Wigner measures and codimension two crossings

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Abstract

This paper gives a semiclassical description of nucleonic propagation through codimension two crossings of electronic energy levels. Codimension two crossings are the simplest energy level crossings, which affect the Born-Oppenheimer approximation in the zeroth order term. The model we study is a two-level Schrödinger equation with a Laplacian as kinetic operator and a matrix-valued linear potential, whose eigenvalues cross, if the two nucleonic coordinates equal zero. We discuss the case of well-localized initial data and obtain a description of the wavefunction's two-scaled Wigner measure and of the weak limit of its position density, which is valid globally in time.

1 Introduction

The quantum-mechanical description of molecular dynamics is given by the time-dependent Schrödinger equation

$$ih\,\partial_t \phi^h = H^h_{mol}\,\phi^h, \quad \phi^h(0) = \phi^h_0. \tag{1}$$

For initial data $\phi^h_0 \in L^2(\mathbb{R}^{3N}, \mathbb{C})$, $N \geq 1$, and an essentially self-adjoint molecular Hamiltonian H^h_{mol}, the spectral theorem yields a unique mild solution

$$\phi^h \in \mathcal{C}(\mathbb{R}, L^2(\mathbb{R}^{3N}, \mathbb{C})).$$

If the molecule consists of k_e electrons and k_n nuclei with $k_e + k_n = N$, the molecular Hamiltonian H^h_{mol} can be written as

$$H^h_{mol} = -\frac{h^2}{2}\Delta_{x_n} + H_e(x_n),$$

where Δ_{x_n} denotes the Laplacian acting on the $3k_n$ nucleonic coordinates, while $H_e(x_n)$ is the electronic Hamiltonian acting on the $3k_e$ electronic coordinates. $H_e(x_n)$ depends parametrically on the nucleonic coordinates x_n and comprises the electrons' kinetics as well as the interaction between electrons and nuclei. The scale-parameter $h > 0$ is given by $h = \sqrt{m_e/M}$, where m_e is the electronic mass and M the average mass of the molecule's nuclei. In the following, we will study the limit

$$h \to 0, \text{ i.e. } M \to \infty.$$

We will concentrate on a closed subset $\sigma_*(x_n)$ of the electronic spectrum $\sigma(H_e(x_n))$, which is the union of two eigenvalues $\lambda_{1,2}(x_n)$ with the same multiplicity k and which is uniformly isolated from the rest of the electronic spectrum. That is, there is a constant $d > 0$, such that

$$\operatorname{dist}\left(\,\sigma_*(x_n),\ \sigma(H_e(x_n)) \setminus \sigma_*(x_n)\,\right) \geq d \quad \text{for all} \quad x_n \in \mathbb{R}^{3k_n}.$$

We denote the spectral projection of $H_e(x_n)$ associated with $\sigma_*(x_n)$ by $P_e(x_n)$ and the extension to $L^2(\mathbb{R}^{3N}, \mathbb{C})$ by $P_* = \int_{\mathbb{R}^{3k_n}}^{\oplus} P_e(x_n)\, dx_n$. If $\{\chi_j(x_n)(\cdot)\}_{j=1}^{2k}$ is a family of normalized eigenfunctions of $H_e(x_n)$ for the eigenvalues $\lambda_{1,2}(x_n)$, then we can write

$$\operatorname{Ran} P_* = \left\{ \sum_{j=1}^{2k} \int_{\mathbb{R}^{3k_n}}^{\oplus} \phi_j(x_n)\chi_j(x_n)\, dx_n \;:\; \phi = (\phi_j)_{j=1}^{2k} \in L^2(\mathbb{R}^{3k_n}, \mathbb{C}^{2k}) \right\}.$$

This description of $\operatorname{Ran} P_*$ induces an isometry $\mathcal{U} : \operatorname{Ran} P_* \to L^2(\mathbb{R}^{3k_n}, \mathbb{C}^{2k})$. Now, time-dependent Born-Oppenheimer theory, as carried out by H. Spohn and S. Teufel in [13], gives the following: If we choose initial data $\phi_0^h \in \operatorname{Ran} P_*$ with $\|\phi_0^h\|_{L^2} = 1$, then the solution ϕ^h of the molecular Schrödinger equation (1) can be approximated by a Born-Oppenheimer solution modulo an error of order h. That is,

$$\|\phi^h(t) - \phi_{BO}^h(t)\|_{L^2} = \mathcal{O}((1 + |t|)\, h),$$

for all times $t \in \mathbb{R}$, where $\phi_{BO}^h(t) = \mathcal{U}^* \exp\left(-i\frac{t}{h} H_{BO}^h\right) \mathcal{U}\, \phi_0^h$. If the eigenfunctions $\chi_j(x_n)(\cdot)$ can be chosen real-valued, then the Born-Oppenheimer Hamiltonian is given by

$$H_{BO}^h = -\frac{h^2}{2}\Delta_{x_n} + V(x_n), \tag{2}$$

where $V(x_n)$ is a potential, whose values are $2k \times 2k$ matrices. In this framework, $\operatorname{Ran} P_*$ is referred to as an adiabatically protected subspace (*adiabatos* $\sim$ impassable). We also note, that this type of observation dates back to the late 1920s and is originally assigned to M. Born, V. Fock, and R. Oppenheimer.

If the eigenvalues λ_1 and λ_2 also satisfy the gap-condition, that is if

$$|\lambda_1(x_n) - \lambda_2(x_n)| \geq d \quad \text{for all} \quad x_n \in \mathbb{R}^{3k_n},$$

then Born-Oppenheimer theory shows again adiabatic decoupling between the subspaces associated with λ_1 and λ_2, and the two-level Hamiltonian (2) splits into two scalar Born-Oppenheimer Hamiltonians, modulo an error of order h. If the preceeding gap-condition is hurt, we have to consider two cases: either the eigenvalues cross, i.e.

$$\exists\, \widetilde{x}_n \in \mathbb{R}^{3k_n} : \lambda_1(\widetilde{x}_n) = \lambda_2(\widetilde{x}_n) \qquad \text{(crossing)},$$

or they do not cross, but cannot be separated uniformly (avoided crossing). For generic crossings with mimimal multiplicity k, general symmetry considerations, as carried out in G. Hagedorn's monograph [8], restrict the codimension of the crossing manifold to be one, two, three, or five:

$$\operatorname{codim}_{\mathbb{R}^{3k_n}} \Big\{ x_n \in \mathbb{R}^{3k_n} \,:\, \lambda_1(x_n) = \lambda_2(x_n) \Big\} = \; 1, 2, 3, \text{ or } 5.$$

Codimension two, three, and five crossings affect Born-Oppenheimer approximation in the zeroth order term. This means, that there is leading order exchange between the eigenspaces associated to λ_1 and λ_2. In the following, we will turn to the simplest model system showing a codimension two crossing and study the Wigner measure associated with its solution. Reducing the nucleonic configuration space $\mathbb{R}^{3k_n}$ to $\mathbb{R}^2$, we study

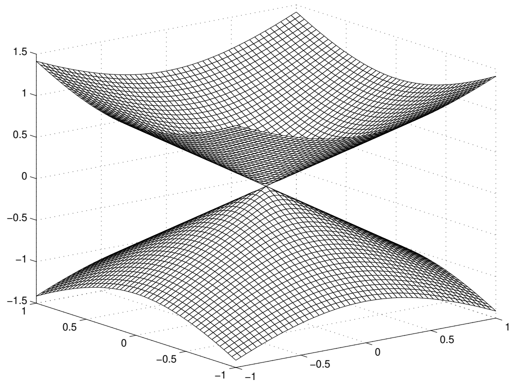
$$ih\, \partial_t \psi^h = -\frac{h^2}{2}\, \Delta_x\, \psi^h + V(x)\psi^h, \quad \psi^h(0) = \psi_0^h, \tag{3}$$

with $(\psi_0^h)_{h>0}$ a bounded family in $L^2(\mathbb{R}^2, \mathbb{C}^2)$, and V a matricial potential of the form

$$V(x) = \begin{pmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{pmatrix}, \quad x \in \mathbb{R}^2.$$

The Hamiltonian $-\frac{h^2}{2}\Delta_x + V(x)$ is an essentially self-adjoint operator on $L^2(\mathbb{R}^2, \mathbb{C}^2)$, and we have a unique mild solution $\psi^h \in \mathcal{C}(\mathbb{R}, L^2(\mathbb{R}^2, \mathbb{C}^2))$. The potential's eigenvalues $\pm|x|$ cross for $x = 0$ as depicted in the figure below, which plots $\pm|x|$ versus x_1 and x_2.

The mathematical analysis of the above model system has been initiated by G. Hagedorn in [8]. His result describes the evolution of the solution ψ^h itself, given special initial data, so called semi-classical wave packets. Recently, C. Fermanian and P. Gérard [6] have studied codimension two crossings from a Wigner measures' point of view. Their method applies to general initial data and covers Hamiltonians of the form $H^W(x, hD_x)$ with symbol $H(x, \xi) = K(\xi) + V(x)$, $K \in \mathcal{C}^\infty(\mathbb{R}^2, \mathbb{R})$.



Here, we aim at applying their result to well-localized initial data and the case, where the kinetics is given by a Laplacian, i.e. for $K(\xi) = |\xi|^2/2$. For this special situation, we will obtain an asymptotic description of the solution $\psi^h(t)$, which is valid *globally in time.*

Actually, we consider for a family of solutions $(\psi^h(t))_{h>0}$ of (3) the Wigner transforms

$$(W^h\psi^h)(t,x,\xi) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} \exp(iy\cdot\xi)\,\psi^h\left(t, x-\frac{h}{2}y\right)\otimes\overline{\psi^h}\left(t,x+\frac{h}{2}y\right)\,dy,$$

where $t\in\mathbb{R}$ and $(x,\xi)\in T^*\mathbb{R}^2 = \mathbb{R}^2\times\mathbb{R}^2$. Since $\psi^h(t,x)$ is a vector in $\mathbb{C}^2$, the Wigner transform is a hermitian matrix in $\mathbb{C}^{2,2}$. The families $(\psi^h(t))_{h>0}$ inherit uniform boundedness in $L^2(\mathbb{R}^2,\mathbb{C}^2)$ for all times $t\in\mathbb{R}$ from the initial data. Therefore, the family $(W^h\psi^h)_{h>0}$ is bounded in $L^\infty(\mathbb{R},\mathcal{S}'(T^*\mathbb{R}^2,\mathbb{C}^{2,2}))$, which means

$$\left|\int_{T^*\mathbb{R}^2}(W^h\psi^h)(t,x,\xi)\,a(x,\xi)\,dxd\xi\right| \le C$$

for all $t\in\mathbb{R}$ and all $a\in\mathcal{S}(T^*\mathbb{R}^2,\mathbb{C}^{2,2})$. Thus, there exist weak*-limit points of $(W^h\psi^h)_{h>0}$ in $L^\infty(\mathbb{R},\mathcal{S}'(T^*\mathbb{R}^2,\mathbb{C}^{2,2}))$. These limit points are called *Wigner measures*, since for fixed times t they are positive matrix-valued Radon measures on the phase space $T^*\mathbb{R}^2$. We refer to [7] for a complete treatment of these measures.

