codimension 3 submanifold*

$$W_2 \subset \text{Sym}(\mathbb{R}^d), \quad W_2 = \{A \mid \dim\ker A = 2\}.$$

This condition is equivalent to $\delta z \mapsto \langle \delta H_{\text{class}}\cdot \mid .\rangle_{|E_0}$ *is a surjective mapping.*

(H3) *Dynamical hypothesis*: *if* $p = \det(H_{\text{class}})$, *the Hamiltonian vector field* $\mathcal{X}_p$ *of* p *vanishes at* z_0 *and its linearization admits a pair of non zero real eigenvalues* $\pm\lambda$.

It implies that $\Sigma = \{z \mid \dim\ker H_{\text{class}} = 2\}$ is a submanifold of codimension 3 of $T^\star\mathbb{R}^n$ on which the symplectic form ω admits a kernel (the characterictic foliation) of dimension 1.

If $d = 2$, we can write H_{class} as

$$H_{\text{class}} = \begin{pmatrix} q+r & s \\ s & q-r \end{pmatrix}. \tag{1}$$

Our assumptions can be rewritten as follows:

(i) $q(0,0) = r(0,0) = s(0,0) = 0$;

(ii) the differentials $\mathrm{d}q$, $\mathrm{d}r$, $\mathrm{d}s$ are linearly independent at the origin;

(iii) the Poisson brackets satisfy $\{q,r\}^2 + \{q,s\}^2 - \{r,s\}^2 > 0$.

LEMMA 1. — *The previous assumptions are* structurally stable. *More precisely, if H_{class} satisfies* (H1), (H2) *and* (H3) *at the point z_0, and $K : T^\star R^n \to \mathrm{Sym}(\mathbb{R}^d)$ is a smooth map, $H_{\text{class}} + \varepsilon K$ satisfies the same hypothesis at some point $z(\varepsilon)$ close to z_0 for ε small enough.*

The generic case includes also the *elliptic case* where the pair of non zero eigenvalues is purely imaginary, see [7].

Property (H2) says that Σ is a smooth submanifold of codimension 3. Let us denote by M the linearization of $\mathcal{X}_p$ at the point z_0.

Because M is of rank 3, M admits an hyperbolic block and a 2-dimensional non trivial Jordan block with 0 as eigenvalue and hence the following linear symplectic normal form at each point of Σ:

$$M = \begin{pmatrix} \begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix} & 0 & 0 \\ 0 & \begin{pmatrix} 0 & 0 \\ 2\lambda & 0 \end{pmatrix} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{2}$$

with $\lambda > 0$. The linear vector field defined by M is the Hamiltonian vector field of the quadratic form $\lambda(x_1\xi_1 - x_2^2)$. In general, the Jordan block could have ± 1 as entries, but here the $+$ sign is forced by the signature $(+,-,-,0,\dots,0)$ of p'' at the points of Σ.

2. Examples.

2.1. Born-Oppenheimer approximation (stationary case).

If

$$\widehat{H} = \widehat{S} \otimes \mathrm{Id} + V(x) \tag{3}$$

where $\widehat{S} = -h^2\Delta_g - E$ is the free stationary Schrödinger equation in $\mathbb{R}^n$ and V is a symmetric $d \times d$ matrix potential which admits a generic crossing of two eigenvalues along a codimension 2 submanifold S in $\mathbb{R}^n$, the previous assumptions are satisfied at the point (x_0, ξ_0), where $x_0 \in S$ and $E - \|\xi_0\|^2$ is the degenerate eigenvalue of $V(x_0)$, if and only if the velocity $2\xi_0\partial_x$ is transversal to S at the point x_0.

2.2. Born-Oppenheimer approximation (time dependent case).

We can also apply our results to the time dependent Schrödinger equation

$$\widehat{H} = \widehat{S} \otimes \mathrm{Id} + V(x,t) \tag{4}$$

where $\widehat{S} = ih\partial_t - h^2\Delta_g$ and V is a symmetric $d \times d$ matrix potential which admits a generic crossing of two eigenvalues along a codimension 2 manifold $S \subset \mathbb{R} \times \mathbb{R}^n$. The previous hypothesis are satisfied at the point $(t_0, \tau_0, x_0, \xi_0)$ if $(t_0, x_0) \in S$, $\tau_0 - \|\xi_0\|^2$ is the degenerate eigenvalue of $V(x_0, t_0)) = 0$ and the vector field $-\partial_t + 2\xi_0\partial_x$ is transversal to S at the point (t_0, x_0).

2.3. Adiabatic limit with extra parameters.

This example is very close to the case studied in our paper [11]. Let us consider the following adiabatic evolution problem:

$$\frac{1}{i}\frac{\mathrm{d}u}{\mathrm{d}\theta} = A(x, \varepsilon\theta)u$$

where $A(x,t)$ is a $d \times d$ real symmetric matrix.

Here x is a real extra parameter close to 0. The goal is to get uniform estimates w.r. to the small parameters ε and x We can transform this equation into a semi-classical problem: by putting $t = \varepsilon\theta$, we get

$$\frac{\varepsilon}{i}\frac{\mathrm{d}u}{\mathrm{d}t} = A(x,t)u$$

where ε is the semi-classical parameter. The principal symbol is $A(x,t) - \tau\mathrm{Id}$. The hypothesis are fulfilled at the point $(0, t_0, \xi_0, \tau_0)$ if and only if $\dim\ker(A(0,t_0) - \tau_0\,\mathrm{Id}) = 2$ and $(x,t,\tau) \mapsto A(x,t) - \tau\,\mathrm{Id}$ is transversal to W_2 at that point.

2.4. Maxwell equations.

We consider the stationary Maxwell equations for an electromagnetic field inside a non homogeneous and non isotropic medium (see [41]). In this case the semi-classical regime is the high frequency regime and the corresponding geometry is the geometrical optic. Let us give a *dielectric tensor* $\varepsilon(x)$ (a Riemannian metric on $\mathbb{R}^3$), $\mu(x)$ the magnetic permeability tensor and $c = 1$ the light velocity, we get the following dispersion matrix (see [41]):

$$M_{\text{class}} = \begin{pmatrix} \mu(x)\tau & \begin{pmatrix} 0 & -\xi_3 & \xi_2 \\ \xi_3 & 0 & -\xi_1 \\ -\xi_2 & \xi_1 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & \xi_3 & -\xi_2 \\ -\xi_3 & 0 & \xi_1 \\ \xi_2 & -\xi_1 & 0 \end{pmatrix} & \varepsilon(x)\tau \end{pmatrix}$$

Generically Σ consists of 4 branches $(t, x; \tau, \pm\tau\xi_j(x)), j = 1, 2$. The algebraic surfaces $p(0, x_0; 1, \xi) = 0$ are called the *Fresnel surfaces*. It is proven in [7], that the hyperbolic case as well as the elliptic case can occur.

2.5. Acoustical waves.

We consider the propagation of acoustical waves in elastic media. The dispersion matrix is given by

$$D(x, \xi) = \rho(x)\,\mathrm{Id} - C(x, \xi)$$

where $\rho(x) > 0$ is the density and $\xi \to C(x, \xi)$, the *elastic tensor*, is a quadratic map on $\mathbb{R}^3$ with values in the positive definite symmetric 3×3 matrices. In this case they are at most 16 singular points on $\det(D(x_0, .)) = 0$ (see [36]). They can be elliptic or hyperbolic (see [7]).

2.6. Oceanography.

The mode conversion problem has also been considered in oceanography, see [35], [49].

2.7. The Landau-Zener model.

We denote by

$$\widehat{H_0} = \begin{pmatrix} D_1 & x_2 \\ x_2 & x_1 \end{pmatrix}$$

with $D_1 = (h/i)\,\partial/\partial x_1$ and by

$$H_0 = \begin{pmatrix} \xi_1 & x_2 \\ x_2 & x_1 \end{pmatrix}$$

its Weyl symbol. Hypothesis (H1), (H2) and (H3) are satisfied at the points $x_1 = x_2 = \xi_1 = 0$.

