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CLOTILDE FERMANIAN-KAMMERER, CAROLINE LASSER, AND DIDIER ROBERT

Abstract. We analyze the propagation of coherent states through general systems of pseudodifferential form associated with Hamiltonian presenting codimension one eigenvalue crossings. In particular, we calculate precisely the non adiabatic effects of the crossing in terms of a transition operator.

1. Introduction

We consider the system of N equations of pseudodifferential form

$$i\varepsilon\partial_t\psi^\varepsilon = \widehat{H}(t)\psi^\varepsilon,\ \ \psi^\varepsilon_{|t=t_0} = \psi^\varepsilon_0 \tag{1}$$

where ψ^ε_0 is a bounded family in $L^2(\mathbb{R}^d,\mathbb{C}^N)$, $\widehat{H}(t)$ the semi-classical Weyl quantization of a Hamiltonian $H(t,x,\xi)$ which is a $N\times N$ matrix satisfying a growth condition of subquadratic type that we explain below. We recall that if $a\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{C}^{N,N})$ with adequate control on the growth of derivatives, the operator $\widehat{a}$ is defined by

$$\mathrm{op}^w_\varepsilon(a)f(x) := \widehat{a}f(x) := (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^d} a\left(\frac{x+y}{2},\xi\right)\mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot(x-y)}f(y)dy\,d\xi,\ \forall f\in\mathcal{S}(\mathbb{R}^d,\mathbb{C}^N).$$

We consider initial data that are wave packets, i.e. $\psi^\varepsilon_0 = \widehat{\vec{V}_0}\mathcal{WP}^\varepsilon_{z_0}\varphi$ where $z_0=(q_0,p_0)\in\mathbb{R}^{2d}$, $\vec{V}_0\in\mathcal{C}^\infty_0(\mathbb{R}^{2d},\mathbb{C}^N)$ and $\varphi\in\mathcal{S}(\mathbb{R}^d,\mathbb{R})$, we set

$$\mathcal{WP}^\varepsilon_z\varphi(x) = \varepsilon^{-d/4}\,\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)}\varphi\left(\frac{x-q}{\sqrt{\varepsilon}}\right). \tag{2}$$

Our aim is to describe the structure of the solutions associated with and for systems presenting codimension 1 crossings.

This question has already been addressed on special cases corresponding to physical settings: Schrödinger type Hamiltonians in [12]:

$$H_S(x,\xi) = \frac{|\xi|^2}{2}\mathbb{I}_{\mathbb{C}^N} + V(x),\ \ V\in\mathcal{C}^\infty(\mathbb{R}^d,\mathbb{C}^{N,N}), \tag{3}$$

and models arising in solid state physics [33]:

$$H_A(x,\xi) = A(\xi) + W(x)\mathbb{I}_{\mathbb{C}^2} \tag{4}$$

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where A is a matrix arising in a Bloch bands decomposition and V a scalar function. We develop here a method which applies for general Hamiltonians H with subquadratic growth situations and for codimension 1 crossings of eigenvalues which have multiplicity larger than 1. In particular, we give a computation of the transfer operator which describe the interactions due to the crossing, that is direct and transparent (see Corollary 2.9).

Our motivation is related with the development of numerical methods using Gaussians, such as the Herman-Kluk and other Gaussian-based methods propagators as developed in the chemical literature [15, 17, 18, 32, 8]. These approximations rely on a good understanding of the propagation of Gaussian states, and have been studied mathematically for scalar systems [29, 28] with applications in numerics [21, 19], that makes this field very active (see for examle [20] and references therein). Therefore theoretical results in this direction should lead in improvement in the understanding of algorithmic realizations of the propagator of systems. For example, we explain here that how to derive a Herman-Kluk realization of the propagator for datas that are polarized along a mode of constant multiplicity (see Corollary 2.5 below).

It turns aout that the propagator $\mathcal{U}^\varepsilon_H(t,t_0)$ associated with $\widehat{H}$ is well defined according to [26] provided that the map $(t,z)\mapsto H(t,z)$ is in $\mathcal{C}^\infty(\mathbb{R}\times\mathbb{R}^{2d},\mathbb{C}^{N\times N})$, valued in the set of self-adjoint matrices and that it has subquadratic growth, i.e.

$$\forall\alpha\in\mathbb{N}^{2d},\ \ |\alpha|\geq 2,\ \ \exists C_\alpha>0,\quad \sup_{(t,z)\in\mathbb{R}\times\mathbb{R}^{2d}}\|\partial^\alpha H(t,z)\|_{\mathbb{C}^{N,N}}\leq C_\alpha. \tag{5}$$

These assumptions guarantee the existence of solutions to equation (1) in $L^2(\mathbb{R}^d,\mathbb{C}^N)$ and, more generally, in the functional spaces

$$\Sigma^k_\varepsilon(\mathbb{R}^d,\mathbb{C}^N)=\{f\in L^2(\mathbb{R}^d,\mathbb{C}^N),\ \ \forall\alpha,\beta\in\mathbb{N}^d,\ \ |\alpha|+|\beta|\leq k,\ \ x^\alpha(\varepsilon\partial_x)^\beta f\in L^2(\mathbb{R}^d,\mathbb{C}^N)\}$$

endowed with the norm

$$\|f\|_{\Sigma^k_\varepsilon}=\sup_{|\alpha|+|\beta|\leq k}\|x^\alpha(\varepsilon\partial_x)^\beta f\|_{L^2}.$$

However, the analysis below could apply in more general settings as long as the classical quantities are well-defined in finite time with some technical improvements that are not discussed here.

Remark 1.1. Indeed, as symbols $a\in\mathcal{C}^\infty(\mathbb{R}^{2d})$ with bounded derivatives define bounded operators $\widehat{a}$ (uniformly in ε) in Σ^k_ε, the propagators of symmetric bounded (or subquadratic) symbols (may be time dependent) are also ε-uniformly-bounded in any Σ^k_ε. This can be easily proved using the symbolic semi-classical calculus and observing that $\Sigma^k_\varepsilon(\mathbb{R}^d)$ is a natural domain of the semi-classical harmonic oscillator and its powers $\left(-\varepsilon^2\triangle+|x|^2\right)^{k/2}$ ([26]).

Assuming that $H(t,x,\xi)$ has a smooth eigenvalue $h_1(t,x,\xi)$, the eigenspace of which admits a smooth eigenprojector $\Pi_1(t,x,\xi)$, the two following cases may happen:

1. *Gap situation*: The eigenvalue $h_1(t,z)$ is separated from the remainder of the spectrum of $H(t)$ by a gap larger than some fixed positive real number δ_0.

(2) *Smooth crossing*: The eigenvalue $h_1(t,z)$ cross another smooth eigenvalue $h_2(t,z)$ which also has a smooth eigenprojector. We shall then assume that the set of these two eigenvalues is separated from the remainder of the spectrum of the matrix $H(t,z)$ by a gap (uniformly in t and z).

