Wigner Measures and Molecular Propagation through Generic Energy Level Crossings

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Abstract. *We study time-dependant Schrödinger equation with matrix-valued potential presenting some generic crossing of type B, I, J or K in Hagedorn's classification. We use two-scale Wigner measures for calculating the Landau-Zener energy transfer which occurs at the crossing. Our method provides a unified framework in which codimension 2, 3 or 5 crossings can be discussed. We recover Hagedorn's result for wave packets, from Wigner measure point of view, and extend them to any data uniformly bounded in L^2. The proof is based on a normal form theorem which reduces the problem to an operator-valued Landau-Zener formula.*

Key words. Energy level crossings, Landau-Zener transitions, Born Oppenheimer approximation, Semi-classical measures (Wigner measures), multi-scale convergence.
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1 Introduction

The quantum description of the dynamics of a molecule consisting on k_n nuclei and k_e electrons, $k_e + k_n = N$, is given by the time dependant Schrödinger equation

$$\left\{ \begin{array}{l} ih\partial_t \Phi^h = H^h_{moll} \Phi^h, \\ \Phi^h(0) = \Phi^h_0, \end{array} \right. \tag{1}$$

with initial data $\Phi^h_0 \in L^2(\mathbf{R}^{3N})$ and where H^h_{moll} is an essentially self-adjoint molecular hamiltonian. The scale parameter h is the square-root of the ratio of the electronic mass m_e on the average mass of the molecule's nuclei,

$$h = \sqrt{\frac{m_e}{M}}.$$

We are concerned with big molecules, more precisely with the limit $M \to +\infty$, i.e. $h \to 0$.

The molecular hamiltonian H^h_{moll} can be written as

$$H^h_{moll} = -\frac{h^2}{2}\Delta_x + H_e(x),$$

where x describes the nuclear configuration, $x \in \mathbf{R}^{3k_n}$. The electronic hamiltonian $H_e(x)$ contains the electrons' kinetics and the interaction between electrons end nuclei. We suppose that H_e depends smoothly on x.

We consider $\sigma_e\left(H_e(x)\right)$ the spectrum of $H_e(x)$ and $\sigma_*(x)$ a closed subset of $\sigma_e\left(H_e(x)\right)$ which is the union of two eigenvalues λ_1 and λ_2 of the same multiplicity k. We denote by $P_*(x)$ the spectral projector of $H_e(x)$ associated with $\sigma_*(x)$, then there exists an isometry $\mathcal{U}:\ \mathrm{Ran}P_* \to L^2(\mathbf{R}^{3k_n}, \mathbf{C}^{2k})$. We suppose that the initial data Φ_0^h belongs to $\mathrm{Ran}(P_*)$. If $\sigma_*(x)$ is isolated from the rest of the spectrum, that is if

$$d\left(\sigma_*(x), \sigma\left(H_e(x)\right)/\sigma_*(x)\right) \geq d, \;\; \forall x \in \mathbf{R}^{3k_n},$$

then $\mathrm{Ran}(P^*)$ is said adiabatically protected: it is possible to approximate Φ^h by a Born-Oppenheimer solution, Φ^h_{BO},

$$\Phi^h_{BO} = \mathcal{U}^*\exp\left(-i\frac{t}{h}H^h_{BO}\right)\mathcal{U}\Phi^h_0,$$

where $H^h_{BO} = -\frac{h^2}{2}\Delta_x + V(x)$ and V is a matrix potential whose values are $2k \times 2k$ matrices. Thus, it is possible to reduce the study of (1) to this of some system of $2k$ equations, of the form

$$\left\{\begin{array}{l} ih\partial_t\psi^h = -\frac{h^2}{2}\Delta_x\psi^h + V(x)\psi^h, \\ \psi^h(0) = \mathcal{U}\Phi^h_0. \end{array}\right. \tag{2}$$

This type of observation dates back to the 1920's and is originally assigned to Born, Fock and Oppenheimer. The reader can refer to [29] for some precise statements of this fact.

We focus more precisely on the case where $\lambda_1(x)$ and $\lambda_2(x)$ cannot be separated because there exists some x_0 such that

$$\lambda_1(x_0) = \lambda_2(x_0).$$

In [18], G. Hagedorn derives normal forms for matrix potential V in such a context. Let us shortly recall his argument.

It is classic to associate with H^h_{moll} its symmetry group G and the subgroup H of unitary elements of G. Two cases occur, either $G = H$, either H is a subgroup of index 2 of G. As $G = H$, standard group representation theory applies and one associates with the eigenvalues λ_1 and λ_2 a unique representation of G. These representations are either unitarily equivalent or not. If $H \neq G$, one uses the theory of corepresentation (see [30] or [25]) of which there exist three types (see [25]). With λ_1 and λ_2, one associates some corepresentation of one of these three types. If these corepresentations are of the same type, they are either unitarily equivalent or not, which gives six different situations. If not, they are of different types, and we have to deal with three new situations. Adding the two different cases which arises as $G = H$, we obtain eleven cases to study. For each of them, assuming that the eigenvalues are of minimal multiplicity, G. Hagedorn derives in [18] some normal forms which are diagonal as soon as the representations or corepresentations associated with the eigenvalues are not unitarily equivalent, i.e. in seven of the derived cases. The four remaining normal forms obtained are not diagonal, they are the following ones.

$$
\begin{aligned}
H_2 &= \mathrm{tr}(H_2) + \begin{pmatrix} p_1 & p_2 \\ p_2 & -p_1 \end{pmatrix} \; - \; (\textit{type } I), \\
H_3 &= \mathrm{tr}(H_3) + \begin{pmatrix} p_1 & p_2 + ip_3 \\ p_2 - ip_3 & -p_1 \end{pmatrix} \; - \; (\textit{type } B), \\
H_{3'} &= \mathrm{tr}(H_{3'}) + \begin{pmatrix} \begin{pmatrix} p_1 & p_2 + ip_3 \\ p_2 - ip_3 & -p_1 \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \begin{pmatrix} p_1 & p_2 - ip_3 \\ p_2 + ip_3 & -p_1 \end{pmatrix} \end{pmatrix} \; - \; (\textit{type } K), \\
H_5 &= \mathrm{tr}(H_5) + \begin{pmatrix} p_4 \, \mathbf{1} & \begin{pmatrix} p_0 + ip_1 & p_2 + ip_3 \\ -p_2 + ip_3 & p_0 - ip_1 \end{pmatrix} \\ \begin{pmatrix} p_0 - ip_1 & -p_2 - ip_3 \\ p_2 - ip_3 & p_0 + ip_1 \end{pmatrix} & -p_4 \, \mathbf{1} \end{pmatrix} \; - \; (\textit{type } J),
\end{aligned}
$$

where for any $j \in \{2, 3, 3', 5\}$, $x \mapsto p(x) \in \mathbf{R}^j$ is a smooth vector-valued function. For these four hamiltonians, the eigenvalues are $\mathrm{tr}(H_j) \pm \mid p \mid$. We shall say that these crossings are generic if

$$
\mathrm{d}p \ \textit{is of maximal rank on} \ p = 0, \tag{A1}
$$

i.e. of rank 2 for $j = 2$, 3 for $j = 3, 3'$ and 5 for $j = 5$. This explains why it is usual to refer to these crossings as to codimension 2, 3 and 5 crossings and enlightens the choice of the index j we made. It will be useful in the following to have some notation for the matrices above, thus we set

$$
k = \mathrm{tr}(H_j), \quad V_j = H_j - k.
$$

For each of these hamiltonians, there occurs energy transfer at leading order between the two modes that G. Hagedorn has precisely calculated in [18] for wave packets passing through the crossing with non vanishing speed (see also [19], [22]). Actually, in [18], G. Hagedorn considers linear functions p. Indeed, wave packets are localized at microlocal scale on one point thus it is enough to deal with the Taylor expansion of p at the point concerned by the crossing. Our aim here is to consider more general initial data, thus we cannot suppose that p is linear without loss of generality.
We shall describe the energy transfer by means of Wigner measure for initial data (ψ_0^h) uniformly bounded in L^2, in the same spirit as in [8], [10] or [11]. Actually, the case of the hamiltonians H_2 and H_3 for which the eigenvalues are of multiplicity 1, are dealt with in [9] and [10] respectively. Our aim here is to generalize these results to codimension 5 crossings and to the case of eigenvalues of higher multiplicity than 1.

In the following we denote by d the dimension of the set of the nuclear configuration, $d = 3k_n$ and we consider system (S_j), $j \in \{2, 3, 3', 5\}$,

$$
(S_j) \left\{ \begin{array}{l} ih\partial_t \psi^h = -\frac{h^2}{2} \Delta_x \psi^h + H_j(x)\psi^h, \quad (t, x) \in \mathbf{R} \times \mathbf{R}^d, \\ \psi^h(0) = \psi_0^h, \end{array} \right.
$$

$(\psi_0^h) \in L^2(\mathbf{R}^d, \mathbf{C}^{N(j)})$ with $N(2) = N(3) = 2$ and $N(3') = N(5) = 4$, $\mid \psi_0^h \mid_{L^2} \leq C$. We suppose that $\mathrm{d}p$ is of rank j above $\{p = 0\}$. We aim at describing Wigner measures of (ψ^h).

1.1 Wigner Measures

We begin by shortly recalling some basic facts about semi-classical measures. We consider observable $a \in \mathcal{C}_0^\infty(\mathbf{R}^{d+1} \times \mathbf{R}^{d+1}, \mathbf{C}^{N,N})$ and we associate with a the semi-classical pseudo-differential operator of symbol a which expresses with Weyl quantification, as

$$\mathrm{op}_h\ (a)f(y) = (2\pi)^{-d} \int a(\frac{y+y'}{2}, \eta)\, \mathrm{e}^{\frac{i}{h}\eta\cdot(y-y')} f(y')\mathrm{d}y'\ \mathrm{d}\eta,$$

with $y = (t,x) \in \mathbf{R}_t \times \mathbf{R}_x^d$, $f \in L^2(\mathbf{R}^{d+1}, \mathbf{C}^N)$. If (v^h) is a uniformly bounded family in $L^2(\mathbf{R}^{d+1}, \mathbf{C}^N)$, there exists h_k, $h_k \underset{k\to+\infty}{\longrightarrow} 0$, and a positive matrix-valued Radon measure μ on $T^*\mathbf{R}^{d+1}$ such that

$$\forall a \in \mathcal{C}_0^\infty(\mathbf{R}^{d+1} \times \mathbf{R}^{d+1}, \mathbf{C}^{N,N}),\ \left(\mathrm{op}_{h_k}\ (a)v^{h_k}\ \mid\ v^{h_k}\right) \underset{k\to+\infty}{\longrightarrow} \mathrm{tr}\,(< a, \mu >)\,.$$

The link with the energy density of (v^{h_k}) is given by

$$\mathrm{w} - \lim \mid v^{h_k}(x) \mid^2 \mathrm{d}x = \int_{\xi\in\mathbf{R}^{d+1}} \mathrm{tr}\,\mu(x, \mathrm{d}\xi),$$

provided some assumption of h-oscillation is fulfilled (see [14]), namely

$$\limsup_{h\to 0} \int_{|\xi|\geq R/h} \mid \widehat{v}^h(\xi) \mid^2 \mathrm{d}\xi \underset{R\to+\infty}{\longrightarrow} 0.$$

The reader can refer to [14] and [24] or to [15] for a survey on Wigner measures.

We endow $T^*\mathbf{R}^{d+1}$ with the symplectic form $\sigma = \mathrm{d}\tau \wedge \mathrm{d}t + \mathrm{d}\xi \wedge \mathrm{d}x$, and we denote by $\{f, g\}$ the Poisson bracket of functions f and g, $\{f\ ,\ g\} = \nabla_{\tau,\xi} f \cdot \nabla_{t,x} g - \nabla_{t,x} f \cdot \nabla_{\tau,\xi} g$. The vector field H_f is the hamiltonian vector field associated with the function f, thus we have $\mathrm{d}g\ H_f = \{f\ ,\ g\} = \sigma(H_f, H_g)$.
A family (ψ^h) solution to (S_j) belongs to $\mathcal{C}(\mathbf{R}_t, L^2(\mathbf{R}^d, \mathbf{C}^{N(j)}))$ and thus to $L^2_{loc}(\mathbf{R}^{d+1}_{t,x})$. We consider semi-classical measures μ of (ψ^h) viewed as a function of (t, x). Matrix-valued measure μ acts on $\mathbf{R}^{2d+2}_{t,x,\tau,\xi}$ and is supported on

$$\Sigma = \left\{\mid p \mid^2 = \left(\tau + k + \frac{1}{2}|\xi|^2\right)^2\right\}.$$

Moreover, according to [15] and [16], μ decomposes as

$$\mu = \mu^+ + \mu^- \ \text{ with } \ \Pi^{\pm,j} \mu^\pm\, \Pi^{\pm,j} = \mu^\pm,$$

where $\Pi^{\pm,j}$ are the spectral projectors associated with matrix H_j for the eigenvalue $k \pm \mid p \mid$

$$\Pi^{\pm,j} = \frac{1}{2}\left[\mathbf{1} \pm \frac{1}{|p|}V_j(p)\right].$$

Moreover, $\mu^{\pm}$ are positive matrix-valued measures which satisfy the localization property

$$\mathrm{Supp}(\mu^{\pm}) \subset \{\tau + k + \frac{1}{2} \mid \xi \mid^2 \pm \mid p \mid = 0\}.$$

Outside

$$S = \{p = 0, \;\; \tau + k + \frac{1}{2} \mid \xi \mid^2 = 0\},$$

these measures propagate along the hamiltonian curves of

$$\lambda^{\pm} = \tau + k + \frac{1}{2} \mid \xi \mid^2 \pm \mid p \mid,$$

and we have

$$H_{\lambda^{\pm}}\mu^{\pm} = [F^{\pm,j} \;,\; \mu^{\pm}], \;\text{ outside }\; S, \tag{3}$$

with

$$F^{\pm,j} = \left[\Pi^{\pm,j} \;,\; \{\tau + k + \frac{|\xi|^2}{2} \pm |p| \;,\; \Pi^{\pm,j}\}\right] = \frac{1}{4|p|}\left[V_j\left(\frac{p}{|p|}\right), V_j(E)\right] \tag{4}$$

where the latter formula comes from the application of the result of [16] p.281. Therefore, as long as the classical trajectories do not reach S, Wigner measures of (ψ^h) are determined by the transport equations. The problem is that there exist classical trajectories which reach S in finite time.