One important property of the Wigner measures $\mu(t,\cdot)$ is their relation to the position density $|\psi^h(t,x)|^2$. Let us consider some fixed time $t\in\mathbb{R}$. If the family of initial data $(\psi_0^h)_{h>0}$ is *h-oscillating,* that is if

$$\limsup_{h\to 0}\int_{|\xi|\ge\frac{R}{h}} |\ \widehat{\psi_0^h}(\xi)\ |^2\ d\xi \underset{R\to+\infty}{\longrightarrow} 0,$$

then $(\psi^h(t))_{h>0}$ inherits this property as well. Roughly speaking, h-oscillating families have frequencies of oscillations, which are of order less or equal to $1/h$. Furthermore, given h-oscillation, the weak limit points of $(\,|\psi^h(t,x)|^2\,)_{h>0}$ in $L^1(\mathbb{R}^2,\mathbb{C}^2)$ can be described by Wigner measures $\mu(t,\cdot)$ of $(\psi^h(t))_{h>0}$ via

$$\mathrm{w}-\lim_{h\to 0}|\ \psi^h(t,x)\ |^2 = \int_{\mathbb{R}^2_\xi} tr(\mu(t,x,d\xi)). \tag{4}$$

In the following, we will perform a *complete* study of the evolution of Wigner measures associated with solutions to (3), assuming specific initial data. This study, for example, covers the case of initial data microlocally localised on a set Σ_0 of the form

$$\Sigma_0 = \left\{(x,\xi)\in T^*\mathbb{R}^2 :\ |\ x\ |= R,\ \ x=\xi,\ \ x\cdot\omega_0>0\right\}$$

with radius $R>0$ and $\omega_0\in\mathbf{S}^1$, which means

$$\forall a\in\mathcal{C}_0^\infty(T^*\mathbb{R}^2\backslash\Sigma_0,\mathbb{C}^{2,2}):\ \int_{T^*\mathbb{R}^2}(W^h\psi_0^h)(x,\xi)\,a(x,\xi)\,dxd\xi \underset{h\to 0}{\longrightarrow} 0.$$

Thus, $(\psi_0^h)_{h>0}$ concentrates asymptotically on a half circle in position space and has asymptotically equal position and momentum. Moreover, we assume that $(\psi_0^h)_{h>0}$ is h-oscillating and localised on the eigenspace associated, say, with the eigenvalue $+|x|$ of $V(x)$. For example, we suppose

$$\Pi^-(x)\psi_0^h(x) \underset{h\to 0}{\longrightarrow} 0$$

strongly in $L^2(\mathbb{R}^2,\mathbb{C}^2)$, where $\Pi^\pm(x) = \frac{1}{2}(\mathrm{Id} \pm V(x)/|x|)$ denote the spectral projectors of $V(x)$ associated with $\pm|x|$. Assuming these initial data, the solution $(\psi^h(t))_{h>0}$ stays localised on the mode plus until it hits the crossing manifold $\{x=0\}$. At the crossing, we observe a Landau-Zener exchange between the eigenspaces, and $(\psi^h(t))_{h>0}$ will be localised on both modes. Our analysis gives the following theorem, which describes the weak limit of the position density globally in time.

Theorem 1 *Let $(\psi_0^h)_{h>0}$ be bounded in $L^2(\mathbb{R}^2,\mathbb{C}^2)$, h-oscillating, microlocally localised on Σ_0, and localised on the mode plus. Let $(\psi^h(t))_{h>0}$ be a family of solutions of (3) given the initial data $(\psi_0^h)_{h>0}$. We denote $C = R^2/2 + R$ and choose a smooth, compactly supported function $\phi \in \mathcal{C}_0^\infty\left(\{x\in\mathbb{R}^2 : |x| > C\},\mathbb{C}\right)$. Then we have*

$$\lim_{h\to 0}\int_{\mathbb{R}^2}\phi(x)\mid \Pi^+(x)\psi^h(t,x)\mid^2\, dx = 0$$

for all times $t\in\mathbb{R}$. Moreover, there exists a positive, increasing sequence $(t_j)_{j\geq 0}$ with $t_j\to+\infty$ as $j\to+\infty$, a sequence $(a_j)_{j\geq 0}$ of positive Radon measures on $\mathbf{S}^1$, and a sequence $(x_j)_{j\geq 0}$ in $\mathcal{C}^0(\mathbb{R},\mathbb{R}^2)$, such that

$$\lim_{h\to 0}\int_{\mathbb{R}^2}\phi(x)\mid \Pi^-(x)\psi^h(t,x)\mid^2\, dx = \sum_{0\leq k\leq j}\int_{\mathbf{S}^1}\phi\left(x_j(t)\omega\right)a_j(d\omega)$$

for $t\in(t_{j-1},t_j)$, $j\in\mathbb{N}_0$, where $t_{-1}=0$.

Thus, on the mode plus the solution asymptotically stays inside the ball of radius C. On the mode minus, points outside the ball are charged recurrently in time. Explicit formulae for the a_j, t_j and x_j are given in Section 4.

We will proceed as follows: In Section 2, we discuss propagation of Wigner measures and study the classical trajectories associated with the Schrödinger equation (3). Section 3 introduces two-scaled Wigner measures and gives some examples for well-localized data. In Section 4, we discuss Landau-Zener transitions between the two eigenspaces at points, where classical trajectories hit the crossing manifold $\{x=0\}$ recurrently in time, and obtain an asymptotic description of the solution's position density, which is valid globally in time.

2 Propagation of Wigner measures

Let $(\psi_0^h)_{h>0}$ be a family of initial data, which is bounded in $L^2(\mathbb{R}^2,\mathbb{C}^2)$, $(\psi^h(t))_{h>0}$ a family of solutions of (3), and $\mu(t,\cdot)$ an associated Wigner measure. The evolution of Wigner measures associated with solutions of a system, whose principal symbol admits eigenvalues of constant multiplicity but no crossings, has been studied in [7]. These results apply to system (3) *outside* the crossing manifold

$$S = \{(x, \xi) \in T^*\mathbb{R}^2 : x = 0\}.$$

We consider initial data $(\psi_0^h)_{h>0}$, such that the asociated Wigner measures μ_0 have support outside the singular set S. By the results of [7], outside S the Wigner measure $\mu(t, \cdot)$ commutes with the projectors $\Pi^\pm$ and thus can be decomposed as

$$\mu(t, \cdot) = \Pi^+ \mu(t, \cdot)\Pi^+ + \Pi^- \mu(t, \cdot)\Pi^-$$

in $\mathcal{D}'(\mathbb{R}, \mathcal{S}'(T^*\mathbb{R}^2, \mathbb{C}^{2,2}))$. Since the eigenspaces are one-dimensional, the decomposition simplifies to

$$\mu(t, \cdot) = \mu^+(t, \cdot)\Pi^+ + \mu^-(t, \cdot)\Pi^-,$$

where $\mu^\pm(t, \cdot) = tr(\Pi^\pm \mu(t, \cdot))$ are scalar positive Radon measures satisfying the transport equations

$$\partial_t \mu^\pm + \xi \cdot \nabla_x \mu^\pm \mp \frac{x}{|x|} \cdot \nabla_\xi \mu^\pm = 0, \quad \mu^\pm(0) = tr(\Pi^\pm \mu_0). \tag{5}$$

These transport equations give continuity of the maps $t \mapsto \mu^\pm(t, \cdot)$ and thus a description of $\mu^\pm(t, \cdot)$ on any given time interval, provided that the supports of $\mu^\pm(t, \cdot)$ do not intersect the crossing manifold S. We consider the flows of the associated Hamiltonian systems

$$\dot{x}^\pm(t) = \xi^\pm(t), \quad \dot{\xi}^\pm(t) = \mp \frac{x^\pm(t)}{|x^\pm(t)|}, \tag{6}$$

which describe the classical motion corresponding to the quantum-mechanical motion issued by the Schrödinger equation (3). Therefore, their solutions are called *classical trajectories.* The following proposition characterizes the trajectories, which touch the singular set S. For this, we will use the symplectic product

$$x \wedge \xi = x^\perp \cdot \xi = x_1\xi_2 - x_2\xi_1$$

for $(x, \xi) \in T^*\mathbb{R}^2$.

Proposition 1 *We consider classical trajectories with initial data $x^\pm(0) = x_0$, $\xi^\pm(0) = \xi_0$, $(x_0, \xi_0) \in T^*\mathbb{R}^2 \setminus \{0\}$.*

1. *If $x_0 \wedge \xi_0 \neq 0$, then $x^\pm(t) \wedge \xi^\pm(t) \neq 0$ for all $t \in \mathbb{R}$, and the classical trajectories do not reach $S = \{x = 0\}$.*

2. If $x_0 \wedge \xi_0 = 0$, then $x^{\pm}(t) \wedge \xi^{\pm}(t) = 0$ for all $t \in \mathbb{R}$, and the trajectory associated with the mode $+|x|$ is the first classical trajectory to hit S for a positive time t_0,

$$t_0 = \xi_0 \cdot \omega + \sqrt{|\xi_0|^2 + 2|x_0|},$$

where $\omega = \frac{x_0}{|x_0|}$ for $x_0 \neq 0$ and $\omega = \frac{\xi_0}{|\xi_0|}$ for $x_0 = 0$. Moreover we have for $t \in (0, t_0)$

$$x^{\pm}(t) = \mp \frac{t^2}{2} \omega + t\,\xi_0 + x_0, \quad \xi^{\pm}(t) = \mp t\omega + \xi_0. \tag{7}$$

Proof. Omitting the plus-minus superscripts for $x(t)$ and $\xi(t)$ unless the context requires, we start with the observation, that the Hamiltonian systems (6) are equivalent to the Newtonian equations

$$\ddot{x}(t) = -\nabla U^{\pm}(x(t)), \quad \dot{x}(0) = \xi_0, \quad x(0) = x_0,$$

with central field $U^{\pm}(y) = \pm|y|$. Motion in a central field conserves the angular momentum. Thus, we have

$$x(t) \wedge \dot{x}(t) = x_0 \wedge \xi_0, \quad \text{i.e.} \quad x(t) \wedge \xi(t) = x_0 \wedge \xi_0 \quad \text{for all } t \in \mathbb{R},$$

and the first assertion follows.