The first case is very well understood and corresponds to adiabatic situations that have been studied by several authors (see in particular [30, 22]). The second case is less studied; some results on the subject focus on the evolution at leading order of quadratic quantities of the wave function for data which are not necessarily wave-packets (see [16, 6] and the references therein). The main results devoted to wave packets in this setting are [12, 33], where the authors show on model problems from physics that one can give a rather explicit description of the wave function itself, exhibiting transitions that occur at the crossing between the two modes at order $\sqrt{\varepsilon}$. We give here a transparent description of these transitions for general systems, through an approximation of $\psi^\varepsilon(t)$ for initial data which are polarized along h_1 with a wave packet structure. Our result (Theorem 2.8 below) shows that if the initial data is a wave packet polarized along $\vec{V}_1$, an eigenvector corresponding to the mode h_1

$$\psi_0^\varepsilon(x) = \widehat{\vec{V}_0} v_0^\varepsilon, \;\; v_0^\varepsilon = \mathcal{WP}^\varepsilon_{z_0}\varphi_0, \;\; (t_0,z_0)\in\mathbb{R}^{2d+1}, \;\; \varphi_0\in\mathcal{S}(\mathbb{R}^d), \tag{6}$$

and $\vec{V}_0 \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ is a function that satisfies in a neighborhood U of z_0:

$$\forall z\in U, \;\; H(t_0,z)\vec{V}_0(z) = h_1(t_0,z)\vec{V}_0(z),$$

then the solution writes

$$\psi^\varepsilon(t) = \widehat{\vec{V}_1(t)}\mathcal{WP}^\varepsilon_{z_1(t)}(\varphi_1^0(t)+\sqrt{\varepsilon}\varphi_1^1(t)) + \sqrt{\varepsilon}\mathbf{1}_{t>t^\flat}\widehat{\vec{V}_2(t)}\mathcal{WP}^\varepsilon_{z_2(t)}\varphi_2(t) + o(\sqrt{\varepsilon})$$

where

(1) the maps $z_1(t)$, $z_2(t)$ are classical trajectories associated respectively with the modes h_1 and h_2 satisfying
$$z_2(t^\flat) = z_1(t^\flat),$$

(2) the time $t^\flat$ is the first time where $z_1(t)$ meets the crossing set
$$\Upsilon = \{(t,z)\in\mathbb{R}^{2d+1}, \; h_1(t,z) = h_2(t,z)\} \tag{7}$$

(3) the profiles of the wave packets $\mathcal{WP}^\varepsilon_{z_1(t)}(\varphi_1^0(t)+\sqrt{\varepsilon}\varphi_1^1(t))$ and $\mathcal{WP}^\varepsilon_{z_2(t)}\varphi_2(t)$ are Schwartz functions $\varphi_1^0(t)$, $\varphi_1^1(t)$ and $\varphi_2(t)$ that solve ε-independent PDEs on $[0,t]$ and $[t^\flat,t]$ respectively, with the property
$$\varphi_2(t^\flat) = \mathcal{T}^\flat\varphi_1^0(t^\flat)$$
for some transfer operator $\mathcal{T}^\flat$ that we prove to be a metaplectic transform (which implies that the structure of Gaussian states is preserved, see Corollary 2.9),

(4) the families $\vec{V}_1(t,z)$ and $\vec{V}_2(t,z)$ are smooth normalized eigenvectors for $h_1(t,z)$ and $h_2(t,z)$ respectively, they are obtained via parallel transport and manifest the polarization of the wave packet along a mode.

We point out that, in the gap case, the solution at time t associated with a polarized data remains polarized along the same mode up to terms of order $O(\varepsilon)$, which is the standard order of the adiabatic approximation, while for smooth crossings a perturbative term of order $O(\sqrt{\varepsilon})$ polarized along the crossing mode has to be taken into account for an $O(\varepsilon)$ approximation.

Before giving a more precise statement of the result, note that the propagation of wave packet has also been studied for nonlinear systems in [3, 13, 14], including situations with avoided crossings [14], however, nonlinear systems with crossings in presence of codimension 1 crossing have not yet been studied and our result should extend in this nonlinear setting with additional assumptions for treating the nonlinearity. Finally, this result opens the way to the derivation of Herman-Kluk realizations of the propagators with the associated algorithmic realizations, as in the adiabatic setting (see Corollary 2.5 below). We postpone this result to further works.

2. Precise statement of the results

Before stating our main results, we recall basic facts about the scalar propagation of wave packets and adiabatic results. That allows us to introduce notations and arguments that we use all other this paper.

2.1. **Scalar propagation and scalar classical quantities.**

The most interesting property of the coherent states is the stability of their structure through evolution, which can be described by means of classical quantities. Note that for all $z \in \mathbb{R}^{2d}$ and $k \in \mathbb{N}$, the operator $\varphi \mapsto \mathcal{WP}^\varepsilon_z \varphi$ is a unitary map in $L^2(\mathbb{R}^d)$ which maps continuously Σ^1_k into Σ^ε_k with a continuous inverse, other elementary properties of the wave-packet transform are listed in Lemma A.1. We shall use the notation

$$J = \begin{pmatrix} 0 & \mathbb{I}_{\mathbb{R}^d} \\ -\mathbb{I}_{\mathbb{R}^d} & 0 \end{pmatrix} \tag{8}$$

and, for smooth functions $f, g \in \mathcal{C}^\infty(\mathbb{R}^{2d})$, that might be scalar-, vector- or matrix-valued, we denote the Poisson bracket by

$$\{f, g\} := J\nabla f \cdot \nabla g = \sum_{j=1}^{d} \left(\partial_{\xi_j} f \partial_{x_j} g - \partial_{x_j} f \partial_{\xi_j} g \right).$$

The Hamiltonian vector field of the eigenvalue $h(t)$ is then defined by

$$\forall f \in \mathcal{C}^\infty(\mathbb{R}^{2d}), \;\; \mathcal{X}_{h(t)} f = \{h(t), f\} = Jdh(t)f.$$

For $(t_0, z_0) \in \mathbb{R}^{2d+1}$ we consider the *classical Hamiltonian trajectory* $z(t) = (q(t), p(t))$ issued from z_0 at time t_0, and defined by the ordinary differential equation

$$\dot{z}(t) = J\partial_z h(t, z(t)) = \mathcal{X}_h(t)(z(t)), \;\; z(t_0) = z_0.$$

The associated *flow map* is then denoted by $\Phi_h^{t,t_0}(z_0)$ and we have

$$\partial_t \Phi_h^{t,t_0} = J\partial_z h(t) \circ \Phi_h^{t,t_0}, \quad \Phi_h^{t_0,t_0} = \mathbb{I}_{\mathbb{R}^{2d}}. \tag{9}$$

We take a notation for the blocks of the Jacobian matrix of the flow map:

$$F(t,t_0,z_0) = \begin{pmatrix} A(t,t_0,z_0) & B(t,t_0,z_0) \\ C(t,t_0,z_0) & D(t,t_0,z_0) \end{pmatrix} := \partial_z \Phi_h^{t,t_0}(z_0), \tag{10}$$

which satisfies the linearized flow equation

$$\partial_t F(t,t_0,z_0) = J\mathrm{Hess}_z h(t,z(t))\, F(t,t_0,z_0), \quad F(t_0,t_0,z_0) = \mathbb{I}_{\mathbb{R}^{2d}},$$

and we associate with it the *metaplectic transformation*

$$\mathcal{M}[F(t,t_0,z_0)] : \ \varphi_0 \mapsto \varphi(t)$$

where φ solves the Schrödinger equation

$$i\partial_t \varphi = \mathrm{op}_1^w(\mathrm{Hess}_z h(t,z(t)) z\cdot z)\varphi, \quad \varphi(t_0) = \varphi_0.$$

We will also use the *action integral*

$$S(t,t_0,z_0) = \int_{t_0}^t (p(s)\cdot \dot q(s) - h(s,z(s)))\, ds. \tag{11}$$

Proposition 2.1. *[5] Let $h(t)$ be a smooth scalar Hamiltonian of subquadratic growth (5) As $\varepsilon \searrow 0$ we have for all $\varphi_0 \in \mathcal{S}(\mathbb{R}^d)$ and $z_0 \in \mathbb{R}^{2d}$ in the norm of Σ_ε^k, $k \geq 0$,*

$$\mathcal{U}_h^\varepsilon(t,t_0)\mathcal{WP}_{z_0}^\varepsilon \varphi_0 = \mathrm{e}^{\frac{i}{\varepsilon}S(t,t_0,z_0)}\mathcal{WP}_{z(t)}^\varepsilon \varphi^\varepsilon(t) + \mathcal{O}(\varepsilon),$$

where the profile function $\varphi^\varepsilon(t)$ is given by

$$\varphi^\varepsilon(t) = \mathcal{M}[F(t,t_0,z_0)]\left(1 + \sqrt{\varepsilon}\, b_1(t,t_0,z_0)\right)\varphi_0, \tag{12}$$

and the correction function $b_1(t,t_0,z_0)$ satisfies

$$b_1(t,t_0,z_0)\varphi_0 = \sum_{|\alpha|=3} \frac{1}{\alpha!}\frac{1}{i}\int_{t_0}^t \partial_z^\alpha h(s,z(s))\, \mathrm{op}_1^w[(F(s,t_0,z_0)z)^\alpha]\,\varphi_0\, ds. \tag{13}$$