1.2 The Geometry of the Crossing

The results of this section are corollaries of those proved in Section 2 of [10] in a larger framework. However, for the convenience of the reader, we give a direct proof of Propositions 1 and 2 in the Annex. In the following, we set $E = \mathrm{d}p(x)\xi$ and we consider the assumption

$$E \neq 0. \tag{$A2$}$$

Note that if $d = j$, the condition $(A2)$ simply reduces to $\xi \neq 0$. In [18], $d = j$ and the wave packets considered are supposed to have non-vanishing speed at the crossing, which means that $\xi \neq 0$ at the crossing points, i.e. that $(A2)$ holds at all the crossing points.

Proposition 1 . *Consider $\rho_0 \in S$ such that $(A1)$ and $(A2)$ hold in ρ_0, then there exist two unique curves ρ_s^+ and ρ_s^- such that*

$$\dot{\rho}_s^{\pm} = H_{\lambda^{\pm}}(\rho_s^{\pm}), \;\; \rho_0^{\pm} = \rho_0.$$

Moreover, $(\rho_s^{\pm})_{s\leq 0}$ can be smoothly continued by $(\rho_s^{\mp})_{s\geq 0}$.

Consider $\rho_0 \in S$ and a neighborhood $\mathcal{V}$ of ρ_0 in S such that $(A1)$ and $(A2)$ hold in $\mathcal{V}$. We define $J^{\pm,in}$ as the union of the curves $(\rho_s^{\pm})_{s<0}$ which reach $\mathcal{V}$, and $J^{\pm,out}$ the union of the curves $(\rho_s^{\pm})_{s>0}$ issued from $\mathcal{V}$. Because of Proposition 1,

$$J := J^{+,in} \cup J^{-,out}, \quad J' := J^{+,out} \cup J^{-,in},$$

are smooth submanifolds of $T^*\mathbf{R}^{d+1}$. We recall that a submanifold I of $T^*\mathbf{R}^{d+1}$ is said involutive if at any point $\rho \in I$, the vectorial subspace TI_ρ contains its orthogonal $TI_\rho^\perp$ for the symplectic form σ.

Proposition 2 . *If $(A1)$ and $(A2)$ hold in $\mathcal{V}$, the submanifolds J and J' are involutive submanifolds of $T^*\mathbf{R}^{d+1}$. Moreover, there exist smooth functions $u = u(t,x,\tau,\xi) \in \mathbf{S}^{j-1}$, $u' = u'(t,x,\tau,\xi) \in \mathbf{S}^{j-1}$ such that*

$$J = \left\{p = \left(\tau + k + |\xi|^2/2\right) u\right\}, \quad J' = \left\{p = \left(\tau + k + |\xi|^2/2\right) u'\right\},$$
$$u_{|S} = -u'_{|S} = -\frac{E}{|E|}.$$

As in [8], the knowledge of the in-coming semi-classical measure is not enough to describe the out-going one. The repartition of the energy depends on the way (ψ^h) concentrates on J or J' at the scale $\sqrt{h}$ which can be described by two-scale Wigner measures for involutive submanifolds. These measures, on which we shall focus now, have been introduced by L. Miller in [26] and studied in [8].

1.3 Two-scale Wigner Measures for Involutive Submanifolds

Let us consider for a while a more general setting and recall results of [8]. Let I be a codimension m involutive submanifold of the cotangent space $T^*\mathbf{R}^D$. We suppose that I is given by some system of equations $f = 0$ where $f = (f_1, \cdots, f_m) \in \mathcal{C}^\infty(\mathbf{R}^{2D}, \mathbf{R}^m)$, $\mathrm{Rank}(df) = m$ on $f = 0$, $\{f_j, f_k\} = 0$.
Let us denote by $\overline{\mathbf{R}^m}$, the sphere obtained by adding a sphere at infinity to $\mathbf{R}^m$. We consider the set $\mathcal{A}$ of symbols $a = a(z,\zeta,\eta) \in \mathcal{C}^\infty(\mathbf{R}^D \times \mathbf{R}^D \times \mathbf{R}^m)$ which are uniformly compactly supported in the variables (z,ζ) with respect to η and which can be extended in a function of $\mathcal{C}^\infty(\mathbf{R}^D \times \mathbf{R}^D \times \overline{\mathbf{R}^m})$ by

$$a(z,\zeta,\infty\omega) = \lim_{R\to+\infty} a(z,\zeta,R\omega), \quad \forall \omega \in \mathbf{S}^{m-1}.$$

With any $a \in \mathcal{A}$, we associate the two–scaled pseudo-differential operator,

$$\mathrm{op}_h{}^I\,(a) := \mathrm{op}_h\left(a(z,\zeta,\frac{f(z,\zeta)}{\sqrt{h}})\right).$$

By the Calderon-Vaillancourt theorem, the family of operators $\mathrm{op}_h{}^I\,(a)$ is a bounded family of bounded operators in $L^2(\mathbf{R}^D)$. If (ϕ^h) is a bounded family in $L^2(\mathbf{R}^D, \mathbf{C}^N)$, $N \in \mathbf{N}$, its concentration on I at the scale $\sqrt{h}$ is characterized two-microlocally by a positive Radon measure on the compactified bundle to I, $\overline{N}(I)$, which describes the evolution as h goes to 0 of

$$K_h(a) := \left(\mathrm{op}_h{}^I\,(a)\phi^h \;\mid\; \phi^h\right).$$

Let us explain which is the bundle $\overline{N}(I)$. We associate with I its tangent bundle TI. Quotienting the tangent space $T(\mathbf{R}^D)\mid_\rho$ above some point ρ of I by $TI\mid_\rho$, we obtain the fiber above ρ of the normal bundle to I, $N(I)$. Then, $\overline{N}(I)_{|\rho}$ is the closed m-dimensional ball obtained by adding a sphere at infinity to $N(I)\mid_\rho$. The choice of the equation f yields local coordinates on $\overline{N}(I)_{|\rho}$ given by the continuation $\overline{\chi}$ of the isomorphism χ,

$$\chi : [\delta\rho] \mapsto \eta = df(\rho)\delta\rho.$$

If ν is a measure on $\overline{N}(I)$, we denote by ν_f the measure on $\overline{\mathbf{R}^m}$ which is the image of ν by $\overline{\chi}$. Let us come back to the limit of $K_h(a)$.

There exist a sequence $h_k \underset{k\to+\infty}{\longrightarrow} 0$, a positive Radon measure ν on $\overline{N}(I)$ such that for all $a \in \mathcal{A}$,

$$K_{h_k}(a) \underset{k\to+\infty}{\longrightarrow} \mathrm{tr}\left(\int_{\overline{\mathbf{R}^m}} a\,\mathrm{d}\nu_f\right) + \mathrm{tr}\left(\int_{f\neq 0} a\left(x,\xi,\frac{f(x,\xi)}{\mid f(x,\xi)\mid}\infty\right)\mathrm{d}\mu\right),$$

where μ is a semi-classical measure of (ϕ^h).

We point out that ν determines μ above I by

$$\mu\mathbf{1}_I = \int_I \nu(x,\xi,\mathrm{d}\eta).$$

Our aim in the following is to calculate two-scale Wigner measures associated with family (ψ^h) solution to (S_j) and the involutive submanifolds J and J'.

1.4 The Landau-Zener Formula

We suppose that $(A1)$ and $(A2)$ hold in some $\rho_0 \in S$. We denote by $\overline{\nu}$ (resp. $\overline{\nu}'$) the measures associated with (ψ^h) and J (resp. J'). We denote by Σ^+, Σ^-, $\dot{J}^{\pm,in}$ and $\dot{J}^{\pm,out}$ the sets

$$\Sigma^\pm = \{\lambda^\pm = 0\},\;\; \dot{J}^{\pm,in} = J^{\pm,in}\backslash S,\;\; \dot{J}^{\pm,out} = J^{\pm,out}\backslash S.$$

We consider the bundles above $\Sigma^\pm$, $\overline{N}_{\Sigma^\pm}(\dot{J}^{\pm,in})$ and $\overline{N}_{\Sigma^\pm}(\dot{J}^{\pm,out})$ obtained respectively by compactification of the fibers of $T\Sigma^\pm/T(\dot{J}^{\pm,in})$ and of $T\Sigma^\pm/T(\dot{J}^{\pm,out})$. Because of the properties of localization of semi-classical measures, there exist scalar positive Radon measures $\nu^{\pm,in}$ and $\nu^{\pm,out}$ supported on $\overline{N}_{\Sigma^\pm}(\dot{J}^{\pm,in})$ and $\overline{N}_{\Sigma^\pm}(\dot{J}^{\pm,out})$ respectively such that

$$\overline{\nu} = \nu^{+,in} + \nu^{-,out},\;\; \overline{\nu}' = \nu^{-,in} + \nu^{+,out},$$
$$\Pi^\pm\nu^{\pm,in}\Pi^\pm = \nu^{\pm,in},\;\; \Pi^\pm\nu^{\pm,out}\Pi^\pm = \nu^{\pm,out}.$$

Moreover, if $\mathcal{L}^{\pm,in}(H_{\lambda^\pm})$ (resp. $\mathcal{L}^{\pm,out}(H_{\lambda^\pm})$) is the linearized hamiltonian flow of $\lambda^\pm$ transversally to $J^{\pm,in}$ (resp. $J^{\pm,out}$), in $\Sigma^\pm$, the measures $\nu^{\pm,in}$ (resp. $\nu^{\pm,out}$) satisfies

$$\begin{aligned} \mathcal{L}^{\pm,in}(H_{\lambda^\pm})\nu^{\pm,in} &= [\nu^{\pm,in}\ ,\ F^{\pm,j}], \\ \mathcal{L}^{\pm,out}(H_{\lambda^\pm})\nu^{\pm,out} &= [\nu^{\pm,out}\ ,\ F^{\pm,j}]. \end{aligned}$$

These propagation properties result from [15] and [8]. Observe that (4) and Proposition 2 yield that

$$\begin{aligned} F^{\pm,j} &= \frac{1}{4|p|}\mathrm{sgn}(\tau + k + \frac{|\xi|^2}{2})\,[V_j(u), V_j(E)] \text{ on } J, \\ F^{\pm,j} &= \frac{1}{2|p|}\mathrm{sgn}(\tau + k + \frac{|\xi|^2}{2})\,[V_j(u'), V_j(E)] \text{ on } J'. \end{aligned}$$

Since u and u' are colinear to E on S, $F^{\pm,j} = O(1)$ near S. Therefore, the transversality of the hamiltonian flows to S implies that, in the set of distributions, these measures have traces on S that we denote by $\nu_S^{\pm,in}$ and $\nu_S^{\pm,out}$. These four traces can be identified to measures on one set in which we can study the existing link between $\nu_S^{\pm,out}$ and $\nu_S^{\pm,in}$.

Lemma 1 . *For $\rho_0 \in S$, consider $\mathcal{P}(\rho_0) \in \mathcal{L}(\mathbf{R}^j)$, the orthogonal projection on the normal hyperplane to $E(\rho_0)$. The map*

$$\begin{aligned} \eta : T(T^*(\mathbf{R}^{d+1}))_{|\rho_0} &\to \mathbf{R}^j \\ \delta\rho &\mapsto \mathcal{P}(\rho_0)\,(\mathrm{d}p\,\delta\rho) \end{aligned}$$

induces some isomorphism between the limits of the fibres of $\overline{N}_{\Sigma^\pm}(\dot{J}^{\pm,in})$ and $\overline{N}_{\Sigma^\pm}(\dot{J}^{\pm,out})$ above some point ρ which goes to ρ_0 and this hyperplane.

This lemma is proved in the Annex.
Using this isomorphism η, the connection between $\nu_S^{\pm,in}$ and $\nu_S^{\pm,out}$ near the point ρ_0 is described by the following Theorem.

Theorem 1 . *If $\nu_S^{+,in}$ and $\nu_S^{-,in}$ are mutually singular, then*

$$\left\{ \begin{aligned} \nu_S^{+,out} &= T\nu_S^{-,in} + (1-T)\,\mathcal{R}_j\,\nu_S^{+,in}\,\mathcal{R}_j, \\ \nu_S^{-,out} &= T\nu_S^{+,in} + (1-T)\,\mathcal{R}_j\,\nu_S^{-,in}\,\mathcal{R}_j, \end{aligned} \right. \tag{5}$$

with for $\eta = \mathcal{P}(\mathrm{d}p\,\delta\rho)$.

$$T = \exp\left(-\frac{\pi}{|\,E\,|}|\eta|^2\right),$$

and for $\eta \neq 0$,

$$\mathcal{R}_j = V_j\left(\frac{\eta}{|\eta|}\right).$$

Remark 1 . *We emphasize that the part of the energy two-microlocally localized above $\eta = 0$ propagates along the smooth curves $(\rho_s^{\pm})_{s<0} \cup (\rho_s^{\mp})_{s>0}$, while the part localized on $|\eta| = +\infty$ is utterly reflected and is not at all transferred to the other mode.*

Remark 2 . *The results stated above can easily be generalized to time-dependant hamiltonians (i.e. $k = k(t,x)$, $p = p(t,x)$) provided the assumptions $(A1)$ and $(A2)$ are satisfied with*

$$E = \partial_t p + \nabla_x p \, \xi.$$

With such notation, Theorem 1 holds and the proof below applies easily.