We turn to the case $x_0 \wedge \xi_0 = 0$. Inserting a Taylor expansion of $x(t)$ into (6), we get

$$\frac{x(t)}{|x(t)|} \underset{t \to 0^+}{\longrightarrow} \omega = \begin{cases} \frac{x_0}{|x_0|} & \text{if} \quad x_0 \neq 0, \\ \frac{\xi_0}{|\xi_0|} & \text{if} \quad x_0 = 0. \end{cases}$$

We rewrite $x(t), \xi(t)$ for small $t > 0$ as $x(t) = k(t)\omega$, $\xi(t) = l(t)\omega$ with $k(t), l(t) \in \mathbb{R}$, and are left with

$$\dot{k}^{\pm}(t) = l^{\pm}(t), \quad \dot{l}^{\pm}(t) = \mp 1, \quad k(0) = k_0, \quad l(0) = l_0.$$

Since $x(t) = t\xi_0 + o(t)$, we have $k_0 = |x_0|$. Moreover $l_0 = \operatorname{sgn}(x_0 \cdot \xi_0)|\xi_0|$ if $x_0 \neq 0$ and $l_0 = |\xi_0|$ if $x_0 = 0$. Thus, we have $l^{\pm}(t) = \mp t + l_0$, $k^{\pm}(t) = \mp\frac{t^2}{2} + l_0 t + k_0$ for small $t > 0$. The determinant for the zeros of $k^{\pm}(t)$ is $l_0^2 \pm 2k_0$. We distinct different cases.

If $l_0^2 < 2k_0$, then only the plus-trajectory hits S for some positive time t_0, i.e. for $t_0 = l_0 + \sqrt{l_0^2 + 2k_0}$.

If $l_0^2 = 2k_0$, then the plus-trajectory hits S for some $t_0 > 0$, before the minus-trajectory does so. The hitting time is given by $t_0 = l_0 + |l_0|\sqrt{2}$.

If $l_0^2 > 2k_0$, then we have to distinguish two cases. If $\operatorname{sgn}(l_0) > 0$, then only the plus-trajectory has a positive hitting time t_0, and we get again $t_0 = l_0 + \sqrt{l_0^2 + 2k_0}$. If $\operatorname{sgn}(l_0) < 0$, then the minus-trajectory also has a positive hitting time $s_0 = |l_0| - \sqrt{l_0^2 - 2k_0}$. However, an easy calculation gives $t_0 < s_0$, and we are done.

The preceeding proof contains the following easy observation concerning the trajectory associated with the mode $-|x|$, which will be useful later on.

Remark 1 *The minus-trajectory with initial data $x^-(0) = 0$, $\xi^-(0) = \xi_0$ with $\xi_0 \neq 0$ is given for positive times $t \in \mathbb{R}^+$ by*

$$x^-(t) = \left(\frac{t^2}{2|\xi_0|} + t\right)\xi_0, \quad \xi^-(t) = \left(\frac{t}{|\xi_0|} + 1\right)\xi_0.$$

This trajectory does not hit S for times $t \in \mathbb{R}^+$.

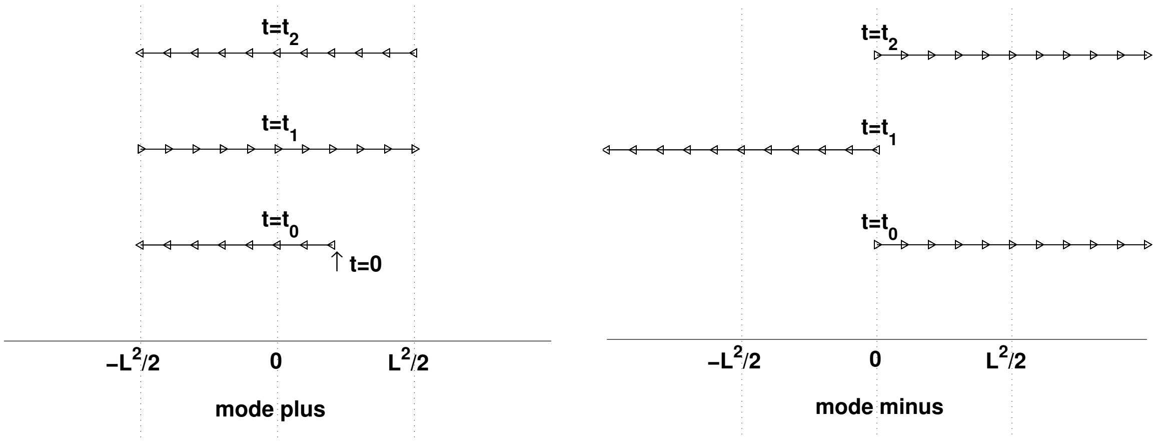
Next, we consider the plus-trajectory with initial data (x_0, ξ_0), $x_0 \wedge \xi_0 = 0$, $x_0 \neq 0$. By Proposition 1, we can also calculate the plus-trajectory after the first hitting time t_0. For this, we set again $\omega = \frac{x_0}{|x_0|}$ and

$$L = \sqrt{|\xi_0|^2 + 2|x_0|}, \qquad t_j = \xi_0 \cdot \omega + (2j+1)L \quad (j \in \mathbb{N}_0).$$

Remark 2 *The positive times, at which the plus-trajectory hits S, are given by t_j, $j \in \mathbb{N}_0$, and we have for $t \in (t_j, t_{j+1})$, $j \in \mathbb{N}_0$*

$$x^+(t) = (-1)^j \left(\frac{(t-t_j)^2}{2} - L(t-t_j)\right)\omega, \quad \xi^+(t) = (-1)^j (t - t_j - L)\,\omega.$$

We point out, that at any hitting time t_j we have $\xi^+(t_j) = (-1)^{j+1} L\omega \neq 0$. Thus, the preceeding remark is an immediate consequence of Proposition 1, using the change of sign of the fraction $\frac{x^\pm(t)}{|x^\pm(t)|}$ at the hitting times $t = t_j$.



The above figure summarizes our discussion, depicting the trajectories' x-component: Classical trajectories touching the singular set S are contained in the hypersurface

$$I = \left\{(x,\xi) \in T^*\mathbb{R}^2 : x \wedge \xi = 0\right\}.$$

Starting a plus-trajectory with initial data $(x_0, \xi_0) \in I \setminus S$, its x-component runs along the straight line given by ω. It hits S at time $t = t_0$ for the first time, and we start a minus-trajectory going off in the opposite direction. The plus-trajectory hits S again at time $t = t_1$, and the mode minus goes off in the opposite direction, and so on.

If we consider initial data $(\psi_0^h)_{h>0}$ for the Schrödinger equation (3), such that the associated Wigner measures μ_0 are supported in $\{(x_0, \xi_0)\}$ with $(x_0, \xi_0) \in I \setminus S$, then the transport equations (5) describe the evolution of the measures $\mu^\pm(t, \cdot)$ until the hitting time t_0. When arriving on S, we will observe some exchange between the plus- and the minus-mode, a Landau-Zener phenomenon. This quantum-mechanical effect has been described quantitatively for the first time by L. Landau in [11] and C. Zener in [14], independently from each other. The work of C. Fermanian and P. Gérard [6] shows, that this transfer does not depend on microlocal i.e. phase space information only, but that a second level of observation, which can be called "two-microlocal", must be taken into account as well. Their Landau-Zener type formula relies on some two-scaled variant of Wigner measures, which we will focus on in the following, such that we can continue the evolution of $\mu^\pm(t, \cdot)$ for times $t > t_0$ in the manner described for the classical trajectories above.

These two-scaled Wigner measures quantify the way a wave packet concentrates on the hypersurface I by introducing a new variable $\eta \in \overline{\mathbb{R}}$, which roughly speaking describes the distance of the core of a wave packet from I versus the scale $\sqrt{h}$, that is

$$\eta = \frac{x \wedge \xi}{\sqrt{h}}.$$

We note, that for all types of crossings, avoided and real crossings, the scale $\sqrt{h}$ is known to play an important role, see the work of Y. Colin de Verdière, M. Lombardi, J. Pollet [1], G.Hagedorn [8], G. Hagedorn, A. Joye [9], A. Joye [10], P. Exner, A. Joye [3] or P. Martin, G. Nenciu [12].

3 Two-scaled Wigner measures

The critical hypersurface $I = \{x \wedge \xi = 0\}$ is an involutive (or coisotropic) submanifold of $T^*\mathbb{R}^2$, i.e. we have $(T_z I)^\perp \subset T_z I$ for all $z \in I$, where $(T_z I)^\perp$ denotes the symplectic complement of the tangent space $T_z I$ in $T_z \mathbb{R}^2$. This is an immediate consequence of the obvious fact, that $(T_z I)^\perp$ is the linear span of the Hamiltonian vector field associated with the function

$$g : T^*\mathbb{R}^2 \to \mathbb{R}, \quad (x, \xi) \mapsto x \wedge \xi.$$

We now define a two-scaled Wigner transform of $(\psi^h)_{h>0}$ for $I = \{x \wedge \xi = 0\}$ with scale $\sqrt{h}$ by

$$W_2^h \psi^h(x, \xi, \eta) = W^h \psi^h(x, \xi) \otimes \delta\left(\eta - \frac{x \wedge \xi}{\sqrt{h}}\right), \quad (x, \xi, \eta) \in T^*\mathbb{R}^2 \times \mathbb{R},$$

which acts on the following class of test functions

$$\mathcal{A} = \big\{ a \in \mathcal{C}^\infty(T^*\mathbb{R}^2 \times \mathbb{R}, \mathbb{C}^{2,2}) : \operatorname{supp}(a) \subset K \times \mathbb{R} \text{ for compact } K \subset T^*\mathbb{R}^2 \setminus \{(0,0)\},$$
$$\exists\, a_\infty \in \mathcal{C}^\infty(T^*\mathbb{R}^2 \times \mathbf{S}^1, \mathbb{C}^{2,2}),\ \exists\, R = R(a) \in [0,+\infty),\ \forall x,\xi \in \mathbb{R}^2,\ \forall |\eta| \geq R :$$
$$a(x,\xi,\eta) = a_\infty(x,\xi,\operatorname{sgn}(\eta)) \big\},$$

where $\mathbf{S}^1$ denotes the unit sphere. These test functions differ from standard matrix-valued test functions in two ways: firstly, as functions of (x,ξ) alone they are compactly supported outside $\{(0,0)\}$. This restriction assures, that we are working in regions of the phase space $T^*\mathbb{R}^2$, where the gradient of the function g chosen to describe I does not vanish. Secondly, there is an additional coordinate $\eta \in \mathbb{R}$, which is used for measuring the distance from points in $T^*\mathbb{R}^2$ to the hypersurface I versus the scale $\sqrt{h}$. We denote by $\overline{\mathbb{R}}$ the one point compactification of $\mathbb{R}$ and continue $a(x,\xi,\cdot)$ continuously on $\overline{\mathbb{R}}$.