The special case of *Gaussian states* is of special interest. The *Gaussian states* are wave packets with Gaussian profiles the variance of which is taken in the Siegel state $\mathfrak{S}^+(d)$ of $d\times d$ complex-valued symmetric matrices with positive imaginary part,

$$\mathfrak{S}^+(d) = \left\{\Gamma \in \mathbb{C}^{d\times d},\ \Gamma = \Gamma^\tau,\ \mathrm{Im}\Gamma > 0\right\}.$$

With $\Gamma \in \mathfrak{S}^+(d)$ we associate the Gaussian profile

$$g^\Gamma := c_\Gamma\, \mathrm{e}^{\frac{i}{2}\Gamma x\cdot x}. \tag{14}$$

where $c_\Gamma = \pi^{-d/4}\det^{1/4}(\mathrm{Im}\Gamma)$ is a normalization constant in $L^2(\mathbb{R}^d)$, it is a non-zero complex number whose argument is determined by continuity according to the work environment. By Proposition 2.1, the Gaussian states remain Gaussians through the evolution by $\mathcal{U}_h^\varepsilon$: for $\Gamma_0 \in \mathfrak{S}^+(d)$, we have

$$\mathcal{M}[F(t,t_0,z_0)]g^{\Gamma_0} = g^{\Gamma(t,t_0,z_0)}$$

with $\Gamma(t,t_0,z_0)\in\mathfrak{S}^+(d)$, and the width and the normalization constant of the resulting Gaussian function are determined by initial width Γ_0 and the Jacobian $F(t,t_0,z_0)$ according to

$$\begin{aligned}\Gamma(t,t_0,z_0) &= (C(t,t_0,z_0)+D(t,t_0,z_0)\Gamma_0)(A(t,t_0,z_0)+B(t,t_0,z_0)\Gamma_0)^{-1}\\ c_{\Gamma(t,t_0,z_0)} &= c_{\Gamma_0}\det{}^{-1/2}(A(t,t_0,z_0)+B(t,t_0,z_0)\Gamma_0),\end{aligned}\tag{15}$$

where the branch of the square root in $\det^{-1/2}$ is determined by continuity in time.

2.2. **The case of systems, parallel transport.** For treating systems, one need to consider vector-valued solutions and to take into account the vectorial aspects of the wave packets. For this, we consider initial data at time $t=t_0$ that are wave packets and focalized along a mode, that is of the form (2.3). For this, we need to introduce the following matrices

$$\Omega(t,z)=\Pi(t,z)\{\Pi,H\}(t,z)\Pi(t,z),\tag{16}$$

$$K(t,z)=(\mathbb{I}_{\mathbb{C}^N}-\Pi(t,z))\left(\partial_t\Pi(t,z)+\{h,\Pi\}(t,z)\right)\Pi(t,z)\tag{17}$$

that are smooth and satisfy algebraic properties detailed in Lemma B.1 below. The next result introduce normalized eigenvectors that evolve inside a given mode by the so-called *parallel transport*. This construction generalizes [3, Proposition 1.9], which was inspired by the work of George Hagedorn, see [12, Proposition 3.1]).

Proposition 2.2. *Assume that $\Pi(t)$ is a smooth eigenprojector such that $\Pi(t)H(t)=H(t)\Pi(t)=h(t)\Pi(t)$. Let $\vec V_0\in\mathcal{C}_0^\infty(\mathbb{R}^{2d},\mathbb{C}^N)$ be such that there exists $z_0\in\mathbb{R}^{2d}$ and a neighborhood U_{z_0} of z_0 such that*

$$\forall z\in U_{z_0},\ \ \vec V_0(z)=\Pi(t_0,z)\vec V_0(z).$$

Then, there exists a smooth normalized vector-valued function satisfying

$$\forall z\in\Phi_h^{t,t_0}(U),\ \ \vec V(t,t_0,z)=\Pi(t,z)\vec V(t,t_0,z)$$

such that for all $t\in\mathbb{R}$ and $z\in\mathbb{R}^{2d}$,

$$\partial_t\vec V(t,t_0,z)+\{h,\vec V\}(t,t_0,z)=\Omega(t,z)\vec V(t,t_0,z)+K(t,z)\vec V(t,t_0,z),\ \ \vec V(t_0,t_0,z)=\vec V_0(z).$$

Note that Proposition 2.2 does not require any gap condition, and we will use it also in the crossing situation, with smooth eigenvalues and eigenprojectors.

The parallel transport is enough to describe at leading order the propagation of wave-packets focalized along gapped eigenvalues, that are eigenvalues $h(t,z)$ of the matrix $H(t)$ that are uniformly separated from the remainder of the spectrum: there exists $\delta>0$ such that for all $(t,z)\in\mathbb{R}\times\mathbb{R}^{2d}$,

$$\operatorname{dist}\left(h(t,z),\sigma(H(t,z))\setminus\{h(t,z)\}\right)>\delta.\tag{18}$$

Note that, this gap assumption implies the existence of a contour $\mathcal{C}$ in the complex plane, such that its interior only contains the eigenvalue $h(t,z)$ and no other eigenvalues of $H(t,z)$. Then, one can write the associated eigenprojector as

$$\Pi(t,z) = -\frac{1}{2\pi i}\oint_{\mathcal{C}} (H(t,z)-\zeta)^{-1} d\zeta, \tag{19}$$

which implies the smoothness of $\Pi(t,z)$. Since the works of Kato [K1, K2], numerous works have been devoted to this *adiabatic situation* (see for example the articles [22, 23, 24] and [30]) and one can sum-up these results in the next statement

Theorem 2.3. *[30, 22, 3] Assume the existence of an eigenvalue gap as in Assumption (18) and consider initial data of the form*

$$\psi_0^\varepsilon = \widehat{\vec{V}_0} v_0^\varepsilon + O(\varepsilon) \text{ in } L^2(\mathbb{R}^d, \mathbb{C}^N),$$

where $\vec{V}_0$ is a smooth eigenvector and $v_0^\varepsilon \in L^2(\mathbb{R}^d, \mathbb{C})$. Then, for all $T>0$, there exists $C>0$ such that $\psi^\varepsilon(t) = \mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon$ satisfies the estimate

$$\sup_{t\in[0,T]} \left\| (\widehat{\mathbb{I}_{\mathbb{C}^N} - \Pi}(t))\psi^\varepsilon(t) \right\|_{L^2(\mathbb{R}^d)} + \left\| \psi^\varepsilon(t) - \widehat{\vec{V}(t)} v^\varepsilon(t) \right\|_{L^2(\mathbb{R}^d)} \leq C\varepsilon$$

where $v^\varepsilon(t) = \mathcal{U}_h^\varepsilon(t,t_0)v_0^\varepsilon$. Besides, if there exists $k\in\mathbb{N}$ such that $(\psi_0^\varepsilon)_{\varepsilon>0}$ is a bounded family in Σ_ε^k, then the convergence above holds in Σ_ε^k.

Note that the operator $\widehat{\Pi}(t)$ is no longer a projector. However, it coincides at order $O(\varepsilon)$ with the operators constructed in [22, 30], which are projectors. Besides, the reader will find in [22, 30], various results about the adiabatic approximation, including expansions at any order by means of superadiabatic projectors. The precise time evolution of coherent state itself was studied in the adiabatic setting in [1, 22, 28]. Their result is obtained by constructing an asymptotic quantum diagonalization, in the spirit of the construction of superadiabatic projectors of [30]. However, the leading order approximation is enough for our purpose.