The system $\widehat{H_0}$, which is closely related to the case computed by Landau and Zener, will be our local model.

It will be usefull to denote by $\mathcal{X}_p$ (resp. $\mathcal{X}_0$) the Hamiltonian vector field of p (resp. $p_0 = x_1\xi_1 - x_2^2$). We have:

$$\mathcal{X}_0 = x_1\partial_{x_1} - \xi_1\partial_{\xi_1} + 2x_2\partial_{\xi_2}.$$

2.8. Avoided crossings.

Let us assume that our system $\widehat{H}u = 0$ depends on a real parameter a. We can add a as another coordinate (like some x_{n+1}) and we assume that the new system satisfies our hypothesis (H1), (H2) and (H3). Then we get the normal form $\widehat{H_0}$ and the operator $\hat{a}$ (multiplication by a) commute with it. So we see that the Weyl symbol of $\hat{a}$ is a function of (x_2, x', ξ'). If we assume moreover that $\partial a/\partial x_2 \neq 0$, we can recover x_2 as a function of (a, x', ξ') so that we get a normal form

$$\widehat{H}_a = \begin{pmatrix} \widehat{\xi_1} & P_a \\ P_a^t & x_1 \end{pmatrix}$$

where P_a is an a-dependent pseudo-differential operator w.r.t. to x' only. This way, we see how to recover the results of [33] and [34].

3. Reduction of high dimensional systems to two dimensional systems.

Let us consider a $d \times d$ symmetric matrix of pseudo-differential operators $\widehat{H}$ and assume that its principal symbol $H_{\text{class}}(0)$ at some point 0 is singular with a kernel of dimension 2. Then it is well-known that we can find an invertible matrix A of pseudo-differential operators such that $A^t\widehat{H}A$ splits mod $O(h^\infty)$ into a direct sum of a 2×2 symmetric system $\widehat{H_1}$ whose principal symbol vanishes at the point 0 and a $(d-2) \times (d-2)$ system $\widehat{H_2}$ which is invertible at the point 0 (see for example [7] and [18]).

Hence, we will work in what follows with a 2×2 *system.*

We will derive a semi-classical normal form in the following way: we first work on the classical level where we give a refined version of the Braam-Duistermaat normal form. We then proceed on the semi-classical level.

4. Some notations.

Our canonical coordinates will be $(x_1, \xi_1; x_2, \xi_2; x', \xi')$ with

$$\omega = \mathrm{d}\xi_1 \wedge \mathrm{d}x_1 + \mathrm{d}\xi_2 \wedge \mathrm{d}x_2 + \cdots .$$

The associated Poisson bracket will be denoted by $\{.,.\}$: if $\mathcal{X}_f$ is defined by $\iota(\mathcal{X}_f)\omega = -\mathrm{d}f$, $\{f,g\} = \mathcal{X}_f(g)$. We will denote by Z the hyperplane

$\{x_2 = 0\}$, by Y the subspace $Y = \{x_1 = \xi_1 = 0\}$ and by Σ their intersection

$$\Sigma = Y \cap Z = \{x_1 = \xi_1 = x_2 = 0\}.$$

This notation could seem to be confusing, but this Σ is the previous Σ for the Landau-Zener model.

For $n \in \mathbb{N} \cup \infty$, $f = O_V(n)$ means that f is of order n transversally to the submanifold V, i.e., the Taylor expansion of f starts with terms of degree $\geq n$ along V.

Let us denote by H_N the space of smooth functions of (x, ξ) which are homogeneous polynomials of degree N w.r. to (x_1, ξ_1, x_2).

5. The cohomological equation.

We will need the following lemma:

LEMMA 2. — *Let $p_0 = x_1\xi_1 - x_2^2$ and $\rho \in H_N$. The following equation:*

$$\{U, p_0\} + V p_0 = \rho + O_\Sigma(N+1) \tag{5}$$

admits a solution (U, V) with $U \in \widetilde{H}_N = H_N \oplus C^\infty(\Sigma) x_2^{N-1}$ and $V \in H_{N-2}$.

Proof. — We expand U, V and ρ as polynomials in x_2: $U = \sum_{j=0}^{N-1} U_j x_2^j$ with $U_j \in H_{N-j}$ for $j \leq N-2$ and $U_{N-1} = U' + U''$ with $U' \in H_1$ and $U'' \in C^\infty(\Sigma)$, $V = \sum_{j=0}^{N-2} V_j x_2^j$ with $V_j \in H_{N-j-2}$ and $\rho = \sum_{j=0}^{N} \rho_j x_2^j$ with $\rho_j \in H_{N-j}$, we get the following equations:

• If $0 \leq j \leq N-1$:

$$\{U_j, x_1\xi_1\} + V_j x_1 \xi_1 = \rho_j + V_{j-2}, \tag{$\star j$}$$

where $V_{-1} = V_0 := 0$;

• and:

$$0 = \rho_N + V_{N-2} + 2\frac{\partial U''}{\partial \xi_2}\cdot \tag{$\star N$}$$

Equation $(\star j), j \leq N-1$, can be solved by choosing V_j so that $\rho_j + V_{j-2} - V_j x_1 \xi_1$ admits no "resonant term", i.e., no terms $(x_1\xi_1)^{\frac{1}{2}j}$. Equation $(\star N)$ gives U''. □

6. Finding a gauge transform.

LEMMA 3. — *We define* $z_1 = (x_1, \xi_1)$. *If* $L : \mathbb{R}^3_{z_1,x_2} \to \mathrm{Sym}_2(\mathbb{R})$ *is a linear map such that* $\det(L(z_1,x_2)) = x_1\xi_1 - x_2^2$, *there exists a constant invertible matrix* A *such that* $A^t L(z_1,x_2)A = H_0(\pm z_1, x_2)$.

Proof. — We first restrict to $x_2 = 0$. We put $L = x_1q_1+\xi_1q_2+x_2q_3$ with fixed quadratic forms q_j. We have $\det(q_1) = \det(q_2) = 0$ and $q_1 \neq 0, q_2 \neq 0$. The kernel of q_1 is generated by V_1 and the kernel of q_2 by V_2. (V_1, V_2) are independent because q_1 and q_2 are linearly independent (otherwise $\det(x_1q_1 + \xi_1q_2) = 0$). We can assume that $q_1(V_2) = q_2(V_1) = \pm 1$ (both have the same sign because of the value of the determinant of $L(z_1, 0)$). Hence, by choosing the basis (V_2, V_1), we get

$$L(z_1, 0) = \pm\begin{pmatrix} \xi_1 & 0 \\ 0 & x_1 \end{pmatrix}.$$

We have now $L(z_1, x_2) = H_0(\pm z_1, 0) + x_2M$ and by identification of the determinants we get $L(z_1, x_2) = H_0(\pm z_1, \pm x_2)$. It is easy to change $-x_2$ into $+x_2$ by using the gauge transform $(u, v) \mapsto (u, -v)$. □

LEMMA 4. — *Let* $H = H_0+O_\Sigma(2)$ *and assume that* $\det(H) = \det(H_0)$. *Then there exists a smooth map* $x \mapsto A(x)$ *defined in some neighbourhood of* Σ *such that*

$$A^tHA = H_0.$$

The same result holds in the real analytic and in the formal series settings.

Proof. — We will use Moser's path method.