Let $(\psi^h)_{h>0}$ be a bounded family in $L^2(\mathbb{R}^2,\mathbb{C}^2)$. Théorème 1 in [6] shows, that there exists a subsequence $(h_k)_{k>0}$ with $h_k \to 0$ and a positive matrix-valued Radon measure ν on $I \times \overline{\mathbb{R}}$, such that for all $a \in \mathcal{A}$

$$\begin{aligned}\int_{T^*\mathbb{R}^2\times\mathbb{R}} tr\left(W_2^h\psi^h(x,\xi,\eta)a(x,\xi,\eta)\right)\, dx d\xi d\eta &= \int_{T^*\mathbb{R}^2} tr\left(W^h\psi^h(x,\xi)a(x,\xi,\tfrac{x\wedge\xi}{\sqrt{h}})\right)\, dx d\xi \\ &\overset{h_k\to 0}{\longrightarrow} \int_{T^*\mathbb{R}^2\setminus I} tr\left(a(x,\xi,\operatorname{sgn}(x\wedge\xi)\infty)\,\mu(dx,d\xi)\right) \\ &\qquad + \int_{I\times\overline{\mathbb{R}}} tr\left(a(x,\xi,\eta)\,\nu(dx,d\xi,d\eta)\right),\end{aligned} \tag{8}$$

where μ is a Wigner measure of (ψ^h).

Definition 1 *Let $(\psi^h)_{h>0}$ be a bounded family in $L^2(\mathbb{R}^2,\mathbb{C}^2)$. Then we call the Radon measures ν, which are associated via (8) to the weak*-limit points of $(W_2^h\psi^h)_{h>0}$ in $\mathcal{A}'$, two-scaled Wigner measures of $(\psi^h)_{h>0}$ for $I = \{x\wedge\xi = 0\}$ with scale $\sqrt{h}$.*

We note, that a two-scaled Wigner measure ν depends on the function g chosen to describe the hypersurface I; we consider another function $\widetilde{g} = fg$ with $f(x,\xi) \neq 0$ for all $x,\xi \in \mathbb{R}^2$ to describe the hypersurface I and a two-scaled Wigner measure $\widetilde{\nu}$ associated with $\widetilde{g}$ via (8). Then, we have for $a \in \mathcal{A}$

$$\int_{I\times\overline{\mathbb{R}}} a(x,\xi,\eta)\,\widetilde{\nu}(dx,d\xi,d\eta) = \int_{I\times\overline{\mathbb{R}}} a\left(x,\xi,f(x,\xi)\eta\right)\,\nu(dx,d\xi,d\eta). \tag{9}$$

This relation allows a geometrical interpretation of ν, see Section 1.3 in [6]. For our purpose, however, it will be enough to have relation (9). The key property of two-scaled Wigner measures is

$$\mathbb{1}_I(x,\xi)\,\mu(x,\xi) = \int_{\overline{\mathbb{R}}} \nu(x,\xi,d\eta).$$

That is, we can recover a Wigner measure's μ restriction to I by projecting a two-scaled measure ν onto I. We can derive this easily from the defining limit equation (8): we choose $\tilde{a} \in \mathcal{A}$ with $\tilde{a}(x,\xi,\eta) = a(x,\xi)\cdot 1$, where a is a smooth function compactly supported inside I. Then,

$$\begin{aligned}\int_{T^*\mathbb{R}^2\times\overline{\mathbb{R}}} tr(a(x,\xi)\nu(dx,d\xi,d\eta)) &= \int_{I\times\overline{\mathbb{R}}} tr(a(x,\xi)\nu(dx,d\xi,d\eta)) \\ &= \lim_{h_k\to 0}\int_{T^*\mathbb{R}^2} tr\left(W^h\psi^h(x,\xi)a(x,\xi)\right)\,dxd\xi - \int_{T^*\mathbb{R}^2\setminus I} tr(a(x,\xi)\mu(dx,d\xi)) \\ &= \int_I tr(a(x,\xi)\mu(dx,d\xi)).\end{aligned}$$

In [8], G. Hagedorn has also studied molecular propagation through codimension three and five crossings. For those systems, the codimension of the associated critical submanifold I is greater than one, but the submanifolds I are still involutive, and two-scaled Wigner measures of the same type as here can be applied. We refer to [6] for a definition of two-scaled Wigner measures associated with general involutive submanifolds. However, for Dirac systems different types of crossings occur, and the associated critical submanifolds are no more involutive but symplectic; see [5] for an analysis of a 2×2 Dirac system using two-scaled Wigner measures for symplectic submanifolds. We note, that those measures are close to the two-microlocal Wigner measures, which have been introduced without emphasizing a second scale [4].

In the following, we discuss some examples for two-scaled Wigner measures associated with $I = \{x \wedge \xi = 0\}$. For simplicity, the considered functions are all scalar-valued.

3.1 Some coherent states

We start with some coherent states of the form

$$\psi^h(x) = h^{-\beta}\Phi\left(\frac{x - x_0 - h^\gamma \eta_0}{h^\beta}\right)\exp\left(\tfrac{i}{h}\,\xi_0\cdot x\right)$$

with $\Phi \in L^2(\mathbb{R}^2,\mathbb{C})$, $0 < \beta \le 1$, $0 < \gamma < \beta$, and $x_0, \xi_0, \eta_0 \in \mathbb{R}^2$ with $x_0 \wedge \xi_0 = 0$.

If we choose $\beta = \frac{1}{2}$, $\eta_0 = 0$, and $\Phi(x) = \exp\left((x\cdot BA^{-1}x)/2\right)$ with $A, B \in \mathbb{C}^{2,2}$ invertible, then ψ^h is a semiclassical wave packet as considered by G. Hagedorn in [8]. Moreover, $(\psi^h)_{h>0}$ is h-oscillating, and we have for scalar-valued test functions $a \in \mathcal{A}$

$$\begin{aligned}&\int_{T^*\mathbb{R}^2} W^h\psi^h(x,\xi)a\left(x,\xi,\frac{x\wedge\xi}{\sqrt{h}}\right)\,dxd\xi = \\ &\qquad (2\pi)^{-2}\int_{T^*\mathbb{R}^2\times\mathbb{R}^2} \exp(iy\cdot\xi)\Phi(x-y/2)\overline{\Phi}(x+y/2)\times\end{aligned}$$

$$\times a\left(x_0 + h^\beta x + h^\gamma \eta_0, \xi_0 + h^{1-\beta}\xi, \frac{d(x,\xi)}{\sqrt{h}}\right) dydxd\xi,$$

where $d(x,\xi) = hx \wedge \xi + h^\beta x \wedge \xi_0 + h^{1-\beta} x_0 \wedge \xi + h^{1+\gamma-\beta}\eta_0 \wedge \xi + h^\gamma \eta_0 \wedge \xi_0$, so that

$$\frac{d(x,\xi)}{\sqrt{h}} = h^{\beta-\frac{1}{2}}\, x \wedge \xi_0 + h^{\frac{1}{2}-\beta}\, x_0 \wedge \xi + h^{\gamma-\frac{1}{2}}\, \eta_0 \wedge \xi_0 + o(h^{\frac{1}{2}-\beta}) + o(1). \tag{10}$$

Ignoring the η-component of a, we obtain the Wigner measure of (ψ^h)

$$\mu(x,\xi) = \|\Phi\|_{L^2}^2\ \delta(x - x_0) \otimes \delta(\xi - \xi_0),$$

which shows, that (ψ^h) concentrates on $I = \{x \wedge \xi = 0\}$.

However, the two-scaled measure for I with scale $\sqrt{h}$ depends on η_0 and γ. If $\beta = \frac{1}{2}$ and $\eta_0 \wedge \xi_0 = 0$, then the concentration of (ψ^h) on I is issued from finite distance. Otherwise, the concentration occurs from infinite distance (versus $\sqrt{h}$). Below, we discuss some significant cases. For simplicity, we assume $|x_0| = |\xi_0| = 1$.

$\beta = \frac{1}{2}$ and $\eta_0 \wedge \xi_0 = 0:$ The dominating term in (10) is $x \wedge \xi_0 + x_0 \wedge \xi$. For $t \in \mathbb{R}$ and $z \in \mathbb{R}^2$, we set $\Psi(x) = \exp\left(-\frac{i}{2}|x|^2 \mathrm{sgn}(x_0 \cdot \xi_0)\right)\Phi(x)$. Then,

$$\nu(x,\xi,\eta) = \delta(x - x_0) \otimes \delta(\xi - \xi_0) \otimes (2\pi)^{-2} \left(\int_{\mathbb{R}} |\ \widehat{\Psi}(tx_0 + \eta x_0^\perp)\ |^2\ dt\right) d\eta.$$

$\gamma < \beta = \frac{1}{2}$ and $\eta_0 \wedge \xi_0 \neq 0:$ The dominating term in (10) is $h^{\gamma-1/2}\eta_0 \wedge \xi_0$ and

$$\nu(x,\xi,\eta) = \mu(x,\xi) \otimes \delta(\eta - \mathrm{sgn}(\eta_0 \wedge \xi_0)\,\infty).$$

$\gamma < \beta < \frac{1}{2}:$ The dominating term in (10) is $h^{\gamma-1/2}\eta_0 \wedge \xi_0$ if $\eta_0 \wedge \xi_0 \neq 0$ and $h^{\beta-1/2}x \wedge \xi_0$ if $\eta_0 \wedge \xi_0 = 0$. In the first case we obtain as before

$$\nu(x,\xi,\eta) = \mu(x,\xi) \otimes \delta(\eta - \mathrm{sgn}(\eta_0 \wedge \xi_0)\,\infty).$$

In the second case we have to consider

$$\int_{\mathbb{R}^2} |\Phi(x)|^2 a(x_0, \xi_0, \mathrm{sgn}(x \wedge \xi_0)\infty)\, dx = \int_{\mathbb{R}^2} |\Phi(t\xi_0 + \eta\xi_0^\perp)|^2 a(x_0, \xi_0, -\mathrm{sgn}(\eta)\infty)\, dtd\eta.$$

Therefore,

$$\nu(x,\xi,\eta) = \delta(x - x_0) \otimes \delta(\xi - \xi_0) \otimes \left[\left(\int_{x\cdot\xi_0^\perp > 0} |\Phi(x)|^2\, dx\right) \delta(\eta + \infty) + \left(\int_{x\cdot\xi_0^\perp < 0} |\Phi(x)|^2\, dx\right) \delta(\eta - \infty)\right].$$

The case $\beta > \frac{1}{2}$ leads to a similar discussion with results depending on the sign of $\gamma - (1 - \beta)$.