It is also interesting to notice that Theorem 2.3 is enough to describe the dynamics of an initial data of the form (2.3) focalized on a gapped eigenvalue by means of the scalar classical quantities introduced in section 2.1 and by use of the parallel transport. This is stated in the next Corollary; our aim is to give a similar description in the case of systems presenting a codimension 1 crossing.

Corollary 2.4. *In the situation of Theorem 2.3, for any $k\in\mathbb{N}$, $z_0\in\mathbb{R}^{2d}$ and $\varphi\in\mathcal{S}(\mathbb{R}^d)$, we have in $\Sigma_\varepsilon^k(\mathbb{R}^d,\mathbb{C}^N)$,*

$$\mathcal{U}_{H(t)}^\varepsilon\, \widehat{\vec{V}_0}\, \mathcal{WP}_{z_0}^\varepsilon(\varphi) = \mathrm{e}^{\frac{i}{\varepsilon}S(t,t_0,z_0)} \widehat{\vec{V}(t,t_0)}\, \mathcal{WP}^\varepsilon_{\Phi_h^{t,t_0}(z_0)}(\varphi^\varepsilon(t)) + O(\varepsilon),$$

where the profile $\varphi^\varepsilon(t)$ is given by (12) and all the classical quantities are associated with the function $h(t)$.

We close this section devoted to parallel transport to derive another consequence of the adiabatic theorem in terms of numerical realizations of the propagator by a Herman-Kluk approach. Indeed, the gaussian frame is at the root of the Herman-Kluk approximation of a Schrödinger propagator as proved in [27, 29]. Let $g^\varepsilon_z = \mathcal{WP}^\varepsilon_z(g^{i\mathbb{I}})$ denotes a Gaussian wave packet centered in $z=(q,p)$ with variance $\sqrt{\varepsilon}$, the family of wave packets $(g^\varepsilon_z)_{z\in\mathbb{R}^{2d}}$ forms a continuous frame and provides the reconstruction formula

$$\phi^\varepsilon_0(x) = (2\pi\varepsilon)^{-d}\int_{z\in\mathbb{R}^{2d}} \langle g^\varepsilon_z, \phi^\varepsilon_0\rangle g^\varepsilon_z(x)dz.$$

The results of [27, 29] about the Herman-Kluk approximation for scalar Schrödinger propagators and Proposition 2.2 imply the convergence of a Herman-Kluk approximation for the propagator of a system of Schrödinger equations, when the data is focalized on a gaped eigenmode.

Corollary 2.5. *In the situation of Theorem 2.3, in the norm of* $L^2(\mathbb{R}^d,\mathbb{C}^N)$

$$\mathcal{U}^\varepsilon_H(t,t_0)\psi^\varepsilon_0 = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} \langle g^\varepsilon_z,\psi\rangle \vec{A}(t,t_0,z)\mathrm{e}^{\frac{i}{\varepsilon}S(t,t_0,z)} g^\varepsilon_{\Phi_h^{t,t_0}(z)}dz + O(\varepsilon),$$

where the vector valued Herman–Kluk prefactor $\vec{A}(t,t_0,z)$ *is given by*

$$\vec{A}(t,t_0,z) = \vec{V}(t,t_0,z)a(t,t_0,z)$$

with $$a(t,t_0,z) = 2^{-d/2}\,\det{}^{1/2}\left(A(t,t_0,z)+D(t,t_0,z)+i(C(t,t_0,z)-B(t,t_0,z))\right).$$

The proof of Theorem 2.3 will be performed in a refined manner that takes into account the size of the gap in Section 3. As it is well-known, it extends to the situation where a subset of eigenvalues are isolated from the remainder of the spectrum (see Proposition 3.5 below). For this reason, in the next section, we reduce to the case of matrices admitting two eigenvalues that differ outside a hypersurface Υ and we study the dynamics of wave packets through this codimension 1 crossings, which is our main result.

2.3. Main result: propagation of wave packets through codimension 1 crossings.

We assume here that the Hamiltonan H writes

$$H(t,z) = v(t,z)\mathbb{I} + H_0(t,z),\quad v(t,z) = \frac{1}{N}\mathrm{tr}H(t,z), \tag{20}$$

where $(t,z)\mapsto v(t,z)\in\mathbb{R}$ and $(t,z)\mapsto H_0(t,z)$ are smooth functions of subquadratic growth valued respectibely in $\mathbb{R}$ and in the set of $N\times N$ trace-free matrices. We assume that the crossing set Υ is a hypersurface. Such a situation is called a *codimension 1 crossing* (see Hagedorn's classification [12] for example).Then if $(t^\flat,z^\flat)\in\Upsilon$, there exists a neighborhood Ω and a smooth function $(t,z)\mapsto f(t,z)$ defined in Ω such that $f(t,z)=0$ is a local equation of Υ in Ω. As a consequence, $df\neq 0$ and $H_0(t,z) = f(t,z)\tilde{H}_0(t,z)$ for some smooth map $(t,z)\mapsto \tilde{H}_0(t,z)$ valued in the set of trace-free hermitian matrices. We shall assume that the set of eigenvalues of $\tilde{H}_0\neq 0$ consists in two distinct smooth eigenvalues which do not cross on Ω and thus, it has smooth eigenprojectors, which are also those of $H(t,z)$; in other words, $\tilde{H}_0$ is trace-free and invertible on Υ.

To sum up, we make the following assumption.

Assumption 2.6. (1) *The matrix $H(t,z)$ has two distinct smooth eigenvalues which cross on a hypersurface Υ of $\mathbb{R}^{2d+1}$*

(2) *The crossing is non-degenerate in the sense that for any $(t^\flat, z^\flat) \in \Upsilon$ there exists a local equation $f(t,z) = 0$ of Υ in a neighborhood Ω of $(t^\flat, z^\flat)$ such that we have* (20) *and* (22)*for any $(t,z) \in \Omega$. Besides, we assume*

$$\partial_t f + \{v, f\} \neq 0, \tag{21}$$

Note that one can then modify f in Ω so that the functions

$$h_j(t,z) = v(t,z) - (-1)^j f(t,z), \quad j \in \{1,2\} \tag{22}$$

are the two smooth eigenvalues of the matrix $H(t,z)$, with smooth associated eigenprojectors $\Pi_1(t,z)$ and $\Pi_2(t,z)$. We shall choose f in that manner throughout the paper.

Example 2.7. Take $N = 2$ and $u \in \mathcal{C}^\infty(\mathbb{R}^{2d+1}, \mathbb{R}^3)$ of subquadratic growth, and satisfying $|u|^2 > \delta_0 > 0$. Consider the Hamiltonian

$$H(t,z) = v(t,z)\mathrm{Id} + f(t,z) \begin{pmatrix} u_1(t,z) & u_2(t,z) + iu_3(t,z) \\ u_2(t,z) - iu_3(t,z) & -u_1(t,z) \end{pmatrix}.$$

The smooth eigenvalues of H, $v + f|u|$ and $v - f|u|$ cross on the set $\{f = 0\}$ and H satisfies Assumption 2.6 as soon as (21) holds.

Note that the condition (21) implies the transversality of the classical trajectories to the crossing set Υ. We associate with each mode h_j the classical quantities introduced in section 2.1, before that we index by j. We consider an initial data at time $t = t_0$ as in which is a coherent state associated with the first mode h_1 where $(t_0, z_0) \notin \Upsilon$, $z \mapsto \vec{V}_0(z)$ is a smooth map compactly supported in a neighborhood of z_0 and $\vec{V}_0(z_0) = 1$.

We assume that the Hamiltonian trajectory $z_1(t,t_0) = \Phi_1^{t,t_0}(z_0)$ reaches Υ at time $t = t^\flat$ and point $z = z^\flat$ where (21) holds. Therefore, $f(t,z) = 0$ is a local equation of Υ in a neighborhood Ω of $(t^\flat, z^\flat)$and the hypothesis of Assumption 2.6 implies

$$\frac{d}{dt} f(t, z_1(t,t_0)) \neq 0$$

close to $(t^\flat, z^\flat)$ and guarantees that the trajectory $z_1(t,t_0,z_0)$ passes through Υ. A similar behaviour holds for the trajectories $\Phi^{t,t_0}(z)$ starting from z close enough to z_0.