1) Let us first construct a path $H_\tau, 0 \le \tau \le 1$, from H_0 to H with $\det(H_\tau) = \det(H_0)$. Let $H = H_0 + K$ where $K = O_\Sigma(2)$ and $\widetilde{H_\tau} = H_0 + \tau K, 0 \le \tau \le 1$. We have only $\det(\widetilde{H_\tau}) = \det(H_0) + O_\Sigma(3)$. Using the Morse-Bott Lemma to the function $\det(\widetilde{H_\tau})$, we can find a smooth family of diffeomorphisms $\varphi_\tau(x, \xi) = (x, \xi) + O_\Sigma(2)$ with $\varphi_0 = \varphi_1 = \mathrm{Id}$ such that

$$\det(\widetilde{H_\tau}) \circ \varphi_\tau = \det(H_0).$$

We define

$$H_\tau(x, \xi) = \widetilde{H_\tau}(\varphi_\tau(x, \xi)).$$

We have now $\det(H_\tau) = \det(H_0)$ and $H_\tau = H_0 + O_\Sigma(2)$. We put

$$H_\tau = \begin{pmatrix} \Xi_1 & X_2 \\ X_2 & X_1 \end{pmatrix}$$

and let

$$D_\tau = \frac{\mathrm{d}}{\mathrm{d}t} H_\tau = -\begin{pmatrix} r & s \\ s & u \end{pmatrix}.$$

From $\det(H_\tau) = \det(H_0)$, we get

$$u\Xi_1 + rX_1 - 2sX_2 = 0. \tag{6}$$

2) Let us solve the following linear equation:

$$B^t H_\tau + H_\tau B = -D_\tau$$

with $B = O_\Sigma(1)$ and $\mathrm{Tr}(B) = 0$. We put $B = \left(\begin{smallmatrix} a & b \\ c & -a \end{smallmatrix}\right)$. We get the following system of equations:

(i) $2(a\Xi_1 + cX_2) = r$,

(ii) $2(bX_2 - aX_1) = u$,

(iii) $cX_1 + b\Xi_1 = s$.

From equation (6), we get that

$$(\Xi_1 = X_2 = 0) \implies (r = 0),$$
$$(X_1 = X_2 = 0) \implies (u = 0).$$

So there are smooth functions a, c, b', a', such that

$$r = 2(a\Xi_1 + cX_2), u = 2(b'X_2 - a'X_1).$$

Then equation (6) implies $a - a' = \omega X_2$ for some smooth function ω, so, if we define $b = b' + \omega X_1$, we get equation (ii). Equation (iii) is then fulfilled from equation (6). All previous arguments work smoothly with respect to τ.

3) The path method works now as follows: we try to find A_τ such that $A_\tau^t H_\tau A_\tau = H_0$. Taking the derivative and putting $\mathrm{d}A_\tau / \mathrm{d}\tau = B_\tau A_\tau$, we get:

$$B_\tau^t H_\tau + H_\tau B_\tau = -D_\tau$$

which we have already solved with $\mathrm{Tr}(B_\tau) = 0$. □

7. The classical normal form.

7.1. Nelson's result.

For convenience, we recall here an adapted version of the statement of Theorem 8, p. 46 of [47]:

THEOREM 1 (Sternberg's theorem). — *Let X be a smooth vector field on $\mathbb{R}^s$, with $X(0)=0$. Let $X_0 x = DX(0)x$ be the linear part of X at the origin, let $U(t)$ and $U_0(t)$ be the flows generated by X and X_0, and define $X = X_0 + X_1$. We assume that X_1 is compactly supported. Suppose there is a linear subspace N, invariant under X_0, such that $X_1 = O_N(\infty)$. Let*

$$E = \left\{x \in \mathbb{R}^s \mid \lim_{t\to+\infty} \|U_0(t)x - N\| = 0\right\}.$$

Then, for all $j \in \mathbb{N}$ and $x \in E$, $D^j\left(U(-t)U_0(t)\right)x$ converges as $t \to +\infty$ and the limit $W_-(x)(x \in E)$ has a smooth extension G to $\mathbb{R}^s$ such that $G - \mathrm{Id} = O_N(\infty)$ and such that $(G^{-1})_\star X - X_0 = O_E(\infty)$.

Moreover, if X and X_0 are Hamiltonian vector fields, G can be chosen to be symplectic.

7.2. Classical normal form.

THEOREM 2. — *Assuming hypothesis* (H1), (H2) *and* (H3) *of Section* 1, *there exists a germ of canonical transformation $\chi : (T^\star\mathbb{R}^n, 0) \to (T^\star X, z_0)$ and a germ of map $(x,\xi) \mapsto A(x,\xi) \in \mathrm{GL}(d,\mathbb{R})$ at the origin, such that*

$$(A^t H_{\text{class}} A)\circ\chi = \begin{pmatrix} \begin{pmatrix} \xi_1 & x_2 \\ x_2 & x_1 \end{pmatrix} & 0 \\ 0 & K \end{pmatrix}, \tag{7}$$

with K invertible.

The normal form is *local* while in [7] it was only *formal* along the codimension 3 subspace $\Sigma = \{x_1 = \xi_1 = x_2 = 0\}$.

Proof. — Let f and g germs of function near the origin, we will denote $f \sim g$ if there exists a (germ of) canonical transformation χ and a (germ of) non vanishing positive function e such that $f\circ\chi = eg$. Same notation for matrix valued germs by allowing gauge transformations: if H, K are germs of matrix valued maps, we denote $H \sim K$ if there exist a canonical transformation χ and an invertible matrix valued function A such that $H\circ\chi = A^t K A$. This implies $\det(H) \sim \det(K)$ as germs of functions.

The proof splits into several steps. The idea is to start finding a normal form for the ideal generated by the determinant p (the dispersion relation).

1) Assuming hypothesis (H1), (H2) and (H3), we prove first $p \sim p_0 + O_\Sigma(3)$.

Let us denote by M_σ the linearized vector field of $\mathcal{X}_p$ at the point $\sigma \in \Sigma$ and by $\pm\lambda(\sigma), \lambda(\sigma) > 0$ the non zero eigenvalues of M_σ. Using our hypothesis on p, we choose vectors $e_2, f_2 \in T_\sigma T^\star\mathbb{R}^n$ so that $\omega(f_2, e_2) = 1, M_\sigma f_2 = 0, M_\sigma e_2 = \lambda(\sigma) f_2$. There exist local coordinates (ξ_2, x', ξ') on Σ so that $f_2 = \partial_{\xi_2}$ and $\omega_{|\Sigma} = \mathrm{d}\xi' \wedge \mathrm{d}x'$. We extend these coordinates to $T_\Sigma T^\star\mathbb{R}^n$ by choosing $e_1, f_1 \in T_\sigma T^\star\mathbb{R}^n$ so that $M_\sigma e_1 = \lambda(\sigma)e_1$, $M_\sigma f_1 = -\lambda(\sigma) f_1$ and $\omega = f_1^\star \wedge e_1^\star + f_2^\star \wedge e_2^\star + \mathrm{d}\xi' \wedge \mathrm{d}x'$. Applying Weinstein's theorem (see [51], Thm. 4.1), these coordinates can be extended to symplectic coordinates near Σ. We have then clearly $p = \lambda(\sigma)(x_1\xi_1 - x_2^2) + O_\Sigma(3)$.

We remark for later use that x_2 is uniquely defined up to $\pm$ mod $O_\Sigma(2)$ (look at the Hamiltonian vector field of x_2 on Σ).

2) This part is a Birkhoff type normal form transversally to Σ. Using Lemma 2 in order to solve the cohomological equation, we prove that $p \sim p_0 + O_\Sigma(\infty)$: if we assume $p = p_0 + r_N$ where $r_N = O_\Sigma(N)$ and $N \geq 3$, we use χ_N which is the time 1 flow of an Hamiltonian $U \in \widetilde{H}_N$ and $e = 1 - V$ with $V \in H_{N-2}$. We want to solve

$$(p_0 + r_N) \circ \chi_N = (1 - V)p_0 + O_\Sigma(N+1).$$

It is enough to solve

$$\{U, p_0\} + Vp_0 = -r_N + O_\Sigma(N+1)$$

using Lemma 2. We get a new remainder term $r_{N+1} = O_\Sigma(N+1)$ and we proceed by induction. We need the elementary observation that $\{\widetilde{H}_N, p_0\} \subset H_N$ in order to see that higher order terms in $p_0 \circ \chi_N$ like

$$\{U, \{U, \dots, \{U, p_0\}, \dots\}\}$$

with # of brackets ≥ 2 are in $O_\Sigma(N+1)$.(1)

(1) Let us remark that the conclusion of this step is already a corollary of the main result of [7].