3.2 Arbitrary phase

Replacing the linear phase by an arbitrary one, we now consider families of the form

$$\psi^h(x) = h^{-\beta}\Phi\left(\frac{x-x_0}{h^\beta}\right)\exp\left(\tfrac{i}{2h}f(|x|^2)\right)$$

with $\Phi \in L^2(\mathbb{R}^2,\mathbb{C})$, $f \in \mathcal{C}^1(\mathbb{R},\mathbb{R})$, $0<\beta<1$, and $x_0 \in \mathbb{R}^2 \setminus \{0\}$. Again, this family is h-oscillating. Writing

$$\begin{aligned}
&f(|\, x_0 + h^\beta z\,|^2) - f(|\, x_0 + h^\beta z'\,|^2)\\
&\quad = 2h^\beta(z-z')\cdot(x_0 + h^\beta\frac{z+z'}{2})\int_0^1 f'\left(t\,|\, x_0+h^\beta z\,|^2 + (1-t)\,|\, x_0 + h^\beta z'\,|^2\right)\,dt\\
&\quad =: 2h^\beta(z-z')\cdot(x_0+h^\beta\frac{z+z'}{2})l_h(x_0,z,z'),
\end{aligned}$$

for $z,z' \in \mathbb{R}^2$, we calculate for scalar-valued $a \in \mathcal{A}$

$$\begin{aligned}
&\int_{T^*\mathbb{R}^2} W^h\psi^h(x,\xi)a\left(x,\xi,\frac{x\wedge\xi}{\sqrt{h}}\right)\,dxd\xi \;=\\
&\qquad (2\pi)^{-2}\int_{T^*\mathbb{R}^2\times\mathbb{R}^2}\exp(iy\cdot\xi)\Phi(x-y/2)\overline{\Phi}(x+y/2)\,\times\\
&\qquad\qquad \times a\left(x_0+h^\beta x, l_h(x_0,x+\frac{y}{2},x-\frac{y}{2})(x_0+h^\beta x)+h^{1-\beta}\xi, \frac{d(x,\xi)}{\sqrt{h}}\right)\,dydxd\xi,
\end{aligned}$$

with

$$\frac{d(x,\xi)}{\sqrt{h}} \;=\; h^{\frac12-\beta}(x_0+h^\beta x)\wedge\xi \;=\; h^{\frac12-\beta}\,x_0\wedge\xi + o(1) \tag{11}$$

Since $\lim\limits_{h\to 0} l_h(x_0,z,z') = f'(|x_0|^2)$, we obtain the Wigner measure

$$\mu(x,\xi) = \|\Phi\|^2_{L^2}\,\delta(x-x_0)\otimes\delta(\xi - f'(|x_0|^2)\,x_0),$$

and have again concentration on $I=\{x\wedge\xi=0\}$. However, $\sqrt{h}$-concentration is issued from finite distance if and only if $\beta\le\frac12$. We distinguish three different cases, assuming $|x_0|=1$.

$\beta<\frac12$: $\quad \nu(x,\xi,\eta)=\mu(x,\xi)\otimes\delta(\eta)$.

$\beta=\frac12$:

$$\nu(x,\xi,\eta) = \delta(x-x_0)\otimes\delta(\xi-f'(1)\,x_0)\otimes(2\pi)^{-2}\left(\int_{\mathbb{R}}|\,\widehat{\Phi}(tx_0+\eta x_0^\perp)\,|^2\;dt\right)d\eta.$$

$\beta > \frac{1}{2}$:

$$\nu(x,\xi,\eta) = \delta(x-x_0)\otimes\delta(\xi - f'(1)\,x_0)\otimes$$
$$(2\pi)^{-2}\left[\left(\int_{x_0\wedge\xi>0} \mid \widehat{\Phi}(\xi)\mid^2\ d\xi\right)\,\delta(\eta-\infty) + \left(\int_{x_0\wedge\xi<0} \mid \widehat{\Phi}(\xi)\mid^2\ d\xi\right)\,\delta(\eta+\infty)\right].$$

Of course, the above discussion easily extends to families

$$\psi^h(x) = h^{-\beta}\Phi\left(\frac{x-x_0-h^\gamma\eta_0}{h^\beta}\right)\exp\left(\tfrac{i}{2h}f(|x|^2)\right)$$

with $0<\gamma<\beta$ and $\eta_0\in\mathbb{R}^2$.

3.3 Concentration on a circle

Finally, we consider families of the form

$$\psi^h(x) = h^{-\frac{1}{4}}\Phi\left(\tfrac{|x|^2-R^2}{\sqrt{h}}\right)\exp\left(\tfrac{i}{2h}\mid x-h^\gamma x_0\mid^2\right),$$

where $\Phi\in\mathcal{C}_0^\infty(\mathbb{R},\mathbb{C})$, $x_0\in\mathbb{R}^2$, $R>0$ and $0<\gamma<1$. Once again, such families are h-oscillating. We have for scalar-valued $a\in\mathcal{A}$

$$I_h := \int_{T^*\mathbb{R}^2} W^h\psi^h(x,\xi)a\left(x,\xi,\frac{x\wedge\xi}{\sqrt{h}}\right)\,dxd\xi =$$
$$\int_{T^*\mathbb{R}^2\times\mathbb{R}^2}\exp(iy\cdot\xi)\Phi\left(\tfrac{|x-y/2|^2-R^2}{\sqrt{h}}\right)\overline{\Phi}\left(\tfrac{|x+y/2|^2-R^2}{\sqrt{h}}\right)\times$$
$$\times a(x,x-h^\gamma x_0+h\xi,\sqrt{h}x\wedge\xi+h^{\gamma-\frac{1}{2}}x_0\wedge x)\,\frac{dy\,dx\,d\xi}{(2\pi)^2\sqrt{h}},$$

and thus by the Fourier inversion formula

$$I_h = \int a(x,x-h^\gamma x_0+h\xi,\sqrt{h}x\wedge\xi+h^{\gamma-\frac{1}{2}}x_0\wedge x)\widehat{\Phi}(\mu-v/2)\overline{\widehat{\Phi}}(\mu+v/2)\times$$
$$\times\exp(iy\cdot\xi)\exp\left(-\tfrac{2i}{\sqrt{h}}\mu\,x\cdot y-\tfrac{i}{\sqrt{h}}v(|x|^2+\tfrac{|y|^2}{4}-R^2)\right)\,\frac{d\mu\,dv\,dy\,dx\,d\xi}{(2\pi)^4\sqrt{h}}.$$

Substituting ξ by $2h^{-\frac{1}{2}}\mu x+h^{-\frac{1}{4}}\zeta$ and y by $h^{\frac{1}{4}}z$, we obtain

$$I_h = \int a(x,x-h^\gamma x_0+2\sqrt{h}\,\mu\,x+h^{\frac{3}{4}}\zeta,h^{\frac{1}{4}}x\wedge\zeta+h^{\gamma-\frac{1}{2}}x_0\wedge x)\widehat{\Phi}(\mu-v/2)\times$$
$$\times\overline{\widehat{\Phi}}(\mu+v/2)\exp(iz\cdot\zeta-\tfrac{i}{4}v|z|^2)\exp\left(-\tfrac{i}{\sqrt{h}}v(|x|^2-R^2)\right)\,\frac{d\mu\,dv\,dz\,dx\,d\zeta}{(2\pi)^4\sqrt{h}}.$$

Then, the stationary phase method in the variables v and $\rho = |x|$ yields, that

$$I_h \underset{h\to 0}{\sim} (2\pi)^{-2} \|\Phi\|_{L^2}^2 \int_{|x|=R} a(x, x, h^{\gamma-\frac{1}{2}} x_0 \wedge x)\, dx.$$

Therefore, we obtain the Wigner measure

$$\mu(x,\xi) = (2\pi)^{-2} \|\Phi\|_{L^2}^2 \, \mathbb{1}_{\{|x|=R\}}(x)\, dx \otimes \delta(\xi - x),$$

and observe again concentration on $I = \{x \wedge \xi = 0\}$. The two-scaled measure provides additional information concerning the exponent γ and the direction x_0. There are three different cases.

$\gamma < \frac{1}{2}$: $\nu(x,\xi,\eta) = \mu(x,\xi) \otimes \delta(\eta - \mathrm{sgn}(x_0 \wedge x)\infty)$,

$\gamma = \frac{1}{2}$: $\nu(x,\xi,\eta) = \mu(x,\xi) \otimes \delta(\eta - x_0 \wedge x)$,

$\gamma > \frac{1}{2}$: $\nu(x,\xi,\eta) = \mu(x,\xi) \otimes \delta(\eta)$.

4 Landau-Zener transitions at hitting points

4.1 Propagation outside the crossing

Next, we discuss the propagation of two-scaled Wigner measures outside the singular set S. As before, $\Pi^{\pm}(x)$ denote the orthogonal projectors of $V(x)$ corresponding to the eigenvalues $\pm|x|$. The weak*-limit points in $L^\infty(\mathbb{R}, \mathcal{A}')$ of $(W_2^h \psi^h(t))_{h>0}$, which are associated via (8) with solutions $(\psi^h(t))_{h>0}$ of the Schrödinger equation (3), are referred to as two-scaled Wigner measures $\nu(t,\cdot)$ of the family $(\psi^h(t))_{h>0}$.