We associate with $\vec{V}_0(t_0, z)$ the time-dependent eigenvector $(\vec{V}_1(t,z))_{t \geq t_0}$ constructed as in Proposition 2.2 for the mode h_1 with initial data $\vec{V}_0(t_0)$ at time t_0. We also consider the time-dependent eigenvector $(\vec{V}_2(t,z))_{t \geq t^\flat}$ constructed for $t > t^\sharp$ as in Proposition 2.2 for the mode h_2 and with initial data at time $t^\flat$ satisfying

$$\vec{V}_2(t^\flat, z) = \frac{\Pi_2(\partial_t \Pi_2 + \{v, \Pi_2\})\vec{V}_1}{\|\Pi_2(\partial_t \Pi_2 + \{v, \Pi_2\})\vec{V}_1\|_{\mathbb{C}^N}}(t^\flat, z) \tag{23}$$

where $\vec{V}_0$ appears in the definition of the initial data (2.3). Note that the vector $\vec{V}_2(t^\flat, z)$ is in the range of $\Pi_2(t^\flat, z)$.

We introduce a family of transformations which will appear in the crossing process. When $(\mu, \alpha, \beta) \in \mathbb{R} \times \mathbb{R}^{2d}$, we set

$$\mathcal{T}_{\mu,\alpha,\beta}\varphi(y) = \left(\int_{-\infty}^{+\infty} \mathrm{e}^{i\mu s^2} \mathrm{e}^{is(\beta\cdot y - \alpha\cdot D_y)} ds \right) \varphi(y), \tag{24}$$

By the Baker-Campbell-Hausdorff formula, we have

$$\mathrm{e}^{is\beta\cdot y}\mathrm{e}^{-is\alpha\cdot D_y} = \mathrm{e}^{is\beta\cdot y - is\alpha\cdot D_y + is^2\alpha\cdot\beta/2}$$

and we deduce

$$\mathcal{T}_{\mu,\alpha,\beta}\varphi(y) = \int_{-\infty}^{+\infty} \mathrm{e}^{i(\mu - \alpha\cdot\beta/2)s^2} \mathrm{e}^{is\beta\cdot y} \varphi(y - s\alpha) ds \tag{25}$$

We prove in Proposition E.1 that this operator maps $\mathcal{S}(\mathbb{R}^d)$ into itself if only if $\mu \neq 0$. Moreover, for $\mu \neq 0$, it is a metaplectic transformation of the Hilbert space $L^2(\mathbb{R}^d)$, multiplied by a complex number. In particular, for any Gaussian function g^Γ, the function $\mathcal{T}_{\mu,\alpha,\beta} g^\Gamma$ is a Gaussian:

$$\mathcal{T}_{\mu,\alpha,\beta}\, g^\Gamma = c_{\mu,\alpha,\beta,\Gamma}\, g^{\Gamma_{\mu,\alpha,\beta,\Gamma}},$$

where $\Gamma_{\mu,\alpha,\beta,\Gamma} \in \mathfrak{S}^+(d)$ and $c_{\mu,\alpha,\beta,\Gamma} \in \mathbb{C}$ are given in Proposition E.1.

The result is then the following.

Theorem 2.8. *Let Assumption 2.6 holds and assume that the initial data is as in (2.3). Let $T > 0$ be such that the interval $[t_0, t^\flat]$ is strictly included in the interval $[t_0, t_0 + T]$. Then, for all $k \in \mathbb{N}$, there exists a constant $C_{T,k} > 0$ such that*

$$\sup_{t\in[0,T]} \left\| \psi^\varepsilon(t) - \widehat{\vec{V}}_1(t) v_1^\varepsilon(t) - \sqrt{\varepsilon}\mathbf{1}_{t>t^\flat} \widehat{\vec{V}}_2(t) v_2^\varepsilon(t) \right\|_{\Sigma_\varepsilon^k} \leq C_{T,k}\, \varepsilon^m,$$

with an exponent $m \geq 2/3$, $v_1^\varepsilon(t) = \mathcal{U}^\varepsilon_{h_1}(t, 0) v_0^\varepsilon$ and $v_2^\varepsilon(t) = \mathcal{U}^\varepsilon_{h_2}(t, t^\flat) v_2^\varepsilon(t^\flat)$ with

$$v_2^\varepsilon(t^\flat) = \gamma^\flat \mathrm{e}^{iS^\flat/\varepsilon} \mathcal{W}\mathcal{P}^\varepsilon_{z^\flat} \mathcal{T}^\flat \varphi_1(t^\flat), \tag{26}$$

where φ_1 is the profile of the coherent state $v_1^\varepsilon(t)$ given by Proposition 2.1,

$$\mathcal{T}^\flat = \mathcal{T}_{\mu^\flat,\alpha^\flat,\beta^\flat} \tag{27}$$

$$\mu^\flat = \frac{1}{2}\left(\partial_t f + \{v, f\}\right) \tag{28}$$

$$(\alpha^\flat, \beta^\flat) := J df(t^\flat, z^\flat) \tag{29}$$

$$\gamma^\flat = \|\left(\{v, \Pi_2\} + \partial_t \Pi_2\right) \vec{V}_1(t^\flat, z^\flat)\|_{\mathbb{C}^N}. \tag{30}$$

Note that by Assumption 2.6, $\mu^\flat \neq 0$, which guarantees that $\mathcal{T}^\flat \varphi_1(t^\flat)$ is Schwartz class. Besides if the Hamiltonian is not time-dependent, this also implies that $(\alpha^\flat, \beta^\flat) \neq (0,0)$. The coefficient $\gamma^\flat$ describes the distortion of the projector Π_1 during its evolution along the flow h_1. It is a quantitative information about the torsion of the eigenmodes. In particular, we have

$$\gamma^\flat = \| \left(\{v, \Pi_2\} + \partial_t \Pi_2\right) \vec{V}_1(t^\flat, z^\flat)\|_{\mathbb{C}^N} = \| \left(\{v, \Pi_1\} + \partial_t \Pi_1\right) \vec{V}_1(t^\flat, z^\flat)\|_{\mathbb{C}^N}.$$

In particular, if the matrix H is diagonal (or diagonalizes in a fixed orthonormal basis), then $\gamma^\flat = 0$: the equations are decoupled (or can be decoupled), one can then apply the result for two independent equation with a scalar Hamiltonian and, of course, there is no interaction between the modes.

The error estimate stems from the method of the proof which is done in two steps with two types of arguments applying far from the crossing step for the first one, and in a boundary layer of Υ for the other one. The size of the boundary layer is taken of size $\delta > 0$ and we have to balance two kinds of estimates: an error of size $O(\varepsilon\delta^{-1})$ which comes from the adiabatic propagation of wave packets outside the boundary layer, and an error of size $O(\delta^2 + \varepsilon)$ generated by the passage through the boundary. The choice of $\delta = \varepsilon^{1/3}$ optimizes the error.

The result of Theorem 2.8 can be specified to Gaussian states.