3) We want to prove that $p \sim p_0 + O_Y(\infty)$. We have already $p = p_0 + O_\Sigma(\infty)$. Let $\psi : T^\star\mathbb{R}^n \to [0,1]$ a function which is homogeneous of degree 0 w.r. to (x_1, ξ_1, x_2), vanishes in a conical neighbourhood of the cone $p_0 = 0$, is 1 in some conical neighbourhood of Y and the restriction of which to the unit sphere is smooth. We define e as follows:

$$e = (1-\psi) + \psi \frac{p}{p_0} \cdot$$

One can check that e is smooth and non vanishing near Σ and we have $p = ep_0 + O_Y(\infty)$.

4) We use Nelson's Theorem 8 (p. 46 of [47]) (see also Subsection 7.1):

• With "X_0" $= \mathcal{X}_{p_0}$, "X" $= \mathcal{X}_p$, where $p - p_0 = O_Y(\infty)$ and $p - p_0$ compactly supported, and "N" $= Y$. We get $p \sim p_0 + O_{\{x_1=0\}}(\infty)$.

• With "X_0" $= -\mathcal{X}_{p_0}$, "X" $= -\mathcal{X}_p$, where $p - p_0 = O_{\{x_1=0\}}(\infty)$ and $p - p_0$ compactly supported, and "N" $= \{x_1 = 0\}$. We get conjugacy of flows.

5) We reduce to the 2 dimensional case and we show that by gauge transform $H_{\text{class}} \sim H_0 + O_\Sigma(2)$. This is based on Lemma 3.

We can assume the plus sign in the normal form of Lemma 3 by using the canonical transformation $(z_1, x_2, \xi_2, x', \xi') \to (\pm z_1, x_2, \xi_2, x', \xi')$.

6) We now apply Lemma 4. □

From the previous normal form, we can deduce some geometrical properties: the dynamics of $\mathcal{X}$ admits the codimension 3 submanifold Σ as a singular manifold, Σ admits smooth unstable (resp. stable) manifold Σ_- (resp. Σ_+) which are of codimension 2 and both included into a smooth codimension 1 invariant manifold.

8. Matrix valued cohomological equation.

Lemma 5. — *Let* $R = R_1 + iR_2 : T^\star\mathbb{R}^2 \to \text{Herm}(2 \times 2)$ *such that* $(R_2)_{|\Sigma} = 0$, *there exist smooth functions* $S : T^\star\mathbb{R}^2 \to \mathbb{R}$ *and* $A : T^\star\mathbb{R}^2 \to \text{Mat}_2(\mathbb{C})$ *such that*

$$\{S, H_0\} + A^\star H_0 + H_0 A = R.$$

Proof. — • Splitting $A = A_1 + iA_2$, we get the equations

$$\{S, H_0\} + A_1^t H_0 + H_0 A_1 = R_1 \tag{8}$$

where R_1 is real symmetric, and

$$-A_2^t H_0 + H_0 A_2 = R_2 \tag{9}$$

where R_2 is real and antisymmetric. Equation (9) is easily solved, using the hypothesis $(R_2)_{|\Sigma} = 0$, by Taylor formula.

• Equation (8) is the linearisation of our classical normal form problem. In order to solve it it is enough to solve the classical normal form problem using Theorem 2 for $H_{\text{class}} + tR_1$ smoothly w.r. to t, using Lemma 1, and to take the derivative w.r. to t at $t = 0$. □

9. The semi-classical normal form.

We have the following normal form:

THEOREM 3. — *Under the assumptions* (H1), (H2) *and* (H3) *of Section* 1, *there exist a Fourier integral operator, microlocally unitary,* U, *a symbol of order* 0 *denoted by* $A_h : T^\star R^n \to \mathrm{GL}(d, \mathbb{C})$ (a gauge transform), *and a real valued symbol denoted*

$$\gamma(h) \sim \sum_{j=0}^{\infty} \gamma_j(\xi_2, x', \xi') h^j$$

(*called* the minimal gap) *such that*

$$U^\star \widehat{A_h}^\star \widehat{H} \widehat{A_h} U = \begin{pmatrix} \widehat{H_0} + ih\widehat{\gamma(h)} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & 0 \\ 0 & \widehat{K} \end{pmatrix} + O(h^\infty)$$

with $\widehat{K}$ *elliptic.*

The 2×2 *submatrix of the previous normal form can be written* (weak normal form) *as follows:*

$$\begin{pmatrix} \widehat{\xi_1} & P \\ P^\star & x_1 \end{pmatrix}$$

with P *commuting with the diagonal terms and* $P = x_2 + O(h)$.

Proof. — Using Section 3, we reduce to $d = 2$. Using the classical normal form of Theorem 2 and Egorov theorem, we reduce the system to $\widehat{H_0} + h\widehat{R}$ where $\widehat{R}$ is self-adjoint of order 0. We normalize the next terms (transport equations) by using Lemma 5. □

QUESTION. — It would be nice to know what kind of semi-classical hypothesis do imply that γ vanishes. For example, what happens in the Born-Oppenheimer case?

10. Microlocal description of the solutions of the normal form.

We will assume in this section that $\widehat{\gamma(h)} = 0$. The result can be extended to the general case using the fact that $\widehat{\gamma(h)}$ commutes with $\widehat{x_1}$ and $\widehat{\xi_1}$.

10.1. Some notations.

We will give some notations for the Hamiltonian $\widehat{H}$. All geometric sets defined below are preserved by canonical transformations and by gauge transforms.

C will denote the characteristic manifold $p^{-1}(0)$ where p is the determinant of H_{class}. We have

$$C = \Sigma \cup C_+ \cup C_-$$

which is a disjoint union where C_+ (resp. C_-) is defined by the fact that both eigenvalues of H_{class} close to 0 are $\lambda_- = 0 < \lambda_+$ (resp. $\lambda_- < \lambda_+ = 0$). We will also define $\Sigma_+ \subset C$ (resp. $\Sigma_- \subset C$) as the stable (resp. unstable) manifolds of Σ for the dynamics ϕ_t of $\mathcal{X}_p$.

We will denote by $WF_h(u_h)$ the *semi-classical wave front set* or *microsupport* or *frequency set* of the family u_h. We will write $u_h = 0$ or $u_h = 0(h^\infty)$ in Ω where Ω is an open set in $T^\star\mathbb{R}^n$ if $WF_h(u_h) \cap \Omega = \emptyset$.

Let us choose $z_0 \in \Sigma$ and $a > 0$ small enough. We define $z_{\text{in}}^+ = (0, a, 0, z_0)$, $z_{\text{in}}^- = (-a, 0, 0, z_0)$, $z_{\text{out}}^+ = (a, 0, 0, z_0)$ and $z_{\text{out}}^- = (0, -a, 0, z_0)$.

If $\vec{U}$ a microlocal solution of $\widehat{H}\vec{U} = 0$ in Ω, an open neighbourhood of some point $z_0 \in \Sigma$, we will denote by

- $\vec{U}_{\text{in}}^+$ the restriction of $\vec{U}$ to some neighbourhood of $z_{\text{in}}^+ \in C_+ \cap \Sigma_+$,
- $\vec{U}_{\text{in}}^-$ the restriction of $\vec{U}$ to some neighbourhood of $z_{\text{in}}^- \in C_- \cap \Sigma_-$,
- $\vec{U}_{\text{out}}^-$ the restriction of $\vec{U}$ to some neighbourhood of $z_{\text{out}}^- \in C_- \cap \Sigma_+$,
- $\vec{U}_{\text{out}}^+$ the restriction of $\vec{U}$ to some neighbourhood of $z_{\text{out}}^+ \in C_+ \cap \Sigma_-$.