Proposition 2 *Let $(\psi^h(t))_{h>0}$ be a family of solutions of the Schrödinger equation (3) with given initial data $(\psi_0^h)_{h>0}$, which are bounded in $L^2(\mathbb{R}^2, \mathbb{C}^2)$. Let $\nu(t,\cdot)$ and ν_0 be two-scaled Wigner measures of $(\psi^h(t))_{h>0}$ and $(\psi_0^h)_{h>0}$ for the hypersurface $I = \{x \wedge \xi = 0\}$ and the second scale $\sqrt{h}$. If $\mathrm{supp}(\nu_0) \cap S = \emptyset$, then $\nu(t,\cdot)$ can be decomposed in $\mathcal{D}'(\mathbb{R}, \mathcal{A}')$ as*

$$\nu(t,\cdot) = \nu^+(t,\cdot)\Pi^+ + \nu^-(t,\cdot)\Pi^-, \tag{12}$$

where $\nu^{\pm}(t,\cdot)$ are scalar-valued positive Radon measures supported on $I \times \overline{\mathbb{R}}$ satisfying

$$\partial_t \nu^{\pm} + \xi \cdot \nabla_x \nu^{\pm} \mp \frac{x}{|x|} \cdot \nabla_\xi \nu^{\pm} = 0, \qquad \nu^{\pm}(0) = tr(\nu_0 \Pi^{\pm}). \tag{13}$$

The decomposition (12) holds, until the Hamiltonian flow associated with the transport equations (13) touches $S = \{x = 0\}$.

Proposition 2 is a consequence of Théorème 2' in [6]. We note, however, that Théorème 2' shows transport terms in η-direction, which vanish in our case. This is due to the fact, that $\{ |\xi|^2/2 \pm |x| \, , \, x \wedge \xi \} = 0$. For the convenience of the reader, we give a proof of Proposition 2 in Appendix A.

From the above transport equations (13) we deduce the continuity of the map $t \mapsto \nu^\pm$ on any given time interval, provided the support of $\nu^\pm$ does not intersect the singular set S. Moreover, $\nu^\pm$ propagates along the classical trajectories associated with the mode $\pm|x|$. Thus, $\nu^\pm$ reaches S, if its initial support intersects the critical hyperface I. The work in [6] provides us with a local result describing the branching of $\nu^\pm$ near some point $(0,\xi_0) \in S \setminus \{(0,0)\}$, which we shall explain next.

4.2 A local Landau-Zener formula

We consider some hitting point $(0,\xi_0) \in S \setminus \{(0,0)\}$ and some neighbourhood $W \subset T^*\mathbb{R}^2$ of $(0,\xi_0)$, such that any classical trajectory included in W crosses S at most once for some given bounded time interval. Such an open set W exists due to the geometry of the trajectories described in Section 2. We denote by $J^{\pm,p}$ ($p \sim$ past) the sets of classical trajectories, which go into $S \cap W$,

$$J^{\pm,p} = \left\{ (x,\xi) \in T^*\mathbb{R}^2 \, : \, \exists (0,\zeta_0) \in S \cap W, \; \exists s \in (-\infty, 0), \; x = x^\pm_{\zeta_0}(s), \; \xi = \xi^\pm_{\zeta_0}(s) \right\},$$

where $(x^\pm_{\zeta_0}(s), \xi^\pm_{\zeta_0}(s))$ are the plus-minus trajectories with initial datum $(0,\zeta_0)$. Similarly, we define the sets $J^{\pm,f}$ ($f \sim$ future) of classical trajectories, which go out of $S \cap W$,

$$J^{\pm,f} = \left\{ (x,\xi) \in T^*\mathbb{R}^2 \, : \, \exists (0,\zeta_0) \in S \cap W, \; \exists s \in (0, +\infty), \; x = x^\pm_{\zeta_0}(s), \; \xi = \xi^\pm_{\zeta_0}(s) \right\}.$$

Measures $\nu^\pm$, which have support in W, are supported in $(J^{\pm,p} \cup J^{\pm,f}) \cap W$, and we denote by $\nu^{\pm,p}$ and $\nu^{\pm,f}$ their traces on S. According to Théorème 3 in [6] we have, if $\nu^{+,p}$ and $\nu^{-,p}$ are mutually singular on $\{| \, \eta \, | < +\infty\}$,

$$\begin{pmatrix} \nu^{+,f} \\ \nu^{-,f} \end{pmatrix} = \begin{pmatrix} 1-T & T \\ T & 1-T \end{pmatrix} \begin{pmatrix} \nu^{+,p} \\ \nu^{-,p} \end{pmatrix} \quad \text{in} \quad S \cap W, \tag{14}$$

with $T = T(\xi,\eta) = \exp(-\frac{\pi\eta^2}{|\xi|^3})$. We point out, that we have described I by the function $g(x,\xi) = x \wedge \xi$, while in the framework of [6] the hypersurface I is specified by $\widetilde{g}(x,\xi) = |\xi|^{-1}(x \wedge \xi)$. Thus, our transfer coefficient T is different from the one in [6]. It is obtained using relation (9).

The proof [6] of the above Landau-Zener formula reduces the Schrödinger equation (3) to a diffusion problem, which is close to the original system studied by Landau [11] and Zener [14] in the early 1930s. For this diffusion problem, the scattering problem can be solved explicitly; see the Appendix of [6]. The reduction is achieved by a change of symplectic time-space coordinates $(t, x, \tau, \xi) \mapsto (s, z, \sigma, \zeta)$, such that in the new coordinates

$$\begin{aligned} J^{\pm,p} &= \{\sigma \pm s = 0, \ \ \zeta_2 = 0, \ \ s < 0\}, \\ J^{\pm,f} &= \{\sigma \mp s = 0, \ \ \zeta_2 = 0, \ \ s > 0\}, \\ I = \{\zeta_2 = 0\}, &\ \ S = \{\sigma = s = \zeta_2 = 0\}. \end{aligned}$$

The system (3) reduces to

$$ih\, \partial_s v^h = Q^W(s, z, hD_s, hD_z) v^h$$

with

$$Q = \begin{pmatrix} s & \alpha(\sigma, z)\zeta_2 \\ \alpha(\sigma, z)\zeta_2 & -s \end{pmatrix},$$

$\alpha(z, \sigma) \neq 0$ for all $z \in \mathbb{R}^2$, $\sigma \in \mathbb{R}$, and $v^h = U\psi^h$, where U is a suitably chosen unitary, matricial Fourier integral operator. Of course, most of the work in [6] deals with the σ-dependance of the function α.

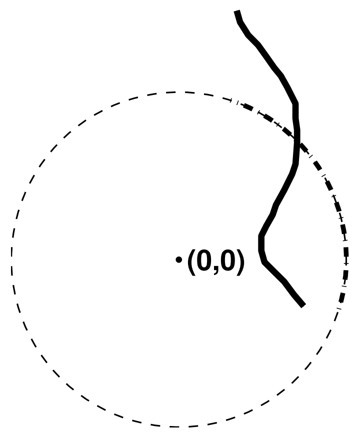
Roughly speaking, the singularity condition on the incident measures $\nu^{+,p}$ and $\nu^{-,p}$ excludes $\sqrt{h}$-interferences between $\Pi^+\psi^h$ and $\Pi^-\psi^h$ at the crossing. One might expect, that after one hitting time this seemingly restrictive condition does not hold any more. However, the following result shows, that for several interesting cases the singularity condition is indeed satisfied for all hitting times. Thus, the local result (14) can be used to describe the evolution of two-scaled Wigner measures *globally in time.* Recovering the Wigner measure from the two-scaled measure, we also obtain a global description of the weak limit of the position density via relation (4).

4.3 A global result

To give a sufficient condition on the initial data guaranteeing, that the Landau-Zener formula (14) can be applied recurrently in time, we need some notation first. Let $\Omega \subset \mathbf{S}^1$, such that $\omega \in \Omega \Rightarrow -\omega \notin \Omega$. Let $k, l : \Omega \to \mathbb{R}$ with $k > 0$. We consider a family of initial data (ψ_0^h), which is uniformly bounded in $L^2(\mathbb{R}^2, \mathbb{C}^2)$. The support of its Wigner measure μ_0 shall satisfy

$$I \cap \operatorname{supp}(\mu_0) = \Sigma,$$

where $\Sigma = \{(k(\omega)\omega, l(\omega)\omega) \in T^*\mathbb{R}^2 \, : \, \omega \in \Omega\}$. This means, that the points of concentration, which will be carried by classical trajectories into S, are localised in a way guaranteeing different arrival times at S for different starting points.



The figure on the right hand side shows a possible scenario in the $\mathbb{R}^2_x$-plane: the thick curve depicts the set $\{k(\omega)\omega \in \mathbb{R}^2 : \omega \in \Omega\}$. If we also assume localisation in the mode plus, we have an associated two-scaled Wigner measure ν_0 of the form

$$\nu_0(x,\xi,\eta) = \left(\int_\Omega \rho_0(\eta, d\omega) \otimes \delta(x - k(\omega)\omega) \otimes \delta(\xi - l(\omega)\omega)\right) \Pi^+(x), \tag{15}$$

where ρ_0 is a positive Radon measure on $\overline{\mathbb{R}} \times \mathbf{S}^1$.

In this situation there are two types of classical trajectories, which carry the energy. The first type are plus-trajectories with initial data (x_0, ξ_0) for $x_0 = k(\omega_0)\omega_0$, $\xi_0 = l(\omega_0)\omega_0$ with $\omega_0 \in \Omega$. The second type consists of minus-trajectories, which are issued by plus-trajectories hitting S. By Remarks 1 and 2, there are two important facts:

- At any of the hitting points $(t, 0, \xi, \eta)$, the incident energy is only carried into S by the plus-trajectories, so that the required singularity assumption holds.
- At any of the hitting points $(t, 0, \xi, \eta)$ we have $\xi \neq 0$, so that we can use the Landau-Zener formula (14).