Remark 3 . *Observe that if at $t = 0$, the initial data is localized on the $+$ mode and supported outside S, then we will have $\nu^{-,in} = 0$ when some classical trajectory will reach S for the first time. Therefore, the measures $\nu_S^{+,in}$ and $\nu_S^{-,in}$ will be mutually singular and Theorem 1 will apply. If one supposes moreover that $x \mapsto |p(x)|^2$ is convex, then, one can prove that the minus trajectories issued from point of S where $(A1)$ and $(A2)$ hold never reach S again. Therefore, the assumptions of Theorem 1 will be fulfilled above any point of S as soon as $(A1)$ and $(A2)$ are satisfied and the local result of Theorem 1 yields global results. Such phenomenon has already been described by the author and C. Lasser in [11] for linear codimension 2 crossings.*

The proof of this Theorem is mainly inspired by [10]. It crucially uses some reduction theorem which turns J and J' into vectorial subspaces. Since the reduction theorems for H_2 and H_3, $H_{3'}$ are direct consequences of the results of [9] (see also [4]) and [10] respectively, we focus on the proofs in the case of H_5.
This article is organized as follows. The Section 2 is devoted to the proof of the reduction Theorem. In Section 3, we prove the reflection of the measure for $\mid \eta \mid = \infty$ and, in Section 4, the Landau-Zener formula for $\mid \eta \mid < \infty$. Finally, the results concerning the geometry of the crossing are proved in the Annex.

Notations . For $\tilde{y} = (y_0, y') = (y_0, y_1, y_2, y_3) \in \mathbf{R}^4$, we denote by $q(\tilde{y})$ the quaternion

$$q(\tilde{y}) = \begin{pmatrix} y_0 + iy_1 & y_2 + iy_3 \\ -y_2 + iy_3 & y_0 - iy_1 \end{pmatrix}.$$

We shall use the following relations

$$\forall \tilde{y} \in \mathbf{R}^4, \;\; q(\tilde{y}) + q(\tilde{y})^* = 2y_0,$$
$$\forall \tilde{y} \in \mathbf{R}^4, \;\; q(\tilde{y}) q(\tilde{y})^* = \mid \tilde{y} \mid^2$$
$$\forall \tilde{y} \in \mathbf{R}^4, \;\; \forall \tilde{v} \in \mathbf{R}^4, \;\; q(\tilde{v}) q(\tilde{y}) = q(v_0 y_0 - v' \cdot y', v_0 y' + y_0 v' - v' \wedge y'),$$

where $v' \wedge y' = (v_2 y_3 - v_3 y_2, v_3 y_1 - v_1 y_3, v_1 y_2 - v_2 y_1)$.
For $y = (\tilde{y}, y_4) \in \mathbf{R}^5$, we set

$$V(y) = \begin{pmatrix} y_4 & q(\tilde{y}) \\ q(\tilde{y})^* & -y_4 \end{pmatrix}.$$

Therefore, we have $H_5 = k + V(p)$.

2 A Reduction Theorem in Codimension 5

We recall that if κ is a canonical transform of $T^*\mathbf{R}^{d+1}$, there exists some semi-classical Fourier integral operator $K = K_h$, called *associated with* κ, which satisfies: $\forall f \in L^2(\mathbf{R}^{d+1})$, $\forall a \in \mathcal{C}_0^\infty(\mathbf{R}^{2d+2})$,

$$K^* \text{ op}_h\ (a)Kf = \text{op}_h\ (a \circ \kappa)f + O(h^2)||f||_{L^2} \text{ in } L^2(\mathbf{R}^{d+1}). \tag{6}$$

The reader can refer to [28] for a complete study of semi-classical Fourier Integral Operator or to [8] where a self-contained approach is included, and where this claim is proved.

Theorem 2 . *Let ρ_0 be such that $(A1)$ and $(A2)$ hold in ρ_0, there exist a local canonical transform κ mapping a neighborhood of ρ_0 into some neighborhood Ω of* 0,

$$\kappa : (t, x, \tau, \xi) \mapsto (s, z, \sigma, \zeta), \ \ \kappa(\rho_0) = 0,$$

a semi-classical Fourier integral operator K associated with κ and a matrix A such that $v^h = K \text{ op}_h\ (A)\psi^h$ satisfies for any $\phi \in \mathcal{C}_0^\infty(\Omega)$,

$$\text{op}_h\ (\phi) \text{ op}_h \begin{pmatrix} -\sigma + s & q(\Gamma\tilde{\zeta}) \\ q^*(\Gamma\tilde{\zeta}) & -\sigma - s \end{pmatrix} v^h = O(h) \ \ in \ \ L^2(\mathbf{R}^d), \tag{7}$$

where $\zeta = (\tilde{\zeta}, \zeta_4, \cdots, \zeta_{d-1}) \in \mathbf{R}^d$ with $\tilde{\zeta} = (\zeta_0, \zeta_1, \zeta_2, \zeta_3) = (\zeta_0, \zeta') \in \mathbf{R}^4$ and where Γ is a smooth invertible matrix, $\Gamma \in \mathcal{C}^\infty(\mathbf{R}^{2d+2}_{s,z,\sigma,\zeta}, \mathbf{C}^{4,4})$. Moreover if $I = \{\tilde{\zeta} = 0\}$, then we have

$$J \cup J' = \{\sigma^2 = s^2\} \cap I,$$
$$J^{\pm,in} = \{\sigma \mp s = 0, \ s > 0\} \cap I, \ \ J^{\pm,out} = \{\sigma \pm s = 0, s < 0\} \cap I.$$

Remark 4 . *The above normal form is to compare with the normal forms obtained for (H_2), (H_3) and thus $(H_{3'})$ in [9], [4] and [10] :*

$$\begin{aligned} N_2 &= \begin{pmatrix} -\sigma + s & \alpha\zeta_1 \\ \alpha\zeta_1 & -\sigma - s \end{pmatrix}, \ \text{for } H_2, \\ N_3 &= \begin{pmatrix} -\sigma + s & \gamma_1\zeta_1 + \gamma_2\zeta_2 \\ \overline{\gamma}_1\zeta_1 + \overline{\gamma}_2\zeta_2 & -\sigma - s \end{pmatrix}, \ \text{for } H_3, \end{aligned}$$

where the real-valued function α does not vanish and the complex-valued functions γ_1 and γ_2 satisfy $\mathcal{I}m(\gamma_1\overline{\gamma}_2) \neq 0$.

The proof of this Theorem follows the proof of Theorem 2 in [10] which states the reduction result for codimension 3 crossings. The first step consists in taking advantage of algebraic properties of H_5 to turn this hamiltonian into some new one where equations of J and J' appear. Then, it remains to define the canonical transform and to reduce the study of (S_5) to this of (7) by means of semi-classical pseudo-differential calculus. We shall emphasize the first step which is specific to codimension 5 while the remainder of the proof is quite similar to the proof of Theorem 2 in [10]. Finally, at the end of this section, we use Theorem 2 to translate Theorem 1 in the coordinates (s, z, σ, ζ) in order to obtain an equivalent statement on the proof of which we shall focus in the following.

2.1 An Algebraic Lemma

We use the equations of J and J',

$$J = \{p = (\tau + k + \frac{1}{2}|\xi|^2)u\}, \quad J' = \{p = (\tau + k + \frac{1}{2}|\xi|^2)u'\}.$$

Observe that if $e = \frac{u'-u}{|u'-u|}$, and

$$L = \{p - (\tau + k + \frac{1}{2}|\xi|^2)u = \lambda e; \quad \lambda \in \mathbf{R}\},$$

then $J \cup J' = L \cap \Sigma$. Moreover we have

$$e_{|S} = -\frac{E}{|E|}. \tag{8}$$

Lemma 2 . *There exist a smooth matrix $A_1 = A_1(t, x, \tau, \xi)$, a smooth function*

$$\alpha = \alpha(t, x, \tau, \xi) = (\alpha_0, \alpha_1, \alpha_2, \alpha_3)$$

and equations of L, $g = (g_0, g_1, g_2, g_3)$, such that $H_5 = A_1^* H_5' A_1$ with

$$H_5' = \tau + k + \frac{1}{2}|\xi|^2 + \alpha \cdot g + \begin{pmatrix} (1-|\theta|^2)^{-1/2} p \cdot e & q(g) \\ q(g)^* & -(1-|\theta|^2)^{-1/2} p \cdot e \end{pmatrix}.$$

Moreover $\alpha_{|S} = 0$ and ${A_1}^*_{|S} = {A_1}^{-1}_{|S}$ with

$$\forall y \in \mathbf{R}^5, \;\; (A_1)_{|S} V(y) (A_1)^*_{|S} = V\left(l(y), -y \cdot \frac{E}{|E|}\right) \tag{9}$$

where the vector of $\mathbf{R}^4$, $l(y)$, consists in the coordinates of $\mathcal{P}(y)$, the orthogonal projection of y on the hyperplane normal to E in some orthonormal basis of this hyperplane.

Proof: The proof relies on two Lemmas. We consider the subset $\mathcal{U}$ of $U_4(\mathbf{R})$ defined by

$$\mathcal{U} = \left\{ U(y) = \begin{pmatrix} y_4 & q(\tilde{y}) \\ -q(\tilde{y})^* & y_4 \end{pmatrix}; \;\; y = (\tilde{y}, y_4) = (y_0, y', y_4) = (y_0, y_1, y_2, y_3, y_4) \in \mathbf{S}^4 \right\}.$$

Lemma 3 . *For all $y \in \mathbf{S}^4$, there exists $R_5 \in O(5)$ such that for all $v \in \mathbf{R}^5$, we have*

$$U(y) V(v) U(y)^* = V(R_y(v)),$$

with $(R_y(v))_j = v_j - 2y_j(v \cdot y)$, $0 \le j \le 3$ $(R_y(v))_4 = -v_4 + 2y_4(v \cdot y)$.

The proof of this lemma consists in straightforward calculations.
Consider now the vector $e = (e_0, e_1, e_2, e_3, e_4)$. If $e_4(\rho_0) \neq -1$, then $e_4 \neq -1$ near ρ_0 and the function $y = y(t, x, \tau, \xi) = (y_0, y_1, y_2, y_3, y_4)$ defined by

$$y_4 = \sqrt{\frac{1+e_4}{2}}, \quad y_j = \frac{1}{2y_4} e_j, \quad 0 \leq j \leq 3,$$

is a smooth function valued in $\mathbf{S}^4$. Moreover we have for this special y,

$$U(y)V(p)U(y)^* = V(\tilde{l}(p), p \cdot e),$$

where $\tilde{l}(p) \in \mathbf{R}^4$ are the coordinates in some orthonormal basis of the orthogonal projection of p on the hyperplane normal to e.
Let us suppose now that $e_4(\rho_0) = -1$. Since $|e| = 1$, $e_0(\rho_0) = 0$ and $e_0 \neq -1$ near ρ_0. Then we use the fact that

$$\frac{1}{2} \begin{pmatrix} \mathbf{1} & \mathbf{1} \\ \mathbf{1} & -\mathbf{1} \end{pmatrix} V(p) \begin{pmatrix} \mathbf{1} & \mathbf{1} \\ \mathbf{1} & -\mathbf{1} \end{pmatrix} = V(p_4, p_1, p_2, p_3, p_0).$$

Therefore, if we consider the function y defined by

$$y_4 = \sqrt{\frac{1+e_0}{2}}, \quad y_0 = \frac{1}{2y_0} e_4, \quad y_j = \frac{1}{2y_0} e_j, \quad j \in \{1, 2, 3\},$$

then $|y|^2 = 1$, $U(y)$ is smooth near ρ_0 and

$$\frac{1}{2} U(y) \begin{pmatrix} \mathbf{1} & \mathbf{1} \\ \mathbf{1} & -\mathbf{1} \end{pmatrix} V(p) \begin{pmatrix} \mathbf{1} & \mathbf{1} \\ \mathbf{1} & -\mathbf{1} \end{pmatrix} U(y)^* = V(\tilde{l}(p), p \cdot e),$$

where $\tilde{l}(p)$ again denotes the coordinates of the orthogonal projection of p on the hyperplane normal to e in some orthonormal basis.
We conclude on the existence of some smooth unitary matrix $A_2 = A_2(t, x, \tau, \xi)$ such that

$$A_2 H_5 A_2^* = \tau + k + \frac{1}{2}|\xi|^2 + V(\tilde{l}(p), p \cdot e),$$

with

$$\forall y \in \mathbf{R}^5, \quad |y|^2 = (y \cdot e)^2 + |\tilde{l}(y)|^2. \tag{10}$$

Let us denote by $\theta = \theta(t, x, \tau, \xi) = (\theta_0, \theta') = (\theta_0, \theta_1, \theta_2, \theta_3)$ the vector of $\mathbf{R}^4$ such that

$$\theta = \tilde{l}(u).$$

Observe that since $u_{|S} = -u'_{|S} = -e_{|S}$ and because of (10) we have

$$\theta_{|S} = 0. \tag{11}$$

We set

$$S(\theta) = \begin{pmatrix} \mathbf{1} & q(\theta) \\ q(\theta)^* & \mathbf{1} \end{pmatrix}.$$

We obtain

$$A_2 H_5 A_2^* = \left(\tau + k + \frac{1}{2}|\xi|^2\right) S(\theta) + V\left(\tilde{l}\left(p - (\tau + k + \frac{1}{2}|\xi|^2)u\right), p \cdot e\right).$$

Notice that the equations of L appear in this hamiltonian. However, we need to get rid of the matrix $S(\theta)$. Because of (11), matrix $S(\theta)$ is invertible near ρ_0 and we have moreover

$$\begin{aligned}
S(\theta)^{-1} &= (1-|\theta|^2)^{-1} S(-\theta), & (12)\\
\sqrt{S(\theta)} &= aS(b\theta) \text{ with } a = \frac{1}{2}\left(\sqrt{1+|\theta|} + \sqrt{1-|\theta|}\right),\ b = \left(1 + \sqrt{1-|\theta|^2}\right)^{-1} & (13)\\
\sqrt{S(\theta)}^{-1} &= a' S(-b\theta), \text{ with } a' = a(1-|\theta|^2)^{-1/2}. & (14)
\end{aligned}$$

Lemma 4 . $\forall y = (y_0, y', y_4) = (\tilde{y}, y_4) \in \mathbf{R}^5$, $\forall z = (z_0, z') \in \mathbf{R}^4$,

$$S(z)V(y)S(z) = 2z \cdot \tilde{y} + V\left((1-|z|^2)\tilde{y} + 2(z \cdot \tilde{y})z, (1-|z|^2)y_4\right).$$

This lemma comes again from straightforward computations.