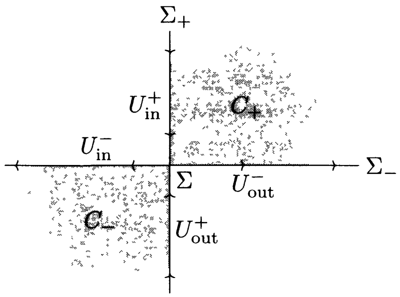

Figure 1. *The microlocal solutions*

We will concentrate on solutions whose component $\vec{U}_{\text{in}}^-$ vanishes.

We will also use a partial Fourier transform w.r. to x_1:

$$\widehat{u}(\xi_1, x_2, x') = (2\pi h)^{-\frac{1}{2}} \int_{\mathbb{R}} \mathrm{e}^{-ix_1\xi_1/h} u(x_1, x_2, x')|\mathrm{d}x_1|.$$

10.2. Special solution.

We will build a special solution of the model problem which will allow to describe all microlocal solutions of $\widehat{H_0}\vec{U} = 0$ near Σ.

Let us consider the solution

$$\vec{U}_0 = \binom{u}{v} \tag{10}$$

of the model equation:

$$D_1 u + x_2 v = 0, \quad x_2 u + x_1 v = 0 \tag{11}$$

given by

- $\vec{U}_{\text{out}}^+$:

$$\begin{cases} u(x_1, x_2) = -i\sqrt{\dfrac{2\pi}{h}}\, Y(x_1) x_2 \Big(\Gamma\Big(1 + i\dfrac{x_2^2}{h}\Big)\Big)^{-1} \\ \qquad\qquad\qquad\qquad\qquad \times\ \mathrm{e}^{\frac{x_2^2}{h}(i \log \frac{x_1}{h} - \frac{1}{2}\pi)}, \\ v(x_1, x_2) = -\dfrac{x_2}{x_1} u(x_1, x_2), \end{cases} \tag{12}$$

where Y is the Heaviside function and Γ the Gamma function. Previous formulae define u as a distribution associated with a locally integrable function and v outside $x_1 = 0$.

The precise definition of the distribution v is given below in term of its partial Fourier transform.

• $\vec{U}_{\text{in}}^{+}$: the h-Fourier transforms $\widehat{u}$ (resp. $\widehat{v}$) with respect to x_1, of u (resp. v) at the non zero values of ξ_1 are given, for $\xi_1 > \mathbf{0}$, by

$$\left\{\begin{aligned} \widehat{u}(\xi_1, x_2) &= -\frac{x_2}{\xi_1}\, \mathrm{e}^{-\frac{i}{h} x_2^2 \log \xi_1}, \\ \widehat{v}(\xi_1, x_2) &= \mathrm{e}^{-\frac{i}{h} x_2^2 \log \xi_1}. \end{aligned}\right. \tag{13}$$

• $\vec{U}_{\text{out}}^{-}$: for $\xi_1 < \mathbf{0}$, by

$$\left\{\begin{aligned} \widehat{u}(\xi_1, x_2) &= \frac{x_2}{|\xi_1|}\, \mathrm{e}^{-\frac{\pi}{h} x_2^2}\, \mathrm{e}^{-\frac{i}{h} x_2^2 \log |\xi_1|}, \\ \widehat{v}(\xi_1, x_2) &= \mathrm{e}^{-\frac{\pi}{h} x_2^2}\, \mathrm{e}^{-\frac{i}{h} x_2^2 \log |\xi_1|}. \end{aligned}\right. \tag{14}$$

The partial Fourier transform of v is the distribution associated with the locally integrable function given by the previous formulae.

One get easily other solutions supported by $x_1 \geq 0$ by multiplying the previous one by an arbitrary function of $(x_2, \ldots, x_n)$.

Remark. 1 — If $\widehat{\gamma(h)}$ does not vanish, our system is replaced by

$$D_1 u + P v = 0, \quad P^\star u + x_1 v = 0, \tag{15}$$

where $P = x_2 + ih\widehat{\gamma(h)}$ commutes with $\widehat{x_1}$ and $\widehat{\xi_1}$. We can do the same calculations where x_2 is replaced at some places by P, at other places by $P^\star$, and x_2^2 is replaced by $P^\star P$ or by $PP^\star$. We get the same kind of formulae from which we can deduce that the results described below also holds in this case.

If $|x_2| \gg \sqrt{h}$ and $x_1 \geq c > 0$, we get

$$u(x_1, x_2) = u_{\mathrm{WKB}}(x_1, x_2)\Big(1 + O\Big(\frac{h}{x_2^2}\Big)\Big)$$

where, by using Stirling's formula (see [1], p. 257):

$$u_{\mathrm{WKB}}(x_1, x_2) = -\operatorname{sign}(x_2)\, \mathrm{e}^{i\frac{\pi}{4}}\, \pi\, \mathrm{e}^{-\frac{i}{h} x_2^2 (\log(\frac{x_2^2}{x_1}) - 1)}. \tag{16}$$

More precisely

$$u(x_1, x_2) = u_{\mathrm{WKB}}(x_1, x_2)\psi\Big(\frac{x_2^2}{h}\Big)$$

where ψ is the smooth function on $]0, +\infty[$, continuous at 0, whose limit at infinity is 1, given by

$$\psi(x) = \frac{\Gamma}{\Gamma_{\mathrm{Stir}}}(1 + ix).$$

Moreover, we can check that

$$\left|u(x_1, x_2)\right|^2 = \left|\psi\Big(\frac{x_2^2}{h}\Big)\right|^2 = 1 - \mathrm{e}^{-2\pi\frac{x_2^2}{h}}.$$

10.3. Microlocal solutions.

In this section, we will describe all microlocal solutions of $\widehat{H_0}\vec{U} = 0$ for which $\vec{U}_{\mathrm{in}}^-$ vanishes using our previous solution $\vec{U}_0$. We get the

THEOREM 4. — *Let $\vec{U}$ be a microlocal solution near the origin of $\widehat{H_0}\vec{U} = 0$, i.e.,*

$$WF_h(\widehat{H_0}\vec{U}) \cap \Omega = \emptyset,$$

where Ω is a neighbourhood of the origin. Let us assume moreover that $\vec{U}_{\mathrm{in}}^- = 0$. Then, if $\varphi_h(x_2, x') = \widehat{v}(\xi_1 = 1, x_2, x')$, we have

$$\vec{U} = \varphi_h(x_2, x')\vec{U}_0$$

microlocally near the origin.

The proof is an extension of an argument given in [12], Prop. 17.

All microlocal solutions near Σ are sums of the previous one's and a similar one whose ingoing part is $\vec{U}_{\mathrm{in}}^-$, i.e. $\vec{U}_{\mathrm{in}}^+ = 0$.