Corollary 2.9. *1- If $v_0^\varepsilon = \mathcal{WP}^\varepsilon_{z_0}(g^{\Gamma_0})$ is a Gaussian state then*

$$v_2^\varepsilon(t^\flat) = c^\flat \mathrm{e}^{iS^\flat/\varepsilon} \mathcal{WP}^\varepsilon_{z^\flat}\left(\mathrm{e}^{i\Gamma^\flat y\cdot y}\right)$$

with

$$c^\flat = \gamma^\flat \sqrt{\frac{2\pi}{i\mu^\flat}}, \quad \Gamma^\flat = \Gamma_1(t^\flat, t_0, z_0) - \frac{(\beta^\flat - \Gamma_1(t^\flat, t_0, z_0)\alpha^\flat) \otimes (\beta^\flat - \Gamma_1(t^\flat, t_0, z_0)\alpha^\flat)}{2\mu^\flat - \alpha^\flat \cdot \beta^\flat + \alpha^\flat \cdot \Gamma_1(t^\flat, t_0, z_0)\alpha^\flat}$$

and $\Gamma_1(t^\flat, t_0, z_0)$ is the image of Γ_0 by the flow map associated with $h_1(t,z)$ by (15) *and* (10)*.*
2- Let $A \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ be a polynomial function, then $\mathrm{op}_1^w(A) g^{\Gamma_0}$ is the product of a polynomial by a Gaussian and choosing $v_0^\varepsilon = \mathcal{WP}^\varepsilon_{z_0}(\mathrm{op}_1^w(A) g^{\Gamma_0})$, we have (with the notations of 1-)

$$v_2^\varepsilon(t^\flat) = c^\flat \mathrm{e}^{iS^\flat/\varepsilon} \mathcal{WP}^\varepsilon_{z^\flat}\left(\mathrm{op}_1^w(A^\flat) g^{\Gamma^\flat}\right)$$

with $A^\flat = A \circ \Phi_{\alpha^\flat,\beta^\flat}(-(4\mu^\flat)^{-1})$ where $\Phi_{\alpha^\flat,\beta^\flat}$ is given by

$$\Phi_{\alpha^\flat,\beta^\flat}(t) = \begin{pmatrix} \mathbb{I} - 2t\beta^\flat \otimes \alpha^\flat & 2t\alpha^\flat \otimes \alpha^\flat, \\ -2t\beta^\flat \otimes \beta^\flat & \mathbb{I} + 2t\alpha^\flat \otimes \beta^\flat \end{pmatrix}. \tag{31}$$

As concluding remarks of this introduction, we want to emphasize that our results are in accordance with those of [12, 33].

(1) In the example (3), denoting by E_A and E_B the two eigenvalues of the potential $V_q(x)$ as in [12], one has
$$\alpha_S^\flat = 0, \quad \beta_S^\flat = \nabla(E_A - E_B)(x), \quad \mu_S^\flat(x,\xi) = \xi \cdot \nabla(E_A - E_B)(x).$$

These coefficients appear in the equation (5.3) of [12]. The latter contribution is devoted to a special type of wave packets which have a profile consisting of a Gaussian multiplied by a Hermite polynomial like in part 2 of Corollary 2.9.

(2) For the example (4), we obtain

$$\alpha^\flat_A = \nabla(E_+ - E_-)(\xi),\ \ \beta^\flat_A = 0,\ \ \mu^\flat_A(x,\xi) = -\frac{1}{2}\nabla W(x)\cdot\nabla(E_+ - E_-)(\xi)$$

where $E_\pm$ are the eigenvalues of $A(\xi)$ as in equation (3.41) of [33] and. The result of Theorem 3.20 (via Definition 3.18) is very a special case of ours.

It is also interesting to notice that in these two examples one of the coefficients $\alpha^\flat$ or $\beta^\flat$ is 0, which is not necessarily the case in our setting since position and momentum variables can be mixed in the coefficient of the matrix part of the Hamiltonian, as long as the symbol satisfies the required growth condition. Actually, it is the case in several physical systems, as Dirac equations with electromagnetic potential (V, A) for example (with the function $\xi - A(t,x)$ appearing in the coefficients of the matrix), or for the equations describing the propagation of acoustical waves in elastic media (the Hamiltonian then is of the form $\rho(x)\mathrm{Id} - \Gamma(x,\xi)$ where $\rho > 0$ is the density and Γ the elastic tensor).

Finally, we want to emphasize that the method of proof we propose here allows to avoid lots of tedious computations which appears in [12] pages 65 to 72 and are also present in [33] via the reference [46] to which the authors refer therein.

2.4. **Organization of the paper.** The proof of Theorem 2.8 is made on two steps: an analysis outside the crossing region in Section 3 and an analysis in the crossing region in Section 4, that allows to conclude the the proof in Section 4.3, together with the one of Corollary 2.9. Finally, we gather in four Appendices various results about wave packets, algebraic properties of the projectors and parallel transport, analysis of the transfer operators $\mathcal{T}_{\mu,\alpha,\beta}$ and technical computations.

3. Adiabatic decoupling outside the crossing region

In this section, we consider a family of solutions to equation (1) in the case where the Hamiltonian $H(t,z)$ satisfies Assumption 2.6 and with an initial data which is a coherent state as in (2.3). We focus here on regions where the classical trajectories associated with the coherent state do not touch the crossing set but are close enough. We prove the next result.

Proposition 3.1. *Let $k \in \mathbb{N}$, $\delta(\varepsilon)$ be such that $\sqrt{\varepsilon} \ll \delta \leq 1$. Let $f(t,z) = 0$ be an equation of Υ in an open set $\Omega \subset \mathbb{R}\times\mathbb{R}^d$. Assume that for $j \in \{1,2\}$,*

$$u^\varepsilon_j = \mathcal{WP}^\varepsilon_{\widetilde z_j}(\widetilde\varphi_j)$$

where $\widetilde\varphi_1$, $\widetilde\varphi_2 \in \mathcal{S}(\mathbb{R}^d)$, $\widetilde z_1$, $\widetilde z_2 \in \mathbb{R}^d$ are such that there exist $s_1, s_2 \in \mathbb{R}$, $c, C > 0$ such that for all $j \in \{1,2\}$ and $t \in [s_1,s_2]$, $z_j(t) := \Phi^{t,s_1}_j(\widetilde z_j) \in \Omega$ with $|f(z_j(t))| > c\delta$ and

$$\left\| \psi^\varepsilon(s_1) - \widehat{\vec V_1(s_1)}u^\varepsilon_1 - \widehat{\vec V_2(s_1)}u^\varepsilon_2 \right\|_{\Sigma^k_\varepsilon} \leq C\varepsilon.$$

Then, for all $k\in\mathbb{N}$, one has

$$\sup_{t\in[s_1,s_2]}\left\|\widehat{\Pi}_j\psi^\varepsilon(t)-\widehat{\vec{V}_j(t)}\mathcal{U}^\varepsilon_{h_j}(t,s_1)u^\varepsilon_j\right\|_{\Sigma^k_\varepsilon}\leq C_k\frac{\varepsilon}{\delta},$$

where the constant C_k does not depend on δ and ε.

For fixed δ, this Proposition implies Theorem 2.8 for $t\in[0,t^\flat[$. We shall choose later $\delta=\varepsilon^{5/12}$. We shall also use this Lemma for $t>t^\flat+\delta$ with some initial data in $t=t^\flat+\delta$.

Proof. Because of the linearity of the equation, it is enough to assume that the contribution of $\psi^\varepsilon(s_1)$ on one of the modes is negligible at the initial time s_1. The roles of the two modes been symmetric, we can choose equivalently one or the other one. For this reason, doing the proof with $v^\varepsilon_1(s_2)=0$ is enough for proving the Proposition, and it is what we assume now. We set

$$w^\varepsilon_1(t)=\widehat{\Pi}_1\psi^\varepsilon(t)-\widehat{\vec{V}_1(t)}v^\varepsilon_1(t),\;\; w^\varepsilon_2(t)=\widehat{\Pi}_2\psi^\varepsilon(t).$$

We introduce the matrices

$$B_j(t)=-2\partial_t\Pi_j(t)-\{h_j(t),\Pi_j(t)\}+\{\Pi_j(t),H(t)\}, \tag{32}$$

that satisfy Lemma B.1 after indexation of the quantities therein by j. We use the next lemma that gives a system satisfied by w^ε_1 and w^ε_2.