We set

$$\phi(\tilde{y}, z) = (1-|z|^2)\tilde{y} + 2(z \cdot \tilde{y})z.$$

Observe that for z such that $|z| \neq 1$, $\phi(y,z) = 0$ if and only if $y = 0$. Lemma 4 and equation (14) yield that if $A_1 = \sqrt{S(\theta)}A_2$, $H_5 = A_1^* H_5' A_1$ with

$$H_5' = \tau + k + \frac{1}{2}|\xi|^2 - 2(a')^2 b\theta \cdot \tilde{l}\left(p - (\tau + k + \frac{1}{2}|\xi|^2)u\right) + (a')^2 V\left(g, (1 - b^2|\theta|^2)p \cdot e\right),$$

and

$$g = \phi\left(\tilde{l}\left(p - (\tau + k + \frac{1}{2}|\xi|^2)u\right), -b\theta\right). \tag{15}$$

Therefore, we have $g = 0$ if and only if $l\left(p - (\tau + k + \frac{1}{2}|\xi|^2)u\right) = 0$. By definition of l, we obtain that $g = 0$ if and only if $p - (\tau + k + \frac{1}{2}|\xi|^2)u$ is colinear to e, thus $g = 0$ is a system of equations of L. Therefore, there exists some vector-valued function α such that

$$\alpha \cdot g = -2(a')^2 b'\theta \cdot l\left(p - (\tau + k + \frac{1}{2}|\xi|^2)u\right).$$

Moreover, equation (11) yields $\alpha_{|S} = 0$ and $(A_1)_{|S} = (A_2)_{|S}$. By definition of A_2, l and because $u_{|S} = -\frac{E}{|E|}$, we obtain

$$(A_1)_{|S} V(y) (A_1)_{|S} = V\left(\tilde{l}_{|S}(y), y \cdot e_{|S}\right).$$

We set $\tilde{l}_{|S} = l$ and we check that

$$(a')^2(1 - b^2|\theta|^2) = (1 - |\theta|^2)^{-1/2},$$

which completes the proof of Lemma 2.

2.2 The Canonical Transform

Proposition 3 . *There exist some function λ, $\lambda > 0$ near ρ_0, and some local canonical transform*

$$\kappa : (t, x, \tau, \xi) \mapsto (s, z, \sigma, \zeta), \;\; \kappa(\rho_0) = 0,$$

such that

$$\begin{aligned} \sigma &= -\lambda(\tau + k + \frac{\mid \xi \mid^2}{2} + \alpha \cdot g), \\ s &= \lambda \frac{p \cdot e}{\sqrt{1 - \mid \theta \mid^2}}, \\ \lambda g &= \Gamma_1 \tilde{\zeta} + (\sigma^2 - s^2)\beta. \end{aligned} \tag{16}$$

where $\zeta = (\zeta_0, \zeta', \zeta_5, \cdots, \zeta_d) = (\tilde{\zeta}, \zeta_5, \cdots, \zeta_d)$, $\beta = \beta(s, z, \sigma, \zeta)$ is a smooth function valued in $\mathbf{R}^4$ and $\Gamma_1 = \Gamma_1(s, \sigma, z, \zeta)$ is a smooth invertible matrix. Moreover

$$\lambda^2_{|S} = 1/|E|. \tag{17}$$

Proof: We set

$$\check{\sigma} = -(\tau + k + \frac{\mid \xi \mid^2}{2} + \alpha \cdot g), \;\; \check{s} = \frac{p \cdot e}{\sqrt{1 - \mid \theta \mid^2}}.$$

Using (8), we obtain

$$\{\check{\sigma}\ ,\ \check{s}\}_{|S} = -\{\tau + k + \frac{|\xi|^2}{2}\ ,\ p\} \cdot e = |E| > 0.$$

Since moreover $\check{\sigma}$ and $\check{s}$ vanish in ρ_0, we can use Lemma 21.3.4. in [21] and we obtain the existence of some function $\lambda > 0$ such that $\{\lambda\check{\sigma}\ ,\ \lambda\check{s}\} = 1$.
By Darboux Theorem, we find functions $\underline{z}, \underline{\zeta}$ such that $(s, \underline{z}, \sigma, \underline{\zeta})$ are local symplectic coordinates near ρ_0. Let us denote by $\underline{f}$ the vector-valued function defined by

$$\underline{f}(s, \underline{z}, \sigma, \underline{\zeta}) = \lambda g(t, x, \tau, \xi).$$

Since $u \cdot e < 0$ and $u' \cdot e > 0$ by definition of e, we have

$$\begin{aligned} \mathrm{sgn}(s) &= -\mathrm{sgn}(\tau + k + |\xi|^2/2) \;\text{ on }\; J, \\ \mathrm{sgn}(s) &= \mathrm{sgn}(\tau + k + |\xi|^2/2) \;\text{ on }\; J'. \end{aligned}$$

Moreover we have $\tau + k + |\xi|^2/2 = \mp|p|$ on $J^{\pm,in} \cup J^{\pm,out}$. Therefore

$$\begin{aligned} \pm\sigma \geq 0 \quad &\text{on} \quad J^{\pm,in} \cup J^{\pm,out}, \\ s \geq 0 \quad &\text{on} \quad J^{+,in} \cup J^{-,in}, \\ s \leq 0 \quad &\text{on} \quad J^{+,out} \cup J^{-,out}. \end{aligned}$$

Moreover on L, we have $g = 0$, thus

$$\lambda^2(\tau + k + |\xi|^2/2)^2 = \sigma^2,$$

$$\begin{aligned}\lambda^2|p|^2 = \lambda^2(p \cdot e)^2 + \lambda^2|l(p)|^2 &= s^2(1 - |\theta|^2) + \lambda^2(\tau + k + |\xi|^2/2)^2|l(u)|^2 \\ &= s^2(1 - |\theta|^2) + \sigma^2|\theta|^2.\end{aligned}$$

Therefore $L \cap \{\sigma^2 = s^2\} = L \cap \Sigma$. Using $L \cap \Sigma = J \cup J'$, we obtain

$$\begin{aligned}J^{\pm,in} &= \{\sigma \mp s = 0, \;\; \underline{f} = 0, \;\; s > 0\}, \\ J^{\pm,out} &= \{\sigma \pm s = 0, \;\; \underline{f} = 0, \;\; s < 0\}.\end{aligned}$$

Since J and J' are involutive submanifolds, we have

$$\{\sigma \pm s \; , \; \underline{f}\} = 0, \;\; \text{on} \;\; \sigma \pm s = 0, \;\; \underline{f} = 0.$$

Arguing as in the proof of Lemma 4 in [10], we obtain that there exists some invertible matrix $\Gamma_2 = \Gamma_2(s, \underline{z}, \sigma, \underline{\zeta})$ and some function β such that

$$\underline{f}(s, \underline{z}, \sigma, \underline{\zeta}) = \Gamma_2(s, \underline{z}, \sigma, \underline{\zeta})\underline{f}(0, \underline{z}, 0, \underline{\zeta}) + (\sigma^2 - s^2)\beta(s, \underline{z}, \sigma, \underline{\zeta}).$$

Observe that the submanifold $\{\underline{f}(0, \underline{z}, 0, \underline{\zeta}) = 0\}$ is involutive. Therefore, there exist symplectic coordinates $z = z(\underline{z}, \underline{\zeta})$, $\zeta = \zeta(\underline{z}, \underline{\zeta})$ and an invertible smooth matrix $M = M(z, \zeta)$ such that

$$\underline{f}(0, \underline{z}, 0, \underline{\zeta}) = M(z, \zeta)\tilde{\zeta}, \;\; \tilde{\zeta} = (\zeta_0, \zeta_1, \zeta_2, \zeta_3),$$

whence (16) with $\Gamma_1(s, z, \sigma, \zeta) = \Gamma_2(s, \underline{z}, \sigma, \underline{\zeta})M(z, \zeta)$. $\diamondsuit$

2.3 Proof of Theorem 2

We set

$$A = \lambda^{-1/2} A_1 \tag{18}$$

and for $(s, z, \sigma, \zeta) = \kappa(t, x, \tau, \xi)$, we denote by $\tilde{f}$ the function defined by

$$\tilde{f}(s, z, \sigma, \zeta) = \lambda g(t, x, \tau, \xi) = \Gamma_1\tilde{\zeta} + (\sigma^2 - s^2).$$

We consider some semi-classical Fourier integral operator U associated with κ and we set

$$v^h = U \;\mathrm{op}_h\; (A)\psi^h.$$

Then, pseudo-differential symbolic calculus and (6) yield that, in $L^2(\mathbf{R}^{d+1})$,

$$\begin{aligned}\mathrm{op}_h \begin{pmatrix} -\sigma + s & q(\tilde{f}) \\ q(\tilde{f})^* & -\sigma + s \end{pmatrix} v^h &= U \;\mathrm{op}_h\; (\lambda H_5')v^h + O(h) \\ &= U \;\mathrm{op}_h\; ((A^*)^{-1}) \;\mathrm{op}_h\; (H_5) \;\mathrm{op}_h\; (A^{-1})v^h + O(h) \\ &= U \;\mathrm{op}_h\; ((A^*)^{-1}) \;\mathrm{op}_h\; (H_5)\psi^h + O(h) \\ &= O(h).\end{aligned}$$

We argue now as in [9], p. 19-20. Consider the symplectic coordinates

$$y = \sigma + s, \quad \eta = \sigma - s,$$

and some semi-classical Fourier integral operator K associated with it. We set $f = \Gamma_2 \tilde{\zeta}$ and

$$D = \sqrt{2} \begin{pmatrix} \eta & \mathbf{0} \\ \mathbf{0} & y \end{pmatrix}, \quad F = \begin{pmatrix} \mathbf{0} & q(f) \\ q(f)^* & \mathbf{0} \end{pmatrix}, \quad B = \begin{pmatrix} \mathbf{0} & q(\beta) \\ q(\beta)^* & \mathbf{0} \end{pmatrix}.$$

With these notations, we are left with system

$$\mathrm{op}_h\ (D - DBD) K v^h = \mathrm{op}_h\ (F) K v^h + O(h), \ \text{ in } \ L^2(\mathbf{R}^{d+1}).$$

Using pseudo-differential symbolic calculus and plugging the latter equation into itself, we get

$$\begin{aligned} \mathrm{op}_h\ (D) K v^h = {} & (\mathrm{op}_h\ (D)\ \mathrm{op}_h\ (B))^2\ \mathrm{op}_h\ (D) K v^h \\ & + \mathrm{op}_h\ (D)\ \mathrm{op}_h\ (B)\ \mathrm{op}_h\ (F) K v^h + \mathrm{op}_h\ (F) K v^h + O(h). \end{aligned}$$

Since BF commutes with D, we obtain

$$\Big(1 - (\mathrm{op}_h\ (D)\ \mathrm{op}_h\ (B))^2 - \mathrm{op}_h\ (B)\ \mathrm{op}_h\ (F)\Big)\ \mathrm{op}_h\ (D) K v^h = \mathrm{op}_h\ (F) K v^h + O(h).$$

Using a parametrix of the operator $P = 1 - (\mathrm{op}_h\ (D)\ \mathrm{op}_h\ (B))^2 - \mathrm{op}_h\ (B)\ \mathrm{op}_h\ (F)$ which exists near 0, one proves the existence of Γ with

$$\Gamma_{|S} = (\Gamma_1)_{|S} \tag{19}$$

such that $\mathrm{op}_h\ (D) K v^h = \mathrm{op}_h \begin{pmatrix} \mathbf{0} & q(\Gamma\tilde{\zeta}) \\ q(\Gamma\tilde{\zeta})^* & \mathbf{0} \end{pmatrix} K v^h + O(h)$, which completes the proof of Theorem 2.$\diamondsuit$

2.4 Consequences of the Reduction Theorem

The reduction Theorem 2 has two important consequences. The first one is that this Theorem provides us with some involutive submanifold of $T^*\mathbf{R}^{d+1}$, $I = \{\tilde{\zeta} = 0\}$, such that

$$J \cup J' = \Sigma \cap I,$$

with transverse intersection. Thus, if ν is the two-scale Wigner measure of (ψ^h) for I, we can identify measures $\overline{\nu}$, (resp. $\overline{\nu}'$) with ν above $\overline{N}(I)_{|J}$ (resp. $\overline{N}(I)_{|J'}$). Actually, if $\overline{N}_\Sigma(J)$ is the bundle above Σ obtained by compactification of the fibers of $T\Sigma/TJ$, the canonical isomorphism from $T\Sigma/TJ$ onto $T(T^*\mathbf{R}^{d+1}_{|J})/TJ_J$ extends in some isomorphism

$$\theta_{\Sigma,I} : \overline{N}_\Sigma(J) \to \overline{N}(I),$$

that we use for identifying $\overline{\nu}$ and $\nu\,\mathbf{1}_{\overline{N}(I)_{|J}}$. The reader can refer to Lemma 4 in [8] for a proof of this fact. Because of this identification, we shall focus in calculating the two-scale Wigner measure of (ψ^h) for I.
The second consequence is that because of the invariance of two-scale Wigner measure through canonical transform (see Lemma 2 in [8]), it is equivalent to study the two-scale Wigner measure of (v^h) for I, or of (ψ^h) for the same set. Indeed, the two-scale Wigner measures $\tilde{\nu}$ of (v^h) and ν of (ψ^h) are linked by

$$\forall a \in \mathcal{A},\ < a\ ,\ \tilde{\nu} >=< a \circ \overline{N}(\kappa)\ ,\ A\nu A^* >, \tag{20}$$

where for $(\rho,\eta) \in \overline{N}(I)$, $\overline{N}(\kappa)(\rho,\eta) = (\kappa(\rho),\eta)$.
We concentrate now on translating Theorem 1 into some result on $\tilde{\nu}$. We set

$$\tilde{\Pi}^{\pm} = \frac{1}{2}\left(1 \pm \frac{1}{\sqrt{s^2+|\Gamma\tilde{\zeta}|^2}} V(\Gamma\tilde{\zeta},s)\right). \tag{21}$$