11. Lagrangian states.

11.1. Qualitative description.

We want to describe solutions for which $\vec{U}_{\mathrm{in}}^-$ vanishes while $\vec{U}_{\mathrm{in}}^+$ is a Lagrangian state associated to a germ of Lagrangian manifold $\Lambda_{\mathrm{in}}^+ \subset T^\star\mathbb{R}^n$ which is contained in C_+ near some point $z \in C_+ \cap \Sigma_+$. We will assume that $\Lambda_{\rm in}^+$ and Σ_+ intersect transversally inside C^+. Their intersection is then an isotropic manifold $W_{\rm in}^+$ of dimension $n-1$. We will denote by

$$W_0 = \left\{ \lim_{t\to+\infty} \phi_t(z) \mid z \in W_{\rm in}^+ \right\}.$$

W_0 is an isotropic submanifold of Σ of dimension $n-2$ transversal to the one dimensional null foliation Ξ of Σ. We will also denote by $W_{\rm out}^- \subset \Sigma^+ \cap C_-$ the isotropic submanifold of dimension $n-1$:

$$W_{\rm out}^- = \left\{ z \mid \lim_{t\to+\infty} \phi_t(z) \in W_0 \right\} \cap C_-.$$

THEOREM 5. — *Let $\vec{U}_{\rm in}^+ \in I^0(\Lambda_{\rm in}^+)$ be a microlocal solution of $\widehat{H_0}\vec{U}_{\rm in}^+ = 0$. There exists a unique microlocal solution of $\widehat{H_0}\vec{U} = 0$ in some neighbourhood of Σ such that $\vec{U}_{\rm in}^-$ vanishes.*

We have the following qualitative description of this solution:

- *The flow-out $\Lambda' \subset C_+$ of $\Lambda_{\rm in}^+ \setminus \Sigma_+$ by ϕ_t is a smooth Lagrangian manifold whose closure is singular along $\Sigma_- \cap C_+$. $\vec{U}$ is a Lagrangian distribution of order 0 on Λ'. Its principal symbol does not extend continuously (in general) along $\Sigma_- \cap C_+$ although Λ' is C^1 (but not C^2).*

- *Along C_-, $\vec{U} = \vec{U}_{\rm out}^-$ is a Gaussian state of order $\frac{1}{2}$ associated to the isotropic manifold $W_{\rm out}^-$ and a positive Lagrangian manifold $\Lambda_{\rm out}^-$.*

Proof. — It is of course enough to prove the theorem for the model. In this case $\vec{U} = \varphi\vec{U}_0$ where $\varphi(x_2, x')$ is any Lagrangian state w.r. to the variables (x_2, x'). The theorem follows directly by examination of the expressions of $\vec{U}_0$ given by Theorem 4. $\square$

11.2. Principal symbols.

We will now describe a construction of the Lagrangian manifold $\Lambda_{\rm out}^-$ as well as of the principal symbol of $\vec{U}_{\rm out}^-$.

11.2.1. *Logarithmic maps.* — Let X be a fixed finite dimensional complex vector space and G_n the Grassmann manifold of its complex subspaces of dimension n. We will say that a map $F :]-a, 0[\to G_n$ is *logarithmic* if there exist maps $f_j :]-a, 0[\to X, j = 1, \dots, n$, such that $f_j(u) = e_j \log|u| + g_j(u)$ with g_j smooth at 0 and $F(u)$ is the vector space freely generated by the $f_j(u)$'s. Such a mapping F admits a formal extension to $u > 0$ defined by $f_j(u) = e_j(\log u + i\pi) + g_j(u)$. This extension, called the *canonical extension of F*, is independent of the choice of the basis as well as invariant by increasing diffeomorphisms ψ in u such that $\psi(0) = 0$.

11.2.2. *The transmission rule for the Lagrangian manifold.* — We will choose a trajectory $\gamma_+(t), t \in]t_0, +\infty[$, of $\mathcal{X}_p$ contained in $\Lambda_{\rm in}^+ \cap \Sigma^+$. This trajectory admits a unique prolongation γ_- as another trajectory contained in $C^- \cap \Sigma^+$ so that the closure of their union is a smooth arc denote by $\gamma(u)$ with u close to 0. We will assume that

- if $u < 0$, then $\gamma(u) = \gamma_+(u) \in C^+$;
- $\gamma(0) \in \Sigma$;
- if $u > 0$, then $\gamma(u) = \gamma_-(u) \in C^-$.

It is clear that $W_{\rm out}^-$ is foliated by the trajectories γ_-. So it is enough to make our constructions along any γ.

We will denote by $L_+(u)$ the tangent plane of $\Lambda_{\rm in}^+$ at the point $\gamma(u), u < 0$.

Similarly $L_-(u)$ will be the complex Lagrangian plane tangent to $\Lambda_{\rm out}^-$ at the point $\gamma(u), u > 0$.

$L_+(u)$ is logarithmic in the sense of the previous section.

PROPOSITION 1. — *$L_-(u), u > 0$, is uniquely defined by its formal expansion which is the canonical extension of $L_+(u)$ and its invariance by the linearization of ϕ_t.*

11.2.3. *The transmission rule for the principal symbol.* — Both limits of $L_\pm(u)$ as $u \to 0$ agree

$$L_0 := \lim_{u \to 0^\mp} L_\pm(u) = TW_0 \oplus \Xi \oplus \Big\langle \frac{\mathrm{d}\gamma}{\mathrm{d}u} \Big\rangle.$$

The following proposition describes the transmission rules for the principal symbol which is an half density on $L_\pm(u)$.

PROPOSITION 2. — *We have*

$$\lim_{u \to 0^+} \big(\log |u|\big)^{\frac{1}{2}} \sigma(\gamma_-(u)) = \lim_{u \to 0^-} \big(\log |u|\big)^{\frac{1}{2}} \sigma(\gamma_+(u)) = \sigma_0 \in \Omega^{\frac{1}{2}}(L_0).$$

Once given the transport equation (see for example [18]), one can check that there exists a unique $\sigma_\pm(u)$ which satisfy the transport equation and such that the previous rule holds. So we have really described the transmission rule for the principal symbol.

12. Gaussian states: "the dromedary becomes a Bactrian"[2].

In this section, we will use the definitions of the Appendix.

12.1. Model problem.

In order to recover Hagedorn's results, one first has to choose an incoming trajectory $\gamma_{\rm in}^+ \subset C_+ \cap \Sigma_+$ of the vector field $\mathcal{X}_p$. We can assume that $\gamma_{\rm in}^+(+\infty) = \gamma_\infty \in \Sigma$.

We have two outgoing trajectories

- $\gamma_{\rm out}^+ \subset C_+ \cap \Sigma_-$ so that $\gamma_{\rm out}^+(-\infty) = \gamma_\infty$,
- $\gamma_{\rm out}^- \subset C_- \cap \Sigma_+$ so that $\gamma_{\rm out}^-(+\infty) = \gamma_\infty$.

THEOREM 6. — *Let $\vec{U}_{\rm in}^+$ be a Gaussian state of order* 0 *based on the isotropic manifold $\gamma_{\rm in}^+$ and assume $\vec{U}_{\rm in}^- = 0$. Then the microlocal solution near σ_0 of $\widehat{H}\vec{U} = 0$ satisfies*

- $\vec{U}_{\rm out}^-$ *is a* Gaussian state *of order* 0 *associated to* $\gamma_{\rm out}^-$,
- $\vec{U}_{\rm out}^+$ *is* non Gaussian *symplectic spinor of order* 0 *associated to* $\gamma_{\rm out}^+$.

Proof. — We look at our model problem. We choose

$$\gamma_{\rm in}^+(t) = (0, \mathrm{e}^{-t}; 0, 0; 0, 0).$$

We have $\gamma_{\rm out}^+(t) = (\mathrm{e}^{t}, 0; 0, 0; 0, 0)$ and $\gamma_{\rm out}^-(t) = (0, -\mathrm{e}^{-t}; 0, 0; 0, 0)$.

A typical "Gaussian state" is given by

$$\vec{U}_{\rm in}^+ = \varphi(x_2, x')(\vec{U}_0)_{\rm in}^+,$$

where

$$\varphi(x_2, x') = Ah^{-\frac{1}{2}(n-1)}\,\mathrm{e}^{Q(x_2,x')/h}$$

with $Q = Q_1 + iQ_2$ and $Q_1 \ll 0$.

- From the explicit formulae, we get that $\vec{U}_{\rm out}^+$ is a coherent state associated to $\gamma_{\rm out}^+$. The symbol of $u_{\rm out}^+$ is

$$A\,\mathrm{e}^{Q(X_2,X')}X_2\Gamma(1 + iX_2^2)^{-1}\,\mathrm{e}^{X_2^2(i\log(x_1/h) - \frac{1}{2}\pi)}$$

apart from trivial factors. The Γ factor prevents $u_{\rm out}^+$ to be Gaussian.