Lemma 3.2. *The family $w^\varepsilon=(w^\varepsilon_1,w^\varepsilon_2)$ satisfies $w^\varepsilon(0)=0$ and*

$$i\varepsilon\partial_t w^\varepsilon_1=\widehat{h_1}w^\varepsilon_1+\frac{\varepsilon}{2i}\widehat{B_1\Pi_1}w^\varepsilon_1+\frac{\varepsilon}{2i}\widehat{B_1\Pi_2}w^\varepsilon_2+O(\varepsilon^2),$$
$$i\varepsilon\partial_t w^\varepsilon_2=\widehat{h_2}w^\varepsilon_2+\frac{\varepsilon}{2i}\widehat{B_2\Pi_2}w^\varepsilon_2+\frac{\varepsilon}{2i}\widehat{B_2\Pi_1}(w^\varepsilon_1+\widehat{\vec{V}_1}v^\varepsilon_1)+O(\varepsilon^2),$$

where the $O(\varepsilon^2)$ holds in $\Sigma^\varepsilon_k(\mathbb{R}^d)$.

We postpone the proof of this lemma in a next subsection and set

$$f^\varepsilon_1=-\frac{1}{2}\widehat{B_1\Pi_1}w^\varepsilon_1-\frac{1}{2}\widehat{B_1\Pi_2}w^\varepsilon_2,$$
$$f^\varepsilon_2=-\frac{1}{2}\widehat{B_2\Pi_2}w^\varepsilon_2-\frac{1}{2}\widehat{B_2\Pi_1}w^\varepsilon_1.$$

Therefore, we have for $t,s\in[s_1,s_2]$, and in $\Sigma^k_\varepsilon(\mathbb{R}^d)$

$$\left\{\begin{array}{lcl} w^\varepsilon_1(t) & = & w^\varepsilon_1(s)+\int_s^t\mathcal{U}^\varepsilon_{h_1}(t,\sigma)f^\varepsilon_1(\sigma)d\sigma+O(\varepsilon),\\ w^\varepsilon_2(t) & = & w^\varepsilon_2(s)+\int_s^t\mathcal{U}^\varepsilon_{h_2}(t,\sigma)f^\varepsilon_2(\sigma)d\sigma-\frac{1}{2}\int_s^t\mathcal{U}^\varepsilon_{h_2}(t,\sigma)\widehat{B_2\Pi_1}\widehat{\vec{V}_1}(\sigma)v^\varepsilon_1(\sigma)d\sigma+O(\varepsilon).\end{array}\right.$$

At this stage of the proof, we take advantage of the special form of the matrix $\Pi_1B_2\Pi_1$ given by (55), i.e.

$$\Pi_1B_2\Pi_1=(h_1-h_2)\Pi_1\{\Pi_1,\Pi_1\}\Pi_1$$

to write in $\mathcal{L}(\Sigma^k_\varepsilon(\mathbb{R}^d))$,

$$\int_s^t \mathcal{U}^\varepsilon_{h_2}(t,\sigma)\widehat{\Pi_1 B_2 \Pi_1}\widehat{\vec{V}_1}(\sigma)\mathcal{U}^\varepsilon_{h_1}(\sigma,0)v_0^\varepsilon d\sigma$$
$$= i\varepsilon \int_s^t \frac{d}{d\sigma}\left(\mathcal{U}^\varepsilon_{h_2}(t,\sigma)\mathrm{op}_\varepsilon\left(\Pi_1\{\Pi_1,\Pi_1\}\Pi_1\vec{V}_1(\sigma)\right)\mathcal{U}^\varepsilon_{h_1}(\sigma,0)\right)v_0^\varepsilon d\sigma + O(\varepsilon) = O(\varepsilon).$$

We deduce that for $s,t\in[s_1,s_2]$, there exists a constant $C>0$ such that

$$\left\| \int_s^t \mathcal{U}^\varepsilon_{h_2}(t,\sigma)\widehat{\Pi_1 B_2 \Pi_1}\widehat{\vec{V}_1}(\sigma)\mathcal{U}^\varepsilon_{h_1}(\sigma,0)v_0^\varepsilon d\sigma\right\|_{\Sigma^k_\varepsilon} \leq C\varepsilon. \tag{33}$$

Therefore, we are left with the equations

$$\left\{\begin{array}{lcl} w_1^\varepsilon(t) & = & w_1^\varepsilon(s) + \int_s^t \mathcal{U}^\varepsilon_{h_1}(t,\sigma)f_1^\varepsilon(\sigma)d\sigma + O(\varepsilon),\\ w_2^\varepsilon(t) & = & w_2^\varepsilon(s) + \int_s^t \mathcal{U}^\varepsilon_{h_2}(t,\sigma)f_2^\varepsilon(\sigma)d\sigma - \frac12\int_s^t \mathcal{U}^\varepsilon_{h_2}(t,\sigma)\widehat{\Pi_2 B_2 \Pi_1}\widehat{\vec{V}_1}(\sigma)v_1^\varepsilon(\sigma)d\sigma + O(\varepsilon).\end{array}\right. \tag{34}$$

Note that for the moment, we have only used the smoothness of the eigenvalues and the eigenprojectors, and not the non-crossing assumption. However, for proving that the source term $\displaystyle\int_s^t \mathcal{U}^\varepsilon_{h_2}(t,\sigma)\widehat{\Pi_2 B_2 \Pi_1}\widehat{\vec{V}_1}(\sigma)v_1^\varepsilon(\sigma)d\sigma$ is small enough, we need the gap assumption. We set $w^\varepsilon(t)=(w_1^\varepsilon(t),w_2^\varepsilon(t))$ and we prove the next Lemma.

Lemma 3.3. *With the assumptions of Proposition 3.1, $\tau\in\mathbb{R}$ and $k\in\mathbb{N}$, there exist constants $C_0,C_1>0$ such that for all $t\in[t_{in},t_{in}+\tau]\subset[s_1,s_2]$,*

$$\|w^\varepsilon(t)\|_{\Sigma^k_\varepsilon} \leq \|w^\varepsilon(t_{in})\|_{\Sigma^k_\varepsilon} + C_0\tau \sup_{t\in[t_{in},t_{in}+\tau]}\|w^\varepsilon(t)\|_{\Sigma^k_\varepsilon} + C_1\varepsilon\delta^{-1}. \tag{35}$$

Then the proof uses a bootstrap argument. We choose some time step τ. Therefore, choosing τ such that $C_0\tau<\frac12$ and $t_{in}=s_1$, we get

$$\sup_{t\in[s_1,s_1+\tau]}\|w^\varepsilon(t)\|_{\Sigma^k_\varepsilon(\mathbb{R}^d)} \leq 2C_1\varepsilon\delta^{-1} := \eta(\varepsilon).$$

As a consequence, we can iterate the argument. We obtain

$$\forall t\in[s_1+\tau,s_1+2\tau],\ \|w^\varepsilon(t)\|_{\Sigma^k_\varepsilon(\mathbb{R}^d)} \leq \eta(\varepsilon) + C_0\tau\sup_{t\in[s_1+\tau,s_1+2\tau]}\|w^\varepsilon(t)\|_{\Sigma^k_\varepsilon(\mathbb{R}^d)} + \frac12\eta(\varepsilon),$$

whence $\displaystyle\sup_{t\in[s_1+\tau,s_1+2\tau]}\|w^\varepsilon(t)\|_{\Sigma^k_\varepsilon(\mathbb{R}^d)} \leq \frac32\eta(\varepsilon)$. Iterating again the argument, until the interval $[s_1,s_2]$ is covered, we obtain that there exists a constant $M>0$ such that

$$\sup_{t\in[s_1,ts_2]}\|w^\varepsilon(t)\|_{\Sigma^k_\varepsilon(\mathbb{R}^d} \leq M\eta(\varepsilon).$$

We have got the estimate of Proposition 3.1 and it only remains to prove Lemma 3.2 and Lemma 3.3. □

3.1. **Proof of Lemma 3.2.**

Proof. By the symbolic calculus for systems we have:

$$\hat{\Pi}_1\hat{H} = \hat{h}_1\hat{\Pi}_1 + \frac{\varepsilon}{2i}\mathrm{op}^w_\varepsilon(\{\Pi_1, H\} - \{h_1, \Pi_1\}) + O(\varepsilon^2).$$