We decompose $\tilde{\nu}$ as $\tilde{\nu} = \tilde{\nu}^+ + \tilde{\nu}^-$ with the commutation's relations

$$\tilde{\Pi}^{\pm}\tilde{\nu}^{\pm}\tilde{\Pi}^{\pm} = \tilde{\nu}^{\pm}, \tag{22}$$

and the localization property: $\tilde{\nu}^{\pm}$ is supported on $J^{\pm,in} \cup J^{\pm,out}$. Let us denote by $\tilde{\nu}^{\pm,in}$ (resp. $\tilde{\nu}^{\pm,out}$) the traces of $\tilde{\nu}^{\pm}$ on $s = 0^+$ (resp. $s = 0^-$). In view of (20), we have

$$\tilde{\nu}^{\pm,out} \circ \overline{N}(\kappa)^{-1} = A_{|S}\,\nu^{\pm,out}\,A^*_{|S},\ \ \tilde{\nu}^{\pm,in} \circ \overline{N}(\kappa)^{-1} = A_{|S}\,\nu^{\pm,in}\,A^*_{|S}.$$

In the coordinates (s,z,σ,ζ) we choose the equations of I, $\tilde{\zeta} = 0$. Let $\rho \in S$, this equation generates coordinates $\tilde{\eta} \in \overline{\mathbf{R}^4}$ on $\overline{N}(I)_{|\rho}$. In the coordinates (t,x,τ,ξ), we characterize $\overline{N}(I)_{|\rho}$ as in Lemma 1. We aim to express the transformation $\overline{N}(\kappa)$ in these systems of coordinates.
Note that, in view of (19) and of Proposition 3, we have

$$\Gamma_{|S}\,\mathrm{d}\tilde{\zeta} = \lambda\,\mathrm{d}g_{|S}.$$

Since $g = \tilde{l}\,(p - (\tau + k + |\xi|^2/2)u)$ with $u_{|S} = e_{|S} = -\frac{E}{|E|}$, we have for $\delta\rho \in TI_{|\rho}$, $\rho \in S$,

$$\Gamma(\rho)\,\mathrm{d}\tilde{\zeta} = \lambda\,\mathrm{d}g(\rho)\delta\rho = \lambda\,l\,(\mathrm{d}p(\rho)\delta\rho)\,,$$

where $l\,(\mathrm{d}p(\rho)\delta\rho)$ are the coordinates of $\mathcal{P}(\mathrm{d}p(\rho)\delta\rho)$, the orthogonal projection of $\mathrm{d}p(\rho)\delta\rho$ on the hyperplane normal to E in the orthonormal basis of this hyperplan introduced in Lemma 2. We denote by $\tilde{\eta}$ the coordinate on $N(I)$ induced by the choice of the equations $\tilde{\zeta}$ of I and we obtain that equations (5) write

$$\left\{\begin{array}{l} \tilde{\nu}^{+,out} = \tilde{T}\,\tilde{\nu}^{-,in} + (1-\tilde{T})\tilde{\mathcal{R}}\,\tilde{\nu}^{+,in}\,\tilde{\mathcal{R}}, \\ \tilde{\nu}^{-,out} = \tilde{T}\,\tilde{\nu}^{+,in} + (1-\tilde{T})\tilde{\mathcal{R}}\,\tilde{\nu}^{-,in}\,\tilde{\mathcal{R}}, \end{array}\right. \tag{23}$$

with,

$$\tilde{T} = T \circ \overline{N}(\kappa), \;\; \tilde{\mathcal{R}} = A_{|S}\mathcal{R}A_{|S}^{-1} \circ \overline{N}(\kappa).$$

By (18), we get

$$\tilde{\mathcal{R}} = A_{1|S}\mathcal{R}A_{1|S}^{-1} \circ \overline{N}(\kappa) = A_{1|S}\mathcal{R}A_{1|S}^{*} \circ \overline{N}(\kappa).$$

Therefore, (17) and (9) yield

$$\tilde{T}(z, \zeta_5, \cdots, \zeta_{d-1}, \tilde{\eta}) = \exp\left(-|\Gamma_{|S}\,\tilde{\eta}|^2\right),$$

$$\tilde{\mathcal{R}}(z, \zeta_5, \cdots, \zeta_{d-1}, \tilde{\eta}) = \frac{1}{|\Gamma_{|S}\tilde{\eta}|}\begin{pmatrix} \mathbf{0} & q(\Gamma_{|S}\,\tilde{\eta}) \\ q(\Gamma_{|S}\,\tilde{\eta})^* & \mathbf{0} \end{pmatrix}.$$

In the following sections, we drop the $\tilde{}$ on $\tilde{\eta}$ and we focus on proving these formula, for $|\eta| = \infty$ first, then for finite η.

Before closing this section, let us state a last result concerning system (7). The dependance on the variable σ of the function Γ does not prevent from dealing with system (7) as a system of evolution equations. Actually, arguing as in [10], Proposition 5, we can prove the following hyperbolic estimate.

Proposition 4 . *Let $\phi \in \mathcal{C}_0^\infty(\mathbf{R})$, $\phi(0) = 1$, then there exist $h_0 > 0$ and $\delta_0 > 0$ such that for any $\delta < \delta_0$, the family* $\mathrm{op}_h\left(\phi\left(\frac{|\zeta|^2}{\delta}\right)v^h\right)_{h<h_0}$ *is bounded in $L^\infty(\mathbf{R}_s, L^2(\mathbf{R}_z^d))$.*

Moreover, arguing as in [10] and [8], the following corollary is straightforward and will be useful in the following.

Corollary 1 . *If $b_h \in \mathcal{C}_0^\infty(\mathbf{R}^{2d+2})$, there exists some constant C such that*

$$\left|\left(\mathrm{op}_h\,(b_h)v^h \mid v^h\right)\right| \le C\int_{-\infty}^{+\infty} \operatorname*{Sup}_{\gamma+|\beta|\le N}\,\operatorname*{Sup}_{z,\sigma,\zeta}\left|\partial_z^\beta\partial_\sigma^\gamma b_h(s,z,\sigma,\zeta)\right|\,\mathrm{d}s.$$

3 Analysis at Infinity

In this section, we aim at proving equations (23) for $|\,\eta\,| = +\infty$, i.e.

$$\tilde{\nu}^{+,out} = \tilde{\mathcal{R}}\,\tilde{\nu}^{+,in}\,\tilde{\mathcal{R}}, \;\; \tilde{\nu}^{-,out} = \tilde{\mathcal{R}}\,\tilde{\nu}^{-,in}\,\tilde{\mathcal{R}}.$$

We follow the method developed in [8] and [10] with modifications induced by the fact that the eigenvalues of matrix V are of multiplicity 2 while it was exactly 1 in the references above. Thus, the proofs therein does not directly apply. However, it is possible to adapt them and the method we use below is not specific to multiplicity 2 and applies for higher multiplicity .

We shall focus on the plus mode, the proof for the minus mode is similar. Let us introduce first some notations. We set

$$\lambda = \sqrt{s^2 + |\Gamma\tilde{\zeta}|^2}, \quad A = V(\Gamma\tilde{\zeta}, s),$$

and we denote by (f^h) the family such that, locally near 0,

$$\frac{h}{i}\partial_s v^h = \mathrm{op}_h\,(A)v^h + hf^h,$$

with $(\mathrm{op}_h\,(\phi)f^h)$ bounded in $L^2_{s,z}$ for any ϕ compactly supported near enough 0. Then, for $\omega \in \mathbf{S}^1$, we denote by X_ω the norm 1 eigenvector of A for the eigenvalue λ defined for $s \neq 0$ or $\tilde{\zeta} \neq 0$ by

$$X_\omega = \frac{1}{\sqrt{2\lambda(\lambda - s)}}\left(q(\Gamma\tilde{\zeta})\omega, (\lambda - s)\omega\right) = \frac{1}{\sqrt{2\lambda(\lambda - s)}}(\lambda + A)\begin{pmatrix} 0 \\ \omega \end{pmatrix}.$$

We shall use the following properties of X_ω.

Lemma 5 **1)** $X_\omega = (0, \omega) + O(|\tilde{\zeta}|)$ *if* $s < 0$, $X_\omega = \left(q\left(\frac{\Gamma\tilde{\zeta}}{|\Gamma\tilde{\zeta}|}\right), 0\right) + O(|\tilde{\zeta}|)$ *if* $s > 0$.

2) *There exists some matrix-valued function ϕ, homogeneous of degree 0 in s, λ and $\tilde{\zeta}$, such that if (ω, ω') is some orthonormal basis of $\mathbf{R}^2$,*

$$\partial_s X_\omega = \frac{1}{2\lambda}\left(\partial_s A - \partial_s \lambda\right) X_\omega + (\phi\,\omega\cdot\omega')X_{\omega'}.$$

Proof: Point **1)** is straightforward by Taylor expansion. Let us focus on point **2)**. Consider $\omega,\ \omega' \in \mathbf{S}^1$ such that $\omega\cdot\omega' = 0$. The vectors X_ω and $X_{\omega'}$ form a orthonormal basis of the subspace of all the eigenvectors of A for the eigenvalue λ. Moreover, using that $X_\omega \cdot X_{\omega'} = 0$, we obtain that

$$\partial_s X_\omega \cdot X_{\omega'} = \frac{1}{2\lambda(\lambda - s)}\left[(\lambda + A)(\partial_s\lambda + \partial_s A)\begin{pmatrix} 0 \\ \omega \end{pmatrix}\right]\cdot\begin{pmatrix} 0 \\ \omega' \end{pmatrix} = 0.$$

We get, through straightforward computation,

$$\partial_s X_\omega \cdot X_{\omega'} = \frac{1}{2\lambda(\lambda - s)}\left(q(\Gamma\tilde{\zeta})^* q(\partial_s\Gamma\tilde{\zeta})\omega\cdot\omega'\right).$$

We set

$$\phi(s, z, \sigma, \zeta) = \frac{1}{2\lambda(\lambda - s)} q(\Gamma\tilde{\zeta})^* q(\partial_s\Gamma\tilde{\zeta}). \tag{24}$$

Since $|X_\omega| = 1$, we also have $\partial_s X_\omega \cdot X_\omega = 0$. Thus, the vector $\partial_s X_\omega$ is of the form

$$\partial_s X_\omega = (\phi\,\omega\cdot\omega')X_{\omega'} + Y,$$

where Y is an eigenvector of A for the eigenvalue $-\lambda$. The derivation in the variable s of the relation $AX_\omega = \lambda X_\omega$ yields

$$(\partial_s\lambda - \partial_s A)X_\omega = (A-\lambda)\partial_s X_\omega = -2\lambda Y = -2\lambda(\partial_s X_\omega - (\phi\omega\cdot\omega')X_{\omega'}),$$

whence **2)** of Lemma 5.$\diamondsuit$

We consider now $\omega,\omega'\in\mathbf{S}^1$ and the matrix

$$\Pi_{\omega,\omega'} = X_\omega \otimes \overline{X}_{\omega'}.$$

Because of (22), measure $\tilde\nu^+$ is utterly determined by the knowledge of $\mathrm{tr}\left(\Pi_{\omega,\omega'}\tilde\nu^+\right)$ for all $\omega,\omega'\in\mathbf{S}^1$. We set

$$\Pi^{in}_{\omega,\omega'} = \begin{pmatrix} q\left(\frac{\Gamma\tilde\zeta}{|\Gamma\tilde\zeta|}\right)\omega \\ 0\end{pmatrix} \otimes \overline{\begin{pmatrix} q\left(\frac{\Gamma\tilde\zeta}{|\Gamma\tilde\zeta|}\right)\omega' \\ 0\end{pmatrix}},\ \ \Pi^{out}_{\omega,\omega'} = \begin{pmatrix} 0\\ \omega\end{pmatrix}\otimes\begin{pmatrix} 0\\ \overline{\omega}'\end{pmatrix},$$

so that we have

$$\Pi_{\omega,\omega'} = \Pi^\infty_{\omega,\omega'} + O(|\tilde\zeta|) \tag{25}$$

with $\Pi^\infty_{\omega,\omega'} = \Pi^{in}_{\omega,\omega'}$ if $s>0$, $\Pi^\infty_{\omega,\omega'} = \Pi^{out}_{\omega,\omega'} + O(|\tilde\zeta|)$ if $s<0$. Consider now $\rho\in\mathcal{C}_0^\infty(\mathbf{R})$, $\rho = 1$ near 0. Since,

$$\tilde{\mathcal{R}}\,\Pi^{in}_{\omega,\omega'}\,\tilde{\mathcal{R}} = \Pi^{out}_{\omega,\omega'},$$

the relations (23) are equivalent to the fact that for all $a_0\in\mathcal{C}_0^\infty(\mathbf{R}^{2d+1}_{z,\sigma,\zeta}\times\mathbf{S}^1)$ and for all $\omega,\omega'\in\mathbf{S}^1$,

$$\begin{aligned}\lim_{\varepsilon\to 0}\ \mathrm{tr}\Big(&< \ \tilde\nu^+\,\mathbf{1}_{|\eta|=\infty}\ ,\ a_0(z,\sigma,\zeta,\frac{\eta}{|\eta|})\,\Pi^{out}_{\omega,\omega'}\,\rho(\frac{s}{\varepsilon})\ >\Big)\\ &= \lim_{\varepsilon\to 0}\mathrm{tr}\Big(<\tilde\nu^+\,\mathbf{1}_{|\eta|=\infty}\ ,\ a_0(z,\sigma,\zeta,\frac{\eta}{|\eta|})\,\Pi^{in}_{\omega,\omega'}\,\rho(\frac{s}{\varepsilon})\ >\Big).\end{aligned} \tag{26}$$

For a_0 as before, $\delta<\delta_0$, (where δ_0 is defined in Proposition 4), $R>0$, $\varepsilon>0$, we define a as

$$a(s,z,\sigma,\zeta,\eta) = \rho\left(\frac{s}{\varepsilon}\right)a_0(z,\sigma,\zeta,\frac{\eta}{|\eta|})\rho\left(\frac{|\tilde\zeta|^2}{\delta}\right)\left(1-\rho\left(\frac{|\eta|}{R}\right)\right).$$

The function a is a symbol of $\mathcal{A}$. Actually, a is smooth despite the term $\frac{\eta}{|\eta|}$ because $\eta\neq 0$ on $\mathrm{Supp}(a)$. For the same reason, the function

$$q_h(s,\sigma,z,\zeta,\eta) = a(s,z,\sigma,\zeta,\frac{\tilde\zeta}{\sqrt{h}})\Pi_{\omega,\omega'}$$

is smooth. Thus the operator $\mathrm{op}_h\,(q_h)$ is well defined. We shall denote it by ${\mathrm{op}_h}^I\,(a\Pi_{\omega,\omega'})$ even though $a\Pi_{\omega,\omega'}\notin\mathcal{A}$. This fact compels us to work in a larger class of symbol than $\mathcal{A}$.