[2] Thanks to George Hagedorn for pointing to me the appropriate names.

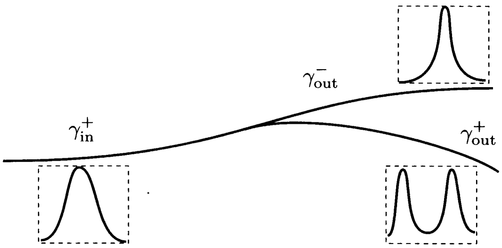

Figure. The squares of the modulus of the solutions

We have

$$|\sigma(u_{\rm out}^+)(X_2, X')|^2 = |A|^2\, \mathrm{e}^{2Q_1(X_2,X')}(1 - \mathrm{e}^{-2\pi X_2^2}), \tag{17}$$

hence a Bactrian!

The rules for the symbol along $\gamma_-^{\rm out}$ are the same as for the Lagrangian states. □

It remains to describe the rules for the principal symbol of the symplectic spinor associated to $\gamma_+^{\rm out}$.

13. The elliptic case.

If we replace in our assumptions of Section 1 the condition (H3) by

(H4) *the linearization of $\mathcal{X}_p$ admits a non zero pair of purely imaginary eigenvalues $\pm i\mu$,*

and (iii) by

(iv) $\{q,r\}^2 + \{q,s\}^2 - \{r,s\}^2 < 0$,

we get that the semi-simple factor is now elliptic. As already observed in [7], this case occurs in Maxwell equations as well as in propagation of waves in elastic media.

On the level of formal series expansions, the same results holds, but we can no more use Sternberg's theorem. We get the

THEOREM 7. — *Assuming* (H1), (H2) *and* (H4), *Theorem* 3 *remains true on the level of formal series transversally to* $\Sigma = \{x_1 = \xi_1 = \xi_2 = 0\}$ *with*

$$H_0 = \begin{pmatrix} \xi_2 - x_1 & \xi_1 \\ \xi_1 & \xi_2 + x_1 \end{pmatrix}.$$

We can describe easily the solutions of the model system

$$\widehat{H_0}\begin{pmatrix} u \\ v \end{pmatrix} = 0$$

by using the unknown functions $w_\pm = u \pm iv$. We get the following equation for w_+:

$$(2\Omega + h)w_+ + h^2 \frac{\partial^2}{\partial x_2^2} w_+ = 0$$

where $\Omega = -h^2\partial_{x_1}^2 + x_1^2$ is an harmonic oscillator. The formal normal form suffices to describe microlocal solutions whose microsupport is Σ; it is enough to developp the value of w_+ at $x_2 = 0$ using the basis of eigenfunctions of Ω.

14. The Hermitian case.

The same method can be applied to other kinds of generic eigenvalues crossings. The main hypothesis in order to get a microlocal normal form is *transversal hyperbolicity*, namely the linearized Hamiltonian vector field should have hyperbolic blocks and Jordan blocks with 0 as eigenvalue only. We give below a sketchy presentation of the Hermitian case which will be the object of [10].

In the Hermitian case, because of the signature $(+,-,-,-,0,\dots,0)$ of p'', there are only four cases. We will classify according the corank of $\omega_{|\Sigma}$ which is assumed to be locally constant:

14.1. Corank 0: the generic case (elliptic-hyperbolic).

The singular stratum Σ of the characteristic manifold is symplectic. The linearization of $\mathcal{X}_p$ do admit two pairs of non vanishing eigenvalues $(\pm\lambda, \pm i\mu)$.

We get moduli in the normal form: we cannot reduce both semi-simple blocks using our equivalence relation. We do not know some physical example of this last case. The normal form should be:

$$H_0 = \begin{pmatrix} \xi_1 & a(x_2^2+\xi_2^2, x', \xi')(x_2 \pm i\xi_2) \\ a(x_2^2+\xi_2^2, x', \xi')(x_2 \mp i\xi_2) & x_1 \end{pmatrix},$$

where $a(\tau, x', \xi')$ is a smooth > 0 function.

Both cases $(\pm)$ are not equivalent: the open cones $C_\pm$ which correspond respectively to $\lambda_- = 0 < \lambda_+$ $(\lambda_- < \lambda_+ = 0)$ are well-defined near Σ. Morse indices differs by 1 on those cones. Moreover, both cones are oriented by $p > 0$. 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.

In the case of two degrees of freedom and analytic data, the normal form for the dispersion relation has been proved to be convergent by Moser [46]. The model problem is studied in [21].

14.2. Corank 2: the hyperbolic case.

The singular manifold is not symplectic and the linearization of $\mathcal{X}_p$ admits one pair of real non vanishing eigenvalues:

$$H_0 = \begin{pmatrix} \xi_1 & x_2 + ix_3 \\ x_2 - ix_3 & x_1 \end{pmatrix}.$$

This normal form is local as in our previous result. We get this model in the Born-Oppenheimer approximation with magnetic field.

14.3. Corank 2: the elliptic case.

The singular manifold is not symplectic and the linearization of $\mathcal{X}_p$ admits one pair of purely imaginary non vanishing eigenvalues.

We get a normal form which is only formal as before. This model is used in the example of spin-orbit interaction (see [19] and [20]). It leads to transition of an eigenstate from one band to another one.

$$H_0 = \begin{pmatrix} x_1 & x_3 + i\xi_3 \\ x_3 - i\xi_3 & x_2 \end{pmatrix}.$$

14.4. Corank 4: the involutive case.

The singular manifold is involutive. A similar case has been studied by Melrose and Uhlmann in [45].

15. Bifurcations.

It would be interesting to describe generic bifurcations which may occur at least for three reasons:

1) The condition 2) is no more satisfied at some points. This imply a singularity of the manifold Σ.

2) There is a change in the normal form involved. For example in the symmetric case, how do we pass generically from the hyperbolic to the elliptic case?

3) For a $d \times d$ system with $d \geq 3$, there exists triply and more degenerated eigenvalue of the classical Hamiltonian at some points.

16. Appendix: coherent states, symplectic spinors and Gaussian states.

16.1. Definitions.

A (semi-classical) *coherent state* is, roughly speaking, a semi-classical state whose microsupport is an isotropic submanifold K of the cotangent space. It is desirable to describe nice families of coherent states for which a so-called *symbolic calculus* is available. Of course, such families should be invariant by Fourier Integral Operators.

There are at least three available theories of coherent states which are closely related:

1) (Semi-classical) *Fourier Integral Operators with complex phase functions* studied by Melin and Sjöstrand [44].

2) (Semi-classical) *Symplectic Spinors* studied by Boutet de Monvel and Guillemin [29] and [6], see also [39].

3) Hagedorn's *Semi-classical Wave Packets* [30], [32] or *Gaussian states.*

The first two theories are better adapted to the context of microlocal analysis being invariant by Fourier Integral Operators. We will use the second one in what follows: we will first give the definition of the *semi-classical symplectic spinors* following closely [29]. Then we will define a subset of it, the so-called *Gaussian states*, associated to some jet of order ∞ of positive complex Lagrangian manifold containing K; they are very close to Hagedorn's semi-classical wave packets. After that, we will define the principal symbols of these objects. All our discussion will be (micro-)local even if it is not always specified.

DEFINITION 1. — • *Let K_0 be the isotropic submanifold of $T^\star(\mathbb{R}^k_x \oplus \mathbb{R}^{n-k}_y)$ defined by*

$$K_0 = \left\{(x, 0; 0, 0) \mid x \in \mathbb{R}^k\right\}.$$

We will say that $a(x, Y, h) \in C^{\infty}(\mathbb{R}^k_x \oplus \mathbb{R}^{n-k}_Y)$ *is a* symbol *in* $\Sigma^{\ell}(K_0)$ *if* $a(x, .\,, h) \in \mathcal{S}(\mathbb{R}^{n-k})$ *and, for all semi-norms* N *of the Schwartz space* $\mathcal{S}(\mathbb{R}^{n-k}_Y)$, *and all* $\varepsilon > 0$, *we have*

$$N(a) = O(h^{\ell+\varepsilon}),$$

uniformly on compacts in $\mathbb{R}^k_x$.