We denote by $(x^+(t,\omega), \xi^+(t,\omega))$ the plus-trajectory described in Remark 2 with initial data $(k(\omega)\omega, l(\omega)\omega)$, $\omega \in \Omega$, and we set

$$L(\omega) = \sqrt{\mid l(\omega) \mid^2 + 2 \mid k(\omega) \mid}, \quad t_j(\omega) = l(\omega) + 2(j+1)L(\omega), \quad j \in \mathbb{N}_0.$$

Moreover, for $t \geq t_j(\omega)$ we denote by $\left(x_j^-(t,\omega), \xi_j^-(t,\omega)\right)$ the minus-trajectory, which has initial data $(0, \xi^+(t_j(\omega), \omega))$ at time $t = t_j(\omega)$. By Remark 1, we have for $t \geq t_j(\omega)$

$$\begin{aligned} x_j^-(t,\omega) &= (-1)^j \left((t - t_j(\omega))^2/2 - L(\omega)\,(t - t_j(\omega))\right)\omega, \\ \xi_j^-(t,\omega) &= (-1)^j\,(t - t_j(\omega) - L(\omega))\,\omega. \end{aligned}$$

Theorem 2 *Let $(\psi^h(t))_{h>0}$ be a family of solutions of the Schrödinger equation (3) with initial data $(\psi_0^h)_{h>0}$, which are bounded in $L^2(\mathbb{R}^2, \mathbb{C}^2)$. Let $(\psi_0^h)_{h>0}$ have a two-scaled Wigner measure ν_0 for $I = \{x \wedge \xi = 0\}$ and scale $\sqrt{h}$, which is of the form (15) and satisfies $\mathrm{supp}(\nu_0) \cap S = \emptyset$. If we decompose a two-scaled Wigner measure $\nu(t,\cdot)$ of $(\psi^h(t))_{h>0}$ for I and scale $\sqrt{h}$ as $\nu(t,\cdot) = \nu^+(t,\cdot)\Pi^+ + \nu^-(t,\cdot)\Pi^-$ in $\mathcal{D}'(\mathbb{R}, \mathcal{A}')$, then we have for all $t \geq 0$*

$$\begin{aligned} \nu^+(t,x,\xi,\eta) &= \int_\Omega \rho^+(t,\eta,d\omega) \otimes \delta\left(x - x^+(t,\omega)\right) \otimes \delta\left(\xi - \xi^+(t,\omega)\right), \\ \nu^-(t,x,\xi,\eta) &= \int_\Omega \rho^-(t,x,\xi,\eta,d\omega). \end{aligned}$$

The positive scalar-valued Radon measures $\rho^{\pm}$ are given by

$$\begin{aligned}
\rho^+(t,\eta,\omega) &= \sum_{j\geq 0} \mathbb{1}_{(t_{j-1}(\omega),t_j(\omega))}(t)\ (1-T(\eta,\omega))^j\ \rho_0(\eta,\omega), \\
\rho^-(t,x,\xi,\eta,\omega) &= \sum_{j\geq 0} \mathbb{1}_{(t_j(\omega),+\infty)}(t)\ T(\eta,\omega)\ (1-T(\eta,\omega))^j\ \rho_0(\eta,\omega)\otimes \\
&\qquad\qquad \otimes\,\delta\left(x-x_j^-(t,\omega)\right)\otimes\delta\left(\xi-\xi_j^-(t,\omega)\right),
\end{aligned}$$

where $T(\eta,\omega)=\exp\left(-\frac{\pi\eta^2}{L(\omega)^3}\right)$ and $t_{-1}(\omega)=0$ for all $\eta\in\overline{\mathbb{R}}$, $\omega\in\Omega$.

Proof. It is enough to prove Theorem 2 for some ν_0, which is of the form

$$\nu_0(x,\xi,\eta)=[\delta(x-x_0)\otimes\delta(\xi-\xi_0)\otimes\rho_0(\eta)]\,\Pi^+(x),$$

i.e. for initial data $(\psi_0^h)_{h>0}$, which are localised in one point. As mentioned before, we just have to use the description of the classical trajectories issued from $(x_0,\xi_0)=(k_0\omega_0,l_0\omega_0)$, $\omega_0\in\mathbf{S}^1$, which is contained in Remarks 1 and 2. We know, that for all $t\in(0,t_0(\omega_0))$ the measure ν^+ propagates along the trajectory $(x^+(t,\omega_0),\xi^+(t,\omega_0))$. Thus, we have

$$\nu(t,x,\xi,\eta)=\left[\delta\left(x-x^+(t,\omega_0)\right)\otimes\delta\left(\xi-\xi^+(t,\omega_0)\right)\otimes\rho_0(\eta)\right]\Pi^+(x)$$

when testing against functions $\phi\in\mathcal{D}'(\mathbb{R},\mathcal{A}')$ with $\mathrm{supp}(\phi)\subset(0,t_0(\omega_0))$. At time $t=t_0(\omega_0)$, there occurs some Landau-Zener partition of energy. Using (14), we obtain

$$\nu(t,x,\xi,\eta)=\nu^+(t,x,\xi,\eta)\,\Pi^+(x)+\nu^-(t,x,\xi,\eta)\Pi^-(x)$$

when testing on $(t_0(\omega_0),t_1(\omega_0))$, where

$$\begin{aligned}
\nu^+(t,x,\xi,\eta) &= (1-T(\eta,\omega_0))\,\rho_0(\eta)\otimes\delta\left(x-x^+(t,\omega_0)\right)\otimes\delta\left(\xi-\xi^+(t,\omega_0)\right), \\
\nu^-(t,x,\xi,\eta) &= T(\eta,\omega_0)\,\rho_0(\eta)\otimes\delta\left(x-x_0^-(t,\omega_0)\right)\otimes\delta\left(\xi-\xi_0^-(t,\omega_0)\right).
\end{aligned}$$

The measure ν^- propagates along $(x_1^-(t,\omega_0),\xi_1^-(t,\omega_0))$ for all $t>t_0(\omega_0)$, while for ν^+ there happens a new Landau-Zener phenomenon at time $t=t_1(\omega_0)$ at the point $(0,L(\omega_0)\omega_0)$. The same arguments apply for any of the hitting points

$$(t_j(\omega_0),0,(-1)^{j+1}L(\omega_0)\omega_0),$$

and therefore Theorem 2 is proved.

Remark 3 *Theorem 2 relies on the specific features of the Hamiltonian curves of the functions $\frac{|\xi|^2}{2}\pm|x|$. Therefore, it will also hold for the linear codimension three and five crossings considered by G. Hagedorn in [8] if a generalisation of the results of [6] to these crossings is performed.*

Remark 4 *We note, that the result of Theorem 2 holds with initial data, such that*

$$\nu_0(x,\xi,\eta) = \nu_0^+(x,\xi,\eta)\Pi^+(x) + \nu_0^-(x,\xi,\eta)\Pi^-(x)$$

with $\mathrm{supp}(\nu_0^-) \subset \{|\eta| = +\infty\}$*, since the singularity assumption for the Landau-Zener formula (14) concerns only the part of the two-scaled measure supported in* $\{|\eta| < +\infty\}$*.*

Remark 5 *If* $\nu_0(\{\eta = 0\}) = 0$*, then* $(1 - T(\eta,\omega))^j$ *goes to zero for* $(\eta,\omega) \in \mathrm{supp}(\rho_0)$ *as* $j \to +\infty$*, and*

$$\int_{\mathbb{R}\times\Omega} \rho^+(t, d\eta, d\omega) \underset{t\to+\infty}{\longrightarrow} 0.$$

Thus, as t goes to $+\infty$ all the energy is transferred from the mode plus to the mode minus.

We close by an immediate corollary concerning the weak $L^1(\mathbb{R}^2, \mathbb{C}^2)$-limit of the position density, which implies Theorem 1 of the introduction when applied to $\Sigma = \Sigma_0$.

Corollary 1 *Let* $C = \sup\left\{ |k(\omega)| + \frac{1}{2}|l(\omega)|^2 : \omega \in \Omega \right\}$*. Then, we have for all times* $t \geq 0$ *and for all* $\phi \in \mathcal{C}_0^\infty(\{x \in \mathbb{R}^2 : |x| > C\}, \mathbb{C})$

$$\begin{aligned}
&\lim_{h\to 0} \int_{\mathbb{R}^2} \phi(x) \mid \Pi^+(x)\psi^h(t,x) \mid^2 \, dx = 0, \\
&\lim_{h\to 0} \int_{\mathbb{R}^2} \phi(x) \mid \Pi^-(x)\psi^h(t,x) \mid^2 \, dx = \int_\Omega \sum_{j\geq 0} \mathbb{1}_{(t_j(\omega),+\infty)}(t)\, \phi(x_j^-(t,\omega))\, a_j(d\omega),
\end{aligned}$$

where $a_j(\omega) = \displaystyle\int_{\mathbb{R}} T(\eta,\omega)(1 - T(\eta,\omega))^j \rho_0(d\eta,\omega)$*.*

We note, that $|k(\omega)| + \frac{1}{2}|l(\omega)|^2 = \frac{L(\omega)^2}{2}$ describes the boundaries of the strip in the $\mathbb{R}_x^2$-plane, between which the plus-trajectory oscillates. In other words, Corollary 1 means, that if we consider $\bar{x} = \varepsilon r \omega$ with $\omega \in \Omega$, $\varepsilon \in \{\pm 1\}$, $r > |k(\omega)| + \frac{1}{2}|l(\omega)|^2$, then the weak limit of $\left(\mid \Pi^-(x)\psi^h(t,x)|^2\right)$ charges $\bar{x}$ recurrently at times

$$t = t_k(\omega) + L(\omega) + \sqrt{L(\omega)^2 + 2 \mid \bar{x} \mid},$$

for $k \in \mathbb{N}$ such that $(-1)^k = \varepsilon$. Moreover, the mass above $\bar{x}$ is $a_k(\omega)$.

A Appendix: Propagation outside the crossing

Proof. Proposition 2 gives a description of the two-scaled Wigner measure ν outside the singular set $S = \{x = 0\}$. Thus, all the test functions $a \in \mathcal{A}$ used in the following have $\mathrm{supp}(a) \cap S = \emptyset$ assuring that in the region under investigation the projectors $\Pi^\pm(x)$ depend smoothly on x. There are two steps:

1. First, we show $[\nu(t,\cdot),\Pi^\pm]=0$ in $\mathcal{D}'(\mathbb{R},\mathcal{A}')$ by analysing

$$L_1^h(t)=\int_{T^*\mathbb{R}^2} tr\left((W^h\psi^h)(t,x,\xi)\,a(x,\xi,\tfrac{x\wedge\xi}{\sqrt{h}})\right)\,dxd\xi$$

for matrix-valued test functions $a\in\mathcal{A}$. Due to this commutativity, we can then decompose $\nu(t,\cdot)$ as $\nu(t,\cdot)=\nu^+(t,\cdot)\Pi^+ + \nu^-(t,\cdot)\Pi^-$ with $\nu^\pm(t,\cdot)=tr(\nu(t,\cdot)\Pi^\pm)$.