Since $\Pi_{\omega,\omega'}$ is an homogeneous function of degree 0 of the variable $(s,\Gamma\tilde{\zeta})$, we have the estimate

$$\left|\partial^{\beta}_{\sigma,z,\zeta_5,\cdots,\zeta_d}\partial^{\alpha}_{s,\tilde{\zeta}}\, q_h\right| \leq C_{\alpha,\beta}(\varepsilon,\delta)\left(\frac{1}{R\sqrt{h}}\right)^{|\alpha|},$$

where we implicitly assumed $R\sqrt{h}\leq 1$. This estimate allows us to use Weyl-Hörmandes symbolic calculus for which we refer to Sections 18.4, 18.5 and 18.6 in [21]. The symbol q_h belongs to the class $S(1,g_h)$ where g_h is the metric

$$g_h = \mathrm{d}z^2 + \frac{\mathrm{d}s^2}{R^2 h} + h^2(\mathrm{d}\sigma^2 + \mathrm{d}\zeta_5^2 + \cdots + \mathrm{d}\zeta_d^2) + h\frac{\mathrm{d}\tilde{\zeta}^2}{R^2}.$$

Since $\frac{g_h}{g_h^\sigma} \leq \left(\frac{\sqrt{h}}{R}\right)^2$, the gain of this symbolic calculus is $\frac{\sqrt{h}}{R}$. Observe that, on the other hand, $\partial_s a\,\Pi_{\omega,\omega'}\in\mathcal{A}$ and by definition of ρ, $\mathbf{1}_{\pm s>0}\,\partial_s a\,\Pi_{\omega,\omega'}\in\mathcal{A}$. Moreover, because of (25), we have

$$\mathrm{tr} < \tilde{\nu}^+\,\mathbf{1}_{|\eta|=\infty}\mathbf{1}_{s>0}\ ,\ \frac{1}{\varepsilon}\rho'\left(\frac{s}{\varepsilon}\right)a_0\Pi^\infty_{\omega,\omega'} >= \lim_{R\to\infty}\lim_{\delta\to 0}\lim_{h\to 0}\left(\mathrm{op}_h{}^I\ (\partial_s a\,\Pi_{\omega,\omega'})\,v^h\,|\,v^h\right).$$

We obtain that (26) is equivalent to

$$\lim_{\varepsilon\to 0}\lim_{R\to\infty}\lim_{\delta\to 0}\lim_{h\to 0}\left(\mathrm{op}_h{}^I\ (\partial_s a\Pi_{\omega,\omega'})\,v^h\mid v^h\right) = 0.$$

The proof of this claim crucially uses Weyl-Hörmander metric g_h defined above and Corollary 1. It is inspired from Section 4.2 in [10] to which the reader can refer. We decompose

$$L_{\varepsilon,R,\delta,h}(a_0) := -\left(\mathrm{op}_h{}^I\ (\partial_s a\Pi_{\omega,\omega'})\,v^h\mid v^h\right)$$

as $L_{\varepsilon,R,\delta,h,0}(a_0) = L^1+L^2+L^3$ with

$$\begin{aligned}
L^1 &= \frac{i}{h}\left(\left[\mathrm{op}_h{}^I\ (a\Pi_{\omega,\omega'})\ ,\ \mathrm{op}_h\begin{pmatrix} s & q(\Gamma\tilde{\zeta})\\ q(\Gamma\tilde{\zeta})^* & -s\end{pmatrix}\right]v^h\mid v^h\right),\\
L^2 &= \left(\mathrm{op}_h{}^I\ (a\partial_s\Pi_{\omega,\omega'})\,v^h\mid v^h\right),\\
L^3 &= i\left(\mathrm{op}_h{}^I\ (a\Pi_{\omega,\omega'})f^h\mid v^h\right) - i\left(\mathrm{op}_h{}^I\ (a\Pi_{\omega,\omega'})v^h\mid f^h\right).
\end{aligned}$$

Then, we prove the convergence to 0 of L^1, L^2 and L^3. For $b=b(s,z,\sigma,\zeta,\eta)\in\mathcal{C}^\infty$, we set

$$b_h^\flat(s,z,\sigma,\zeta) = b(s,z,\sigma,\zeta,\frac{\tilde{\zeta}}{\sqrt{h}}),$$
$$b_h^\sharp(s,z,\sigma,\zeta) = b(s,z,h\sigma,h\zeta,\sqrt{h}\tilde{\zeta}),$$

so that we have for $b\in\mathcal{A}$,

$$\mathrm{op}_h{}^I\ (b) = \mathrm{op}_h\ (b_h^\flat) = \mathrm{op}_1\ (b_h^\sharp).$$

• We begin with L^3. By the Weyl–Hörmander symbolic calculus, if $\chi \in \mathcal{C}_0^\infty(\Omega)$ with $\chi = 1$ near the support of a, we have

$$\mathrm{op}_h{}^I\,(a\Pi_{\omega,\omega'}) = \mathrm{op}_h{}^I\,(a\chi\Pi_{\omega,\omega'}) = \mathrm{op}_h{}^I\,(a\Pi_{\omega,\omega'})\ \mathrm{op}_h\,(\chi) + \mathrm{op}_1\left(S\left(\frac{\sqrt{h}}{R}\right)^N, g_h\right),$$

for all $N \in \mathbf{N}$. On the other hand, we can apply Corollary 1 to the symbol $b_h = a_h^\flat \Pi_{\omega,\omega'}$. Using the explicit expressions of a and of $\Pi_{\omega,\omega'}$, we get

$$| L^3 | \leq C \int_{-\infty}^{+\infty} | \rho(\frac{s}{\varepsilon}) |\ ds + O\left(\left(\frac{\sqrt{h}}{R}\right)^N\right).$$

• Let us consider now L^1. Note that $A_h^\sharp \in S(\lambda_h^\sharp, g_h)$, therefore by symbolic calculus, we obtain

$$L^1 = \frac{1}{2}\left(\mathrm{op}_h\left(\{a_h^\flat \tilde{\Pi}_{\omega,\omega'}, A\} - \{A, a_h^\flat \tilde{\Pi}_{\omega,\omega'}\}\right) v^h \ \mid\ v^h\right) + O(\frac{1}{R^2}).$$

We set

$$b_h = \{a_h^\flat \tilde{\Pi}_{\omega,\omega'}, A\} - \{A, a_h^\flat \tilde{\Pi}_{\omega,\omega'}\}. \tag{27}$$

Observe that $\Pi_{\omega,\omega'} = U(s, \lambda, \Gamma\tilde{\zeta})$ where $U = U(r, t, X)$ is homogeneous of degree 0. Therefore, $\partial_s \Pi_{\omega,\omega'}$ and $\nabla_{\tilde{\zeta}} \Pi_{\omega,\omega'}$ are homogeneous of degree -1 in the variables s, λ and $\tilde{\zeta}$. However, $\partial_\sigma \Pi_{\omega,\omega'}$ and $\nabla_z \Pi_{\omega,\omega'}$ have a better degree of homogeneity, they are homogeneous function of degree 0 in λ, s and $\tilde{\zeta}$. Indeed, we have

$$\partial_\sigma \Pi_{\omega,\omega'} = \partial_\sigma \lambda\, \partial_r U(s, \lambda, \Gamma\tilde{\zeta}) + \nabla_X U(s, \lambda, \Gamma\tilde{\zeta}) \partial_\sigma \Gamma\, \tilde{\zeta},$$

with $\partial_\sigma \lambda = \lambda^{-1} \partial_\sigma \Gamma \tilde{\zeta} \cdot \Gamma \tilde{\zeta}$. Similar relations hold for $\partial_{z_j} \Pi_{\omega,\omega'}$. Note that, in (27), the derivatives $\partial_s \Pi_{\omega,\omega'}$ and $\nabla_{\tilde{\zeta}}$ appear with some factor $\tilde{\zeta}$, which compensates the -1 degree of homogeneity of these functions. Therefore, applying Corollary 1, we obtain the estimate

$$\left|\left(\mathrm{op}_h\,(b_h) v^h\ ,\ v^h\right)\right| \leq C \int_{-\infty}^{+\infty} \rho(\frac{s}{\varepsilon}) \mathrm{d}s = O(\varepsilon).$$

Thus

$$\limsup_{(\varepsilon,\delta)\to(0,0)}\ \limsup_{R\to+\infty}\ \limsup_{h\to 0}\ | L^1 | = 0.$$

• Finally, let us deal with the remainder term L^2. We claim that if $\omega \cdot \omega' = 0$,

$$\begin{aligned}
\partial_s \Pi_{\omega,\omega} &= \left[A, \frac{A}{2\lambda^2} \partial_s \Pi_{\omega,\omega}\right] - (\phi\, \omega \cdot \omega)(\Pi_{\omega',\omega} + \Pi_{\omega,\omega'}), \\
\partial_s \Pi_{\omega,\omega'} &= \left[A, \frac{A}{2\lambda^2} \partial_s \Pi_{\omega,\omega'}\right] - (\phi\, \omega \cdot \omega')(\Pi_{\omega,\omega} + \Pi_{\omega',\omega'}).
\end{aligned} \tag{28}$$

Indeed, because of **2)** of Lemma 5, if $M = \frac{1}{2\lambda}\left((\partial_s A - \partial_s \lambda)\right)$, we have for $\omega \cdot \omega' = 0$,

$$\begin{aligned} \partial_s \Pi_{\omega,\omega'} &= M\Pi_{\omega,\omega'} + \Pi_{\omega,\omega'}M + (\phi\,\omega\cdot\omega')(\Pi_{\omega,\omega} + \Pi_{\omega',\omega'}) \\ \partial_s \Pi_{\omega,\omega} &= M\Pi_{\omega,\omega} + \Pi_{\omega,\omega}M + (\phi\,\omega\cdot\omega)(\Pi_{\omega',\omega} + \Pi_{\omega,\omega'}). \end{aligned}$$

Observe that since

$$\partial_s(A^2) = \partial_s(\lambda^2) = A\partial_s A + A\partial_s A = 2\lambda\partial_s\lambda,$$

we have $AM + MA = 0$. Therefore, using

$$A\Pi_{\omega,\omega'} = \Pi_{\omega,\omega'}A = \lambda\Pi_{\omega,\omega'}, \quad A\Pi_{\omega,\omega} = \Pi_{\omega,\omega}A = \lambda\Pi_{\omega,\omega},$$

we obtain

$$\begin{aligned} A\partial_s\Pi_{\omega,\omega'}A &= -\lambda^2\partial_s\Pi_{\omega,\omega'} + 2\lambda^2(\phi\,\omega\cdot\omega')(\Pi_{\omega,\omega} + \Pi_{\omega',\omega'}), \\ A\partial_s\Pi_{\omega,\omega}A &= -\lambda^2\partial_s\Pi_{\omega,\omega} + 2\lambda^2(\phi\,\omega\cdot\omega)(\Pi_{\omega,\omega'} + \Pi_{\omega',\omega}). \end{aligned}$$

Hence (28).

This latter equation allows to conclude for L^2. Indeed, the homogeneity of ϕ and $\Pi_{\omega,\omega'}$ in s, λ and $\tilde{\zeta}$ yields that

$$\limsup_{(\varepsilon,\delta)\to(0,0)}\ \limsup_{R\to+\infty}\ \limsup_{h\to 0}\ \left|\left(\mathrm{op}_h{}^I\ \left(a(\phi\,\omega\cdot\omega')\Pi_{\omega,\omega'}\right)v^h \ \mid\ v^h\right)\right| = 0.$$

Moreover, we transform the bracket part of $\partial_s\Pi_{\omega,\omega'}$ as in [10] so that we can reuse the equation. In the metric g_h, $\lambda_h^\sharp \geq C\sqrt{h}R$ on $\mathrm{Supp}(a_h^\sharp)$

$$\left(a\lambda^{-2}A\right)_h^\sharp \partial_s\Pi_{\omega,\omega'} \in S\left(\frac{1}{\sqrt{h}R\lambda_h^\sharp}, g_h\right).$$

We obtain

$$\begin{aligned} \mathrm{op}_h{}^I\left(\left[A, \frac{A}{2\lambda^2}\partial_s\Pi_{\omega,\omega}\right]\right) \in \frac{1}{2}\ \mathrm{op}_h\ (A)\ \mathrm{op}_h{}^I\ \left(a\lambda^{-2}A\partial_s\Pi_{\omega,\omega'}\right) \\ -\frac{1}{2}\ \mathrm{op}_h{}^I\ \left(a\lambda^{-2}A\partial_s\Pi_{\omega,\omega'}\right)\mathrm{op}_h\ (A) + \mathrm{op}_1\ \left(S\left(\frac{1}{R^2}, g_h\right)\right). \end{aligned}$$

Therefore, we can use again the equation and we get

$$\begin{aligned} &\left(\mathrm{op}_h{}^I\ \left(\left[A, \frac{A}{2\lambda^2}\partial_s\Pi_{\omega,\omega}\right]\right)v^h \ \mid\ v^h\right) \\ &\qquad = O\left(\frac{1}{R^2}\right) + O(h) - \frac{h}{2i}\left(\mathrm{op}_h{}^I\ \left(\partial_s\left(a\lambda^{-2}A\partial_s\Pi_{\omega,\omega'}\right)\right)v^h \ \mid\ v^h\right). \end{aligned}$$

Since $\mid \partial^\beta_{\sigma,z}\partial_s \left(a\lambda^{-2}A\partial_s\Pi_{\omega,\omega'}\right)^\flat_h \mid\leq \frac{C}{(s^2+hR^2)^{3/2}}$, as h goes to 0,

$$\left(\mathrm{op}_h{}^I\left(\left[A, \frac{A}{2\lambda^2}\partial_s\Pi_{\omega,\omega}\right]\right)v^h \;\mid\; v^h\right)$$
$$= O\left(\frac{1}{R^2}\right) + o(1) + Ch\int_{-\infty}^{+\infty}\frac{ds}{(s^2+hR^2)^{3/2}} = o(1) + O\left(\frac{1}{R^2}\right).$$

Hence, $\limsup\limits_{R\to+\infty}\limsup\limits_{h\to 0} L^2 = 0$. This completes the proof of (23) for $|\eta| = +\infty$.$\diamondsuit$

4 Analysis at Finite Distance

In this section, we aim at proving Landau-Zener formula (23) in $\{|\eta| < +\infty\}$. We proceed in three steps. We begin by stating a normal form which holds in any ball $B\subset \mathbf{R}^4_\eta$. Then we are reduced to deal with some abstract scattering problem that can be solved explicitly. This allows to obtain Landau-Zener formula for measure $\tilde\nu$ and then for ν.