• *A* classical symbol *in* $\Sigma^{\ell}(K_0)$ *is a symbol which admits an asymptotic expansion* $a(x, Y, h) \sim h^{\ell}(\sum_{j=0}^{\infty} h^{\frac{1}{2}j} a_j(x, Y))$. *We will denote by* $\Sigma^{\ell}_{\text{class}}(K_0)$ *this space.*

• *A* symplectic spinor (*resp.* classical symplectic spinor) $u_h(x, y)$ *of order* l *associated with the isotropic manifold* $K_0 = \{(x, 0; 0, 0)\} \subset T^{\star}(\mathbb{R}^k_x \oplus \mathbb{R}^{n-k}_y)$ *is defined by*

$$u_h(x, y) = h^{-\frac{1}{2}(n-k)} a\Big(x, \frac{y}{\sqrt{h}}, h\Big),$$

where $a \in \Sigma^{\ell}(K_0)$ (*resp.* $a \in \Sigma^{\ell}_{\text{class}}(K_0)$). *We will denote* $a \in SS^{\ell}(K_0)$ (*resp.* $a \in SS^{\ell}_{\text{class}}(K_0)$).

• *If* K *is an isotropic submanifold of* $T^{\star}\mathbb{R}^n$ *and* χ *a canonical transformation such that* $\chi(K_0) = K$, *we choose an elliptic FIO of order* 0 *say* A *and define*

$$SS^{\ell}(K) = A(SS^{\ell}(K_0)) \quad \big(\text{resp. } SS^{\ell}_{\text{class}}(K) = A(SS^{\ell}_{\text{class}}(K_0))\big).$$

Remark. 2 — If K is a Lagrangian submanifold, symplectic spinors associated with K are exactly the Lagrangian states (WKB-Maslov states).

The proof of the coherence of the previous definition is an easy adaptation of Guillemin's argument in [29] (see also [6]). It is clear that, if $u_h \in SS^{\ell}(K)$, we have $WF_h(u_h) \subset K$.

An example which is useful in our paper is

$$a(x, Y, h) = a_0(x, Y)\, \mathrm{e}^{iP(Y)\log h}$$

(see formula (17)) where a_0 is in the Schwartz class w.r.t. to Y and P is a real valued polynomial.

Definition 2. — *A positive formal Lagrangian manifold along* K *is a jet of infinite order of complex Lagrangian manifold along* K *whose linear part is a positive Lagrangian subspace of* $((TK)^0/TK) \otimes \mathbb{C}$.

If $K = K_0$, $\Lambda = \Lambda_{\varphi}$ *is defined by a formal series* $\varphi(x, y) = \sum_{j=2}^{\infty} \varphi_j(x, y)$ *where* $\varphi_j(x, y)$ *is homogeneous of degree* j *w.r.t. to* y *and* $\Im\varphi_2(x, .)$ *is a strictly positive quadratic form.*

Definition 3. — *A* Gaussian state *of order* ℓ *associated to* (K_0, Λ_φ) *is defined by*

$$u_h(x, y) = a_h(x, y)\, \mathrm{e}^{i\varphi(x,y)/h}$$

where a *is a classical symbol of order* $\ell - \frac{1}{2}(n-k)$.

We will denote by $\mathrm{GS}^\ell(K_0, \Lambda_\varphi)$ *the corresponding space. We can define* $\mathrm{GS}^\ell(K, \Lambda)$ *using Fourier integral operators.*

Proposition 3. — *A Gaussian state is a symplectic spinor. If* $u \in GS^0(K_0, \Lambda_\varphi)$*, its total symbol is* $\sum_{j=0}^{\infty} A_j(x, Y) h^{\frac{1}{2}j}\, \mathrm{e}^{i\varphi_2(x,Y)}$ *where* $A_j(x, Y)$ *is a polynomial in* Y *of degree less than* $3j$ *and conversely.*

Remark. 3 — The "$3j$" can already be seen in formula (3.2) of [16].

16.3. Principal symbols.

16.2.1. *Symplectic spinors.* — We will now define the principal symbol of a symplectic spinor following [29].

Let K be a k-dimensional isotropic submanifold of $T^\star\mathbb{R}^n$. We will assume as in [29] that K is equipped with a metalinear structure. The vector bundle $E = TK^0/TK$ of dimension $2(n-k)$ over K is symplectic. We will assume that it is equipped with a metaplectic structure. It implies that each Lagrangian subbundle is equipped with a metalinear structure. We assume also that $\mathbb{R}^n$ is equipped with the standard metalinear structure.

We want to define the principal symbol of a semi-classical symplectic spinor which is a half form: $u_h(x, y)\sqrt{\mathrm{d}x\, \mathrm{d}y}$. We start with a direct sum decomposition $E = L \oplus L'$ of E into a sum of two transversal Lagrangian subbundles. The symbol $\sigma(u_h)$ of u_h will be an element $[a_h(x, Y)]\sqrt{\mathrm{d}x\, \mathrm{d}Y}$ where $x \in K$, $Y \in L$ and the equivalent class $[\,.\,]$ is in $\Sigma^0(L)/\Sigma^{\frac{1}{2}}(L)$. We use a local trivialisation of L in order to get functions of (x, Y). If $K = K_0$, $u = h^{-\frac{1}{2}(n-k)} a_h(x, y/\sqrt{h})\sqrt{\mathrm{d}x\, \mathrm{d}y}$, $L = 0 \oplus \mathbb{R}^{n-k}$ and $L' = 0 \oplus (\mathbb{R}^{n-k})^\star$, we have $\sigma(u_h) = [a(x, Y)]\sqrt{\mathrm{d}x\, \mathrm{d}Y}$.

It is now enough to say what is the transformation rule for the symbol under the action of an elliptic Fourier Integral Operatorof order 0: the canonical transformation χ such that $\chi(K_0) = K$ transforms the K_0-bundles $L_0 \oplus L_0' \subset E_0$ into the K-bundles $L \oplus L' \subset E$. It acts in a natural way on principal symbols using the metaplectic representation associated to the linear part of χ. The symbol of $A(u_h)$ using this natural action is just obtained by multiplication by the principal symbol of the Fourier Integral Operator.

It remains to speak about the *transport equation*: we assume that P is a pseudo-differential operator whose principal symbol p vanishes on K and such that $\mathcal{X}_p$ is tangent to K. If $u_h \in \Sigma^0(K)$, $Pu_h \in \Sigma^1(K)$ and its principal symbol is given by the familiar formula

$$\sigma(Pu) = \frac{1}{i}\mathcal{L}_{\mathcal{X}_p}\sigma(u) + \mathrm{sub}(P)\sigma(u)$$

where one need to interpret the Lie derivative properly as in [29]!

In the matrix case, we need a natural extension of the calculus of [18]. For the standard examples (Born-Oppenheimer or adiabatic cases), it is enough to consider the canonical connexion on the polarization bundle.

16.2.2. *Gaussian states.* — The case of Gaussian states is easier to describe: the principal symbol is just a half form on the bundle of Lagrangian spaces $J_1(\Lambda)$ over K. If $K = K_0$ and $\Lambda = \Lambda_\varphi$. $J_1(\Lambda) = \{(x, 0; y, \partial\varphi_2(x,y)/\partial y)\}$ and, if we denote by $\pi : J_1(\Lambda) \to T_{K_0}\mathbb{R}^n$ the canonical projection, the principal symbol of $a_h(x,y)\,\mathrm{e}^{i\varphi(x,y)/h}\sqrt{\mathrm{d}x\mathrm{d}y}$ is $\pi^\star(a_0(x,0)\sqrt{\mathrm{d}x\mathrm{d}y})$.

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