2. Second, we show the transport equations for the scalar-valued measures $\nu^\pm(t,\cdot)$. Thus, we study the evolution of

$$L_2^h(t)=\int_{T^*\mathbb{R}^2} tr\left((W^h\psi^h)(t,x,\xi)\,\Pi^\pm(x)\,a(x,\xi,\tfrac{x\wedge\xi}{\sqrt{h}})\right)\,dxd\xi,$$

for scalar-valued test functions $a\in\mathcal{A}$.

First step. Let $(\psi^h(t))_{h>0}$ be a family of solutions of the Schrödinger equation (3), whose Hamiltonian's symbol will be denoted by $H(x,\xi)=\frac{|\xi|^2}{2}+V(x)$. Testing against functions $a\in\mathcal{A}$, we will use the notation $a_h(x,\xi)=a(x,\xi,\frac{x\wedge\xi}{\sqrt{h}})$. Differentiating for almost all $t\in\mathbb{R}$, we have by the duality of Wigner transformation and Weyl quantization

$$\begin{aligned} ih\,\frac{d}{dt}L_1^h(t) &= \langle\,\psi^h(t)\mid a_h^W(x,hD)\,H^W(x,hD)\,\psi^h(t)\,\rangle_{L^2(\mathbb{R}^2)}\\ &- \langle\,H^W(x,hD)\,\psi^h(t)\mid a_h^W(x,hD)\,\psi^h(t)\,\rangle_{L^2(\mathbb{R}^2)}\\ &= \langle\,\psi^h(t)\mid [a_h^W(x,hD),H^W(x,hD)]\,\psi^h(t)\,\rangle_{L^2(\mathbb{R}^2)}, \end{aligned}$$

where the last equation is due to the symmetry of $H^W(x,hD)$. Analysing this commutator by semiclassical Weyl calculus – see for example Proposition 7.7 in [2] – we apply a cut-off function $\chi\in\mathcal{C}_c^\infty(\mathbb{R}^2,\mathbb{R})$ compensating the linear growth in x of $H(x,\xi)$. We choose χ with support outside $\{x=0\}$, such that $\chi(x)=1$ for all $x\in\mathbb{R}^2$, which lie in the projection of supp(a) onto position space. Since $\chi a=a$ and $a(\nabla_x\chi)=0$, we have

$$a_h^W(x,hD)=a_h^W(x,hD)\,\chi=\chi\,a_h^W(x,hD)$$

and therefore

$$\begin{aligned} [a_h^W(x,hD),V] &= [a_h^W(x,hD),\chi V]\\ &= [a_h,\chi V]^W(x,hD)+\tfrac{h}{2i}\left(\{a_h,\chi V\}-\{\chi V,a_h\}\right)^W(x,hD). \end{aligned}$$

Moreover,

$$[a_h^W(x,hD),-\tfrac{h^2}{2}\,\Delta\,]=\tfrac{h}{i}\,\{a_h,\tfrac{|\xi|^2}{2}\}^W(x,hD)+h^2R^h,$$

where $(R^h)_{h>0}$ is a sequence of bounded operators on $L^2(\mathbb{R}^2,\mathbb{C}^2)$ built with second order derivatives of a_h. We note, that L^2-continuity here and in the following is always implied by the Theorem of Calderon-Vaillancourt, see for example Theorem 7.11 in [2]. Since every derivative of a_h produces an extra factor $\frac{1}{\sqrt{h}}$, we have

$$[a_h^W(x,hD), H^W(x,hD)] = [a_h, V]^W(x,hD) + \sqrt{h}\, Q^h$$

with $(Q^h)_{h>0}$ a bounded sequence of bounded operators on $L^2(\mathbb{R}^2,\mathbb{C}^2)$. Since we also have $\|\psi^h(t)\|_{L^2} = \|\psi_0^h\|_{L^2}$ for all $t\in\mathbb{R}$, we obtain

$$ih\,\frac{d}{dt}L_1^h(t) = \int_{T^*\mathbb{R}^2} tr\left([(W^h\psi^h)(t,x,\xi), V(x,\xi)]\, a_h(x,\xi)\right) dxd\xi + \sqrt{h}\, q^h(t)$$

with $(q^h)_{h>0}$ a bounded sequence in $L^\infty(\mathbb{R},\mathbb{C})$. Obviously, we have for all $\phi\in\mathcal{C}_0^\infty(\mathbb{R},\mathcal{A}')$

$$ih\int_{\mathbb{R}}\frac{d}{dt}L_1^h(t)\,\phi(t)\,dt \;=\; ih\int_{\mathbb{R}} L_1^h(t)\,\frac{d}{dt}\phi(t)\,dt \underset{h\to 0}{\longrightarrow} 0,$$

since $(L_1^h)_{h>0}$ is bounded in $L^\infty(\mathbb{R},\mathbb{C})$. Therefore, passing to the limit in $\mathcal{D}'(\mathbb{R},\mathcal{A}')$, we have shown $[\nu, V]=0$ and $[\nu,\Pi^\pm]=0$. Since the $\Pi^\pm$ are rank one projectors, we can simplify the decomposition $\nu = \Pi^+\nu\Pi^+ + \Pi^-\nu\Pi^-$ to $\nu = \nu^+\Pi^+ + \nu^-\Pi^-$, where $\nu^\pm = tr(\nu\Pi^\pm)$.

Second step. Now, we consider scalar-valued test functions $a\in\mathcal{A}$. We have

$$\frac{d}{dt}L_2^h(t) = \frac{i}{h}\langle\, \left[\Pi^\pm a_h^W(x,hD)\Pi^\pm\,,\; H^W(x,hD)\right]\; \psi^h(t)\mid \psi^h(t)\,\rangle_{L^2(\mathbb{R}^2)}.$$

We denote $\lambda_\pm(x,\xi) = \frac{|\xi|^2}{2}\pm|x|$. Obviously,

$$\left[\Pi^\pm a_h^W(x,hD)\Pi^\pm\,,\; H^W(x,hD)\right] = \left[\Pi^\pm a_h^W(x,hD)\Pi^\pm\,,\; \lambda_\pm^W(x,hD)\right].$$

We reuse the cut-off function χ and obtain

$$\begin{aligned}
\chi\,\Pi^\pm\,\lambda_\pm^W(x,hD) &= \lambda_\pm^W(x,hD)\,\chi\,\Pi^\pm + \tfrac{h}{2i}\,r^W(x,hD) + o(h)\\
\lambda_\pm^W(x,hD)\,\chi\,\Pi^\pm &= \chi\Pi^\pm\,\lambda_\pm^W(x,hD) - \tfrac{h}{2i}\,r^W(x,hD) + o(h),
\end{aligned}$$

where $r(x,\xi) = \{\chi\Pi^\pm, \frac{|\xi|^2}{2}\}$. Here and in the following, the o-notation refers to the space of bounded operators on $L^2(\mathbb{R}^2,\mathbb{C}^2)$. Therefore,

$$\begin{aligned}
\frac{i}{h}\left[\Pi^\pm a_h^W(x,hD)\Pi^\pm\,,\; \lambda_\pm^W(x,hD)\right] &= \frac{i}{h}\,\chi\,\Pi^\pm\,[a_h^W(x,hD), \lambda_\pm^W(x,hD)]\,\chi\,\Pi^\pm\\
&\quad+\tfrac{1}{2}\left(\chi\,\Pi^\pm a_h^W(x,hD)r^W(x,hD) + r^W(x,hD)a_h^W(x,hD)\chi\,\Pi^\pm\right) + o(1).
\end{aligned}$$

Since $\chi a = a$ and $a(\nabla_x\chi)=0$, we obtain

$$\begin{aligned}
\chi\,\Pi^\pm\, a_h^W(x,hD)r^W(x,hD) + r^W(x,hD)a_h^W(x,hD)\chi\,\Pi^\pm &=\\
\Pi^\pm\, a_h^W(x,hD)r^W(x,hD) + r^W(x,hD)a_h^W(x,hD)\Pi^\pm &= q_h^W(x,hD) + o(1)
\end{aligned}$$

with $q = q(x, \xi, \eta)$,

$$q = a(\Pi^{\pm} r + r\Pi^{\pm}) = a\left(\Pi^{\pm}\left\{\Pi^{\pm}, |\xi|^2/2\right\} + \left\{\Pi^{\pm}, |\xi|^2/2\right\}\Pi^{\pm}\right).$$

Moreover, using $\{x \wedge \xi, \lambda_{\pm}(x, \xi)\} = 0$, we have

$$\frac{i}{h}\chi\left[a_h^W(x, hD)\,,\, \lambda_{\pm}^W(x, hD)\right]\chi \;=\; b_h^W(x, hD) + o(1),$$

with $b(x, \xi, \eta) = -\xi \cdot \nabla_x a \pm \frac{x}{|x|} \cdot \nabla_\xi a$. Thus, the η-dependance drops, and we obtain

$$\begin{aligned}
\lim_{h \to 0} \frac{d}{dt} L_2^h(t) &= \int_{T^*\mathbb{R}^2} tr\left(\left(\Pi(x)^{\pm} b(x, \xi, \eta)\Pi^{\pm}(x) + q(x, \xi, \eta)\right)\nu(t, dx, d\xi, d\eta)\right) \\
&= \int_{T^*\mathbb{R}^2} b(x, \xi, \eta)\,\nu^{\pm}(t, dx, d\xi, d\eta) + \int_{T^*\mathbb{R}^2} tr\left(q(x, \xi, \eta)\,\nu(t, dx, d\xi, d\eta)\right).
\end{aligned}$$

For concluding the proof, it remains to show that $tr(q\,\nu(t, \cdot)) = 0$. Using $(\Pi^{\pm})^2 = \Pi^{\pm}$, we get $\Pi^{\pm}\{\Pi^{\pm}, |\xi|^2/2\}\Pi^{\pm} = \Pi^{\pm}\{\Pi^{\pm}, |\xi|^2/2\}\Pi^{\pm} + \Pi^{\pm}\{\Pi^{\pm}, |\xi|^2/2\}\Pi^{\pm} = 0$. Since traces are invariant under cyclic permutations, and since $[\nu(t, \cdot), \Pi^{\pm}] = 0$, we finally have in $\mathcal{D}'(\mathbb{R}, \mathcal{A}')$

$$tr(q\,\nu(t, \cdot)) = tr(a\,\Pi^{\pm}\left\{\Pi^{\pm}, |\xi|^2/2\right\}\Pi^{\pm}\nu(t, \cdot) + a\,\Pi^{\pm}\left\{\Pi^{\pm}, |\xi|^2/2\right\}\Pi^{\pm}\nu(t, \cdot)) = 0.$$

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