4.1 A Normal Form at Finite Distance

Proposition 5 . *For any ball $B\subset\mathbf{R}^4_\eta$, there exists a matrix $C\in\mathcal{C}^\infty_0(\mathbf{R}^{2d+4}_{s,z,\sigma,\zeta,\eta})$ such that if $u^h = \left(1+\sqrt{h}\,\mathrm{op}_h{}^I\,(C)\right)v^h$, then, in $L^2(\mathbf{R}^{d+1})$,*

$$\forall a\in\mathcal{C}^\infty_0(\mathbf{R}^{2d+2}\times B),\;\; \mathrm{op}_h{}^I\,(a)\,\mathrm{op}_h\begin{pmatrix}-\sigma+s & q(\Gamma_{|S}\tilde\zeta)\\ q(\Gamma_{|S}\tilde\zeta)^* & -\sigma-s\end{pmatrix}u^h = O(h).$$

Remark 5 . *Note that (u^h) and (v^h) have the same two-scale Wigner measure on I.*

Proof: We set $J = \begin{pmatrix}\mathbf{1} & \mathbf{0}\\ \mathbf{0} & \mathbf{-1}\end{pmatrix}\in\mathbf{R}^{4,4}$, $\Gamma^0 = \Gamma(s,z,0,\zeta)$ and $\Gamma^{00} = \Gamma(0,z,0,\zeta)$,

$$\tilde H_5 = \begin{pmatrix}-\sigma+s & q(\Gamma\tilde\zeta)\\ q(\Gamma\tilde\zeta)^* & -\sigma-s\end{pmatrix},\;\; \tilde H_5^0 = \begin{pmatrix}-\sigma+s & q(\Gamma^0\tilde\zeta)\\ q(\Gamma^0\tilde\zeta)^* & -\sigma-s\end{pmatrix},\;\; \tilde H_5^{00} = \begin{pmatrix}-\sigma+s & q(\Gamma^{00}\tilde\zeta)\\ q(\Gamma^{00}\tilde\zeta)^* & -\sigma-s\end{pmatrix}.$$

We prove the following lemma.

Lemma 6 . *There exist two smooth matrices $C_1 = C_1(s,z,\sigma,\zeta,\eta)$ and $C_2 = C_2(s,z,\sigma,\zeta,\eta)$, C_1, $C_2\in\mathcal{C}^\infty_0(\mathbf{R}^{2d+4})$ such that for all $a\in\mathcal{C}^\infty_0(\mathbf{R}^{2d+2}\times B)$,*

$$\|\,\mathrm{op}_h{}^I\,(a)\;\Big[\;\left(1+\sqrt{h}\,\mathrm{op}_h{}^I\,(JC_1J)\right)\mathrm{op}_h\,(\tilde H_5) - \mathrm{op}_h\,(\tilde H_5^0)\left(1+\sqrt{h}\,\mathrm{op}_h{}^I\,(C_1)\right)\Big]\,\|_{\mathcal{L}(L^2)} = O(h), \tag{29}$$

$$\|\,\mathrm{op}_h{}^I\,(a)\;\Big[\;\left(1+\sqrt{h}\,\mathrm{op}_h{}^I\,(C_2)\right)\mathrm{op}_h\,(\tilde H_5^0) - \mathrm{op}_h\,(\tilde H_5^{00})\left(1+\sqrt{h}\,\mathrm{op}_h{}^I\,(C_2)\right)\Big]\,\|_{\mathcal{L}(L^2)} = O(h). \tag{30}$$

This lemma yields Proposition 5 thanks to the following remark. Actually, observe that if a is compactly supported in all the variables $s, z, \sigma, \zeta, \eta$, then we have in $\mathcal{L}(L^2)$,

$$\mathrm{op}_h{}^I\ (a)\ \mathrm{op}_h\ (\zeta_j b) = \sqrt{h}\ \mathrm{op}_h{}^I\ (a\eta_j b) + O(\sqrt{h}).$$

Hence

$$||\ \mathrm{op}_h{}^I\ (a)\ \mathrm{op}_h\ (\zeta_j b)||_{\mathcal{L}(L^2)} = O(\sqrt{h}), \tag{31}$$

for $j \in \{0,1,2,3\}$ and $b \in \mathcal{C}_0^\infty(\mathbf{R}^{2d+2})$. Therefore, writing $\Gamma\tilde{\zeta} = \Gamma_{|S}\tilde{\zeta} + O(|\zeta|^2)$, we obtain that for any a compactly supported in all the variables,

$$||\ \mathrm{op}_h{}^I\ (a)\ \mathrm{op}_h\ \left(q(\Gamma\tilde{\zeta})\right) - \mathrm{op}_h{}^I\ (a)\ \mathrm{op}_h\ \left(q(\Gamma_{|S}\tilde{\zeta})\right) ||_{\mathcal{L}(L^2)} = O(h).$$

Therefore, equations(29) and (30) yield Proposition 5. $\diamondsuit$

Proof of Lemma 6: Equation (29) is equivalent to

$$||\ \mathrm{op}_h{}^I\ (a) \left[\left(1+\sqrt{h}\ \mathrm{op}_h{}^I\ (C_1)\right)\ \mathrm{op}_h\ (J\tilde{H}_5) - \mathrm{op}_h\ (J\tilde{H}_5^0)\left(1+\sqrt{h}\ \mathrm{op}_h{}^I\ (C_1)\right)\right] ||_{\mathcal{L}(L^2)} = O(h).$$

Note that $J\tilde{H}_5 = \begin{pmatrix} -\sigma+s & q(\Gamma\tilde{\zeta}) \\ -q(\Gamma\tilde{\zeta})^* & \sigma+s \end{pmatrix}$. We use symbolic calculus to expand in power of $\sqrt{h}$ the left hand side. Because of (31), we obtain that C_1 must satisfy,

$$\sigma[J, C_1] = \begin{pmatrix} \mathbf{0} & q\left((\Gamma^0-\Gamma)\eta\right) \\ -q\left((\Gamma^0-\Gamma)\eta\right)^* & \mathbf{0} \end{pmatrix}.$$

Therefore, we get

$$C_1 = \frac{1}{2\sigma}\begin{pmatrix} \mathbf{0} & q\left((\Gamma^0-\Gamma)\eta\right) \\ q\left((\Gamma^0-\Gamma)\eta\right)^* & \mathbf{0} \end{pmatrix}\chi(\eta),$$

for some function $\chi \in \mathcal{C}_0^\infty(\mathbf{R}^4_\eta)$ identically equal to 1 on B.
A similar proof determines C_2, whence Lemma 6.$\diamondsuit$

4.2 Landau-Zener Formula

Because of Proposition 5, once given some ball $B \subset \mathbf{R}^4_\eta$, we are reduced to the study of the traces on $s = 0^+$ and $s = 0^-$ of the two-scale Wigner measure of a family (u^h) satisfying

$$\forall a \in \mathcal{C}_0^\infty(\mathbf{R}^{2d+2}\times B),\ \ \mathrm{op}_h{}^I\ (a)\ \mathrm{op}_h \begin{pmatrix} -\sigma+s & q(\Gamma_{|S}\,\tilde{\zeta}) \\ q(\Gamma_{|S}\,\tilde{\zeta})^* & -\sigma-s \end{pmatrix} u^h = O(h)\ \text{ in }\ L^2(\mathbf{R}^{d+1}).$$

Moreover, by applying a cut-off function, we may suppose that Γ is compactly supported and turn $\Gamma_{|S}$ into $\phi(\eta)\Gamma_{|S}$ with ϕ compactly supported and identically equal to 1 on B.

In this way, our system is microlocalized in the ball B, which is enough to calculate the two-scale Wigner measures in B. We are left with a system of the form

$$\frac{h}{i}\partial_s u^h = {\rm op}_h{}^I \begin{pmatrix} s & \phi(\eta)q(\Gamma_{|S}\,\tilde\zeta) \\ \phi(\eta)q(\Gamma_{|S}\,\tilde\zeta)^* & -s \end{pmatrix} u^h + hf^h,$$

where $({\rm op}_h{}^I\ (a)f^h)$ is uniformly bounded in $L^2_{s,z}$ for symbols a compactly supported in $\mathbf{R}^{2d+2}\times B$. However, f^h does not contribute to the description of the traces on $s=0^+$, $s=0^-$ of the two-scale Wigner measure of (u^h). Actually, if $S_h(s,s')$ denotes the evolution operator associated with the free system

$$\frac{h}{i}\partial_s \underline{u}^h = {\rm op}_h{}^I \begin{pmatrix} s & \phi(\eta)q(\Gamma_{|S}\,\tilde\zeta) \\ \phi(\eta)q(\Gamma_{|S}\,\tilde\zeta)^* & -s \end{pmatrix} \underline{u}^h,\ \ \underline{u}^h_{|s=0} = u^h_{|s=0},$$

then we have

$$u^h = \underline{u}^h + i\int_0^s S_h(0,t)f^h(t){\rm d}t.$$

Hence, $u^h = \underline{u}^h + O(\sqrt{|s|})$ in $L^2(\mathbf{R}^d_z)$. Therefore, the traces of the two-scale Wigner measures of (u^h) and $(\underline{u}^h)$ on $s=0^\pm$ are the same. Let us denote by G the compact operator

$$G = {\rm op}_h{}^I \left(\phi(\eta)q(\Gamma_{|S}\,\eta)\right).$$

As a consequence of Proposition 7 in [10], we have the following Lemma.

Lemma 7 *There exist $\alpha_j^h = \alpha_j(z)$, $\omega_j^h = \omega_j^h(z)$, $j\in\{1,2\}$, such that, as h goes to 0, for any $\chi\in\mathcal{C}_0^\infty(\mathbf{R})$, $\chi(GG^*)\alpha_1^h$, $\chi(G^*G)\alpha_2^h$, $\chi(GG^*)\omega_1^h$ and $\chi(G^*G)\omega_2^h$ are bounded and for $s<0$,*

$$\begin{aligned} \chi(GG^*)\begin{pmatrix} u_1^h(s,z) \\ u_2^h(s,z)\end{pmatrix} &= \chi(GG^*){\rm e}^{i\frac{s^2}{2h}}\left|\frac{s}{\sqrt h}\right|^{i\frac{GG^*}{2}}\alpha_1^h + o(1), \\ \chi(G^*G)\begin{pmatrix} u_3^h(s,z) \\ u_4^h(s,z)\end{pmatrix} &= \chi(G^*G){\rm e}^{-i\frac{s^2}{2h}}\left|\frac{s}{\sqrt h}\right|^{-i\frac{G^*G}{2}}\alpha_2^h + o(1), \end{aligned}$$

for $s>0$,

$$\begin{aligned} \chi(GG^*)\begin{pmatrix} u_1^h(s,z) \\ u_2^h(s,z)\end{pmatrix} &= \chi(GG^*){\rm e}^{i\frac{s^2}{2h}}\left|\frac{s}{\sqrt h}\right|^{i\frac{GG^*}{2}}\omega_1^h + o(1), \\ \chi(G^*G)\begin{pmatrix} u_3^h(s,z) \\ u_4^h(s,z)\end{pmatrix} &= \chi(G^*G){\rm e}^{-i\frac{s^2}{2h}}\left|\frac{s}{\sqrt h}\right|^{-i\frac{G^*G}{2}}\omega_2^h + o(1), \end{aligned}$$

Moreover

$$\begin{pmatrix}\omega_1^h \\ \omega_2^h\end{pmatrix} = S^h\begin{pmatrix}\alpha_1^h \\ \alpha_2^h\end{pmatrix} \tag{32}$$

with

$$S^h = \begin{pmatrix} a(GG^*) & -\overline{b}(GG^*)G \\ b(G^*G)G^* & a(G^*G) \end{pmatrix},$$

with $a(\lambda) = \mathrm{e}^{-\pi\frac{\lambda}{2}}$, $b(\lambda) = \frac{2i\mathrm{e}^{i\frac{\pi}{4}}}{\lambda\sqrt{\pi}} 2^{-i\lambda/2}\mathrm{e}^{-\pi\frac{\lambda}{4}}\,\Gamma(1+i\frac{\lambda}{2})\,\mathrm{sh}(\frac{\pi\lambda}{2})$, $a(\lambda)^2 = 1-\lambda|b(\lambda)|^2$.

These formula allow to calculate two-scale Wigner measures thanks to Lemma 8 in [10] which states that for $\chi \in \mathcal{C}_0^\infty(\mathbf{R})$ we have,

$$\mathrm{op}_h{}^I\left(\chi\left(|\,\phi(\frac{\eta}{R})\Gamma_{|S}\eta\,|^2\right)\right) = \chi(GG^*) + o(1) = \chi(G^*G) + o(1). \tag{33}$$

In view of

$$\tilde{\Pi}^+ = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \text{ on } J^{+,in},\ \ \tilde{\Pi}^- = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} \text{ on } J^{-,in},$$
$$\tilde{\Pi}^+ = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} \text{ on } J^{+,out},\ \ \tilde{\Pi}^- = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \text{ on } J^{-,out},$$

we obtain that $\tilde{\nu}^+\,\mathbf{1}_{s>0}$ (resp. $\tilde{\nu}^-\,\mathbf{1}_{s>0}$) is the two-scale Wigner measure of the family $\mathrm{e}^{i\frac{s^2}{2h}}\left|\frac{s}{\sqrt{h}}\right|^{i\frac{GG^*}{2}}(\alpha_1^h,0)$ (resp. $\mathrm{e}^{-i\frac{s^2}{2h}}\left|\frac{s}{\sqrt{h}}\right|^{-i\frac{G^*G}{2}}(0,\alpha_2^h)$). Similarly, $\tilde{\nu}^+\,\mathbf{1}_{s<0}$ (resp. $\tilde{\nu}^-\,\mathbf{1}_{s<0}$) is the two-scale Wigner measure of the family $\mathrm{e}^{-i\frac{s^2}{2h}}\left|\frac{s}{\sqrt{h}}\right|^{-i\frac{G^*G}{2}}(0,\omega_2^h)$ (resp. $\mathrm{e}^{i\frac{s^2}{2h}}\left|\frac{s}{\sqrt{h}}\right|^{i\frac{GG^*}{2}}(\omega_1^h,0)$). We use Lemma 9 in [10]: for every $\chi \in C_0^\infty(\mathbf{R}^{2d+4})$), we have in $\mathcal{L}(L^2)$,

$$|\,\frac{s}{\sqrt{h}}\,|^{-i\frac{GG^*}{2}}\mathrm{op}_h{}^I(\chi)\,|\,\frac{s}{\sqrt{h}}\,|^{i\frac{GG^*}{2}} = |\,\frac{s}{\sqrt{h}}\,|^{-i\frac{G^*G}{2}}\mathrm{op}_h{}^I(\chi)\,|\,\frac{s}{\sqrt{h}}\,|^{i\frac{G^*G}{2}} + o(1) = \mathrm{op}_h{}^I(\chi) + o(1).$$

Therefore, $\tilde{\nu}^{+,in}$ (resp. $\tilde{\nu}^{-,in}$) is the two-scale Wigner measure of the family $(\alpha_1^h,0)$ (resp. $(0,\alpha_2^h)$). Similarly, $\tilde{\nu}^{+,out}$ (resp. $\tilde{\nu}^{-,out}$) is the two-scale Wigner measure of the family $(0,\omega_2^h)$ (resp. $(\omega_1^h,0)$). Observe that equation (32) yields,

$$\begin{pmatrix} \omega_1^h(z) \\ 0 \end{pmatrix} = a(GG^*)\begin{pmatrix} \alpha_1^h(z) \\ 0 \end{pmatrix} - b(GG^*)\begin{pmatrix} \mathbf{0} & G \\ G^* & \mathbf{0} \end{pmatrix}\begin{pmatrix} 0 \\ \alpha_2^h(z) \end{pmatrix},$$
$$\begin{pmatrix} 0 \\ \omega_2^h(z) \end{pmatrix} = a(G^*G)\begin{pmatrix} 0 \\ \alpha_2^h(z) \end{pmatrix} + b(G^*G)\begin{pmatrix} \mathbf{0} & G \\ G^* & \mathbf{0} \end{pmatrix}\begin{pmatrix} \alpha_1^h(z) \\ 0 \end{pmatrix}.$$

These relations yield (23) via (33), which completes the proof of Theorem 1.$\diamondsuit$

5 Appendix: The Geometry of the Crossing

Proof of Proposition 1: Consider $\rho_0 = (t_0, x_0, \tau_0, \xi_0) \in S$ such that $E(x_0,\xi_0) \neq 0$ and let us prove the local existence of some integral curves $\rho_s^\pm = (t_0+s, x_s^\pm, \xi_s^\pm, \tau_0)$ of $H_{\lambda^\pm}$. We must have

$$\dot{x}_s^\pm = \xi_s^\pm,\ \ \dot{\xi}_s^\pm = -\nabla k(x_s^\pm) \mp {}^t\nabla p(x_s^\pm)\frac{p(x_s^\pm)}{|p(x_s^\pm)|}.$$

In order to define $(\rho_s^+)_{s<0}$ and $(\rho_s^-)_{s>0}$, we aim at proving the existence of functions $\tilde{x}_s$, $\tilde{\xi}_s$ such that

$$\begin{cases} \tilde{x}_s = x_s^+,\ \ \tilde{\xi}_s = \xi_s^+ & \text{for}\ \ s<0,\\ \tilde{x}_s = x_s^-,\ \ \tilde{\xi}_s = \xi_s^- & \text{for}\ \ s>0.\end{cases}$$

Therefore, we have to solve

$$\frac{\mathrm{d}}{\mathrm{d}s}\tilde{x}_s = \tilde{\xi}_s,$$
$$\frac{\mathrm{d}}{\mathrm{d}s}\tilde{\xi}_s = -\nabla k(\tilde{x}_s) + \mathrm{sgn}(s)\, {}^t\nabla p(\tilde{x}_s)\frac{p(x_s^\pm)}{|p(x_s^\pm)|},$$
$$\frac{\mathrm{d}}{\mathrm{d}s}\left(p(\tilde{x}_s)\right) = E(\tilde{x}_s, \tilde{\xi}_s).$$

Necessarily, $p(\tilde{x}_s) = \int_0^s E(\tilde{x}_\sigma, \tilde{\xi}_\sigma)\mathrm{d}\sigma = s\int_0^1 E(\tilde{x}_{st}, \tilde{\xi}_{st})\mathrm{d}t$ and thus

$$\tilde{\xi}_s = \xi_0 - \int_0^s \left(\nabla k(\tilde{x}_\sigma) + {}^t\nabla p(\tilde{x}_\sigma)\frac{\int_0^1 E(\tilde{x}_{\sigma t}, \tilde{\xi}_{\sigma t})\,\mathrm{d}t}{|\int_0^1 E(\tilde{x}_{\sigma t}, \tilde{\xi}_{\sigma t})\,\mathrm{d}t|}\right)\mathrm{d}\sigma,\ \ \tilde{x}_s = x_0 + \int_0^s \tilde{\xi}_\sigma\,\mathrm{d}\sigma.$$

Since $E(\rho_0) \neq 0$, a fixed point argument can be ruled out on these latter equations. One defines $\tilde{x}_s$, $\tilde{\xi}_s$ and thus ρ_s^+ for $s<0$ and ρ_s^- for $s>0$. We argue similarly for ρ_s^-, $s<0$ and ρ_s^+, $s>0$.$\diamondsuit$

Let us denote by H and H' the limits of the two hamiltonian flows along J and J' above S, we have

$$\lim_{s\to 0^-} H_{\lambda^+}(\rho_s^+) = \lim_{s\to 0^+} H_{\lambda^-}(\rho_s^-) = H_{\tau+k+|\xi|^2/2} - \frac{E}{|E|}\cdot H_p := H,$$
$$\lim_{s\to 0^+} H_{\lambda^+}(\rho_s^+) = \lim_{s\to 0^-} H_{\lambda^-}(\rho_s^-) = H_{\tau+k+|\xi|^2/2} + \frac{E}{|E|}\cdot H_p := H'.$$

Proof of Proposition 2: Let us focus on J, the case of J' is similar. By definition, J is a codimension j submanifold of $T^*\mathbf{R}^{d+1}$. Moreover, since $H_{\lambda^\pm}$ are hamiltonian vector fields, J is an involutive submanifold if and only if for any $\rho \in S$, $TJ_{|\rho}$ is an involutive subspace. Since $TJ_{|\rho} = TS_{|\rho} \oplus \mathbf{R}\,H$, we have $(TJ_{|\rho})^\perp = (TS_{|\rho})^\perp \cap H^\perp$. Observe that

$$TS_{|\rho} = \mathrm{Vect}\left\{H_{\tau+k+|\xi|^2/2},\ H_{p_i},\ 0\le i\le j\right\},\ \ H = H_{\tau+k+|\xi|^2/2} - \frac{E}{|E|}\cdot H_p.$$

Simple calculation shows that if $\delta\rho \in (TJ_{|\rho})^\perp$, there exists $X \in \mathbf{R}^j$ such that

$$\begin{aligned}\delta\rho &= X\cdot H_p - X\cdot\frac{E}{|E|}H_{\tau+k+|\xi|^2/2}\\ &= -\left(X\cdot\frac{E}{|E|}\right)H + \left(X - X\cdot\frac{E}{|E|}\,\frac{E}{|E|}\right)\cdot H_p.\end{aligned}$$

Since $X' = X - X\cdot\frac{E}{|E|}\frac{E}{|E|}$ satisfies $X'\cdot E = 0$, $X'\cdot H_p \in TS_{|\rho}$. Thus, $\delta\rho \in TS_{|\rho}\oplus \mathbf{R}H = TJ_{|\rho}$ and $(TJ_{|\rho})^{\perp} \subset TJ_{|\rho}$, which proves that J is an involutive submanifold.

Since p is of rank j, there exists a function $y = y(t,x,\tau,\xi) \in \mathbf{R}^{2d-j+1}$ such that

$$(t,x,\tau,\xi) \mapsto (\tau + k + |\xi|^2/2, p, y)$$

is a local diffeomorphism near $\rho_0 \in S$. We claim that

$$\begin{aligned} J &\to \mathbf{R}^{2d-j+2} \\ \rho &\mapsto (\tau + k + |\xi|^2/2, y) \end{aligned}$$

also is a local diffeomorphism. Indeed, let $\delta\rho \in TJ$ be a null vector for the differential of this mapping at $\rho \in S$. We have $\delta\rho = \delta s + \lambda H$ with $\delta s \in TS_{|\rho}$ and $\lambda \in \mathbf{R}$. Thus

$$0 = \mathrm{d}(\tau + k)\delta\rho = \lambda\, \mathrm{d}(\tau + k + |\xi|^2/2)H = \lambda\sigma(H, H_{\tau+k+|\xi|^2/2}) = \lambda|E|.$$

Therefore $\lambda = 0$ and $\mathrm{d}y\,\delta s = 0$, whence $\delta s = 0$ in view of the definition of y.
As a consequence, there exist equations of J of the form $p = \phi(\tau + k + |\xi|^2/2, y)$. Since $|p| = |\tau + k + |\xi|^2/2|$ on J, there exists some smooth vector $u = u(t,x,\tau,\xi) \in \mathbf{S}^{j-1}$ such that $\phi(\tau + k + |\xi|^2/2, y) = (\tau + k + |\xi|^2/2)u$.

Observe that

$$\begin{aligned} E &= \lim_{s\to 0^-} \mathrm{d}p(x_s^+)H_{\lambda^+}(\rho_s^+) \\ &= \lim_{s\to 0^-} \mathrm{d}(\tau + k + |\xi|^2/2)(\rho_s^+)H_{\lambda^+}(\rho_s^+)\, u \\ &= -\lim_{s\to 0^-} \{\tau + k + |\xi|^2/2\ ,\ p\}\cdot\frac{p}{|p|}(\rho_s^+)u \quad = \quad -|E|\, u. \end{aligned}$$

Therefore we have $u_{|S} = -\frac{E}{|E|}$, which completes the proof of Proposition 2.$\diamondsuit$

Proof of Lemma 1: Let us study the limits of the fibers of $\overline{N}_{\Sigma^\pm}(j^{\pm,in})$ and $\overline{N}_{\Sigma^\pm}(j^{\pm,out})$ above some point ρ which goes to S. Consider $H^{\perp}$ and $(H')^{\perp}$ the orthogonal of H and H' respectively for the symplectic form on $T(T^*\mathbf{R}^{d+1})$. The measures $\nu_S^{+,in}$ and $\nu_S^{-,out}$ are measures on the compactified of $H^{\perp}/TJ$ and measures $\nu_S^{-,in}$ and $\nu_S^{+,out}$ on $(H')^{\perp}/TJ'$. Note that $TJ = TS\oplus\mathbf{R}H$ and $TJ' = TS\oplus\mathbf{R}H'$, therefore if we set

$$F = TJ + TJ' = TS\oplus\mathbf{R}H\oplus\mathbf{R}H',$$

the $(j-1)$ dimension spaces $H^{\perp}/TJ$ and $(H')^{\perp}/TJ'$ can be identified to $T(T^*\mathbf{R}^{d+1})/F$. Observe that

$$F^{\perp} = TJ^{\perp}\cap H^{\perp}\cap H'^{\perp} = \{W = X\cdot H_p,\ \ X\cdot E = 0,\ \ X\in\mathbf{R}^j\}.$$

Moreover, if $W = X \cdot H_p$ and $\delta\rho \in T(T^*\mathbf{R}^{d+1})_{|\rho}$, $\rho \in S$,

$$\sigma(W, \delta\rho) = -X \cdot \mathrm{d}p\, \delta\rho.$$

Therefore, if $\mathcal{P} \in \mathcal{L}(\mathbf{R}^j)$ is the orthogonal projection on the normal hyperplane to E, the class modulo F of $\delta\rho$ is utterly determined by the knowledge of $\mathcal{P}(\mathrm{d}p\, \delta\rho)$. We choose some orthonormal basis of the hyperplane normal to E, the map

$$\begin{aligned} \eta : T(T^*(\mathbf{R}^{d+1})) &\to \mathbf{R}^{j-1} \\ \delta\rho &\mapsto \mathcal{P}\left(\mathrm{d}p\, \delta\rho\right) \end{aligned}$$

defines a system of coordinates on $T(T^*\mathbf{R}^{d+1})/F$.

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