Therefore, we have in $\Sigma^k_\varepsilon(\mathbb{R}^d)$

$$\begin{aligned} i\varepsilon\partial_t w_1^\varepsilon &= i\varepsilon\widehat{\Pi}_1\partial_t\psi^\varepsilon + i\varepsilon\widehat{\partial_t\Pi_1}\psi^\varepsilon - i\varepsilon\widehat{\vec{V}_1}\partial_t v_1^\varepsilon - i\varepsilon\partial_t\widehat{\vec{V}_1}v_1^\varepsilon \\ &= (\widehat{h}_1\widehat{\Pi}_1\psi^\varepsilon + \frac{\varepsilon}{2i}\widehat{B}_1\psi^\varepsilon) - \widehat{\vec{V}}_1\widehat{h}_1 v_1^\varepsilon - i\varepsilon\partial_t\widehat{\vec{V}}_1 v_1^\varepsilon + O(\varepsilon^2) \\ &= \widehat{h}(w_1^\varepsilon + \widehat{\vec{V}_1}v_1^\varepsilon) + \frac{\varepsilon}{2i}\widehat{B}_1(w_1^\varepsilon + w_2^\varepsilon + \widehat{\vec{V}}_1 v_1^\varepsilon) - \widehat{\vec{V}}_1\widehat{h}v_1^\varepsilon - i\varepsilon\partial_t\widehat{\vec{V}}_1 v_1^\varepsilon + O(\varepsilon^2) \\ &= \widehat{h}_1 w_1^\varepsilon + \frac{\varepsilon}{2i}\widehat{B}_1(w_1^\varepsilon + w_2^\varepsilon) + \frac{\varepsilon}{2i}\widehat{B}_1\widehat{\vec{V}}_1 v_1^\varepsilon - \frac{\varepsilon}{i}\widehat{\{\vec{V}_1, h_1\}}v_1^\varepsilon - i\varepsilon\partial_t\widehat{\vec{V}}_1 v_1^\varepsilon + O(\varepsilon^2) \\ &= \widehat{h}_1 w_1^\varepsilon + \frac{\varepsilon}{2i}\widehat{B}_1\widehat{\Pi}_1 w_1^\varepsilon + \frac{\varepsilon}{2i}\widehat{B}_1(\widehat{\mathbb{I} - \Pi_1})w_2^\varepsilon + \frac{\varepsilon}{i}\left(\frac{1}{2}\widehat{B_1\Pi_1}\widehat{V}_1 + \partial_t\widehat{\vec{V}}_1 - \widehat{\{\vec{V}_1, h_1\}}\right)v_1^\varepsilon + O(\varepsilon^2) \end{aligned}$$

We observe that by (2) of Lemma B.1 and Proposition 2.2 (with $\Omega_1(t) = -\frac{1}{2}\Pi_1(t)B_1(t)\Pi_1(t)$), the vector $\vec{V}_1(t)$ is chosen in order to have

$$\partial_t\widehat{\vec{V}}_1 + \widehat{\{h_1, \vec{V}_1\}} = -\frac{1}{2}\widehat{B_1\Pi_1}\widehat{V}_1 = -\frac{1}{2}\widehat{\Pi_1 B_1\Pi_1}\widehat{V}_1 - \frac{1}{2}(\widehat{\mathbb{I} - \Pi_1)B_1\Pi_1}\widehat{V}_1.$$

Remark 3.4. At that point, it is important to notice that we could made another choice. An alternative would have been to choose $\vec{V}_1(t)$ satisfying

$$\partial_t\widehat{\vec{V}}_1 + \widehat{\{h_1, \vec{V}_1\}} = -\frac{1}{2}(\widehat{\mathbb{I} - \Pi_1)B_1\Pi_1}\widehat{V}_1$$

and $i\varepsilon\partial v_1^\varepsilon(t) = \widehat{h_{\Omega_1}}v_1^\varepsilon(t)$ with $h_{\Omega_1} = h_1 + \frac{\varepsilon}{2i}\Pi_1 B_1\Pi_1$ (which is self-adjoint according to Lemma B.1).

Therefore, we are left with

$$i\varepsilon\partial_t w_1^\varepsilon \;=\; \widehat{h}_1 w_1^\varepsilon + \frac{\varepsilon}{2i}\widehat{B}_1\widehat{\Pi}_1 w_1^\varepsilon + \frac{\varepsilon}{2i}\widehat{B}_1\widehat{\Pi_2}w_2^\varepsilon + O(\varepsilon^2)$$

and a similar calculus holds for $w_2^\varepsilon(t)$. □

3.2. **Proof of Lemma 3.3.**

Proof. Let $k \in \mathbb{N}$. We work in $\Sigma^k_\varepsilon(\mathbb{R}^d, \mathbb{C}^N)$ on the term

$$A_\varepsilon \;:=\; \int_s^t \mathcal{U}^\varepsilon_{h_2}(t,\sigma)\widehat{\Pi_2 B_2\Pi}_1\widehat{\vec{V}_1}(\sigma)v_1^\varepsilon(\sigma)d\sigma. \tag{36}$$

We recall that $\delta \gg \sqrt{\varepsilon}$. We are going to use that the matrix $(H - h_1\Pi_2)$ is invertible on $\mathbb{I}_{\Omega\cap\{f\geq\delta\}}\mathrm{Ran}\,\Pi_2$ with an inverse that we denote by of $(H - h_1\Pi_2)^{-1}|_{\mathrm{Ran}\,\Pi_2}$ which has a norm of size δ^{-1}. Besides, by assumption, there exists $c > 0$ such that $f(t, z_1(t)) > c\,\delta$ for $t \in [s_1, s_2]$. The family v_1^ε being a wave packet, we can restrict its analysis in close to the points $z_1(t)$ for $t\in[s_1,s_2]$ (see Remark A.2, (53)). On this compact, there exists $M>0$ such that $|f(t,z)-f(t,z_1(t))|<M|z-z_1(t)|$, whence

$$|f(t,z)|>c\delta-MR\sqrt{\varepsilon}\ \text{ if }\ |z-z_1(t)|<R\sqrt{\varepsilon}.$$

In view of these considerations, we introduce a cut-off function $\chi\in\mathcal{C}_0^\infty(\mathbb{R})$ so that $0\le\chi\le 1$ and $\chi=1$ close to 0 and we set

$$v_1^{\varepsilon,R}(t)=\widehat{k}_R^\varepsilon(t)v_1^\varepsilon(t),\quad k_R^\varepsilon(z,t)=\chi\left(\frac{z-z_1(t)}{R\sqrt{\varepsilon}}\right). \tag{37}$$

Then, by (53), we have in $\Sigma_\varepsilon^k(\mathbb{R}^d,\mathbb{C}^N)$ and for $t\in[t_{in},t_{in}+\tau]$,

$$v_1^\varepsilon(t)=v_1^{\varepsilon,R}(t)+O(\varepsilon)+O(R^{-N}) \tag{38}$$

and $v_1^{\varepsilon,R}(t)$ is compactly supported in $|z-z_1(t)|\le R\sqrt{\varepsilon}$. Using $\delta\gg\sqrt{\varepsilon}$, we can choose R such that $MR\sqrt{\varepsilon}=\frac{c}{2}\delta$ and we obtain that the matrix $(H-h_1\Pi_2)^{-1}$ is invertible with a norm of size δ^{-1} on the support of $\Pi_2k_\varepsilon^R(t)$ for all $t\in[t_{in},t_{in}+\tau]$. Therefore, we write

$$\begin{aligned}A_\varepsilon&=\int_s^t\mathcal{U}_{h_2}^\varepsilon(t,\sigma)\mathrm{op}_\varepsilon(\Pi_2B_2\Pi_1\vec{V}_1)(\sigma)v_1^{\varepsilon,R}(\sigma)d\sigma+O(\varepsilon)+O(R^{-N})\\&=\int_s^t\mathcal{U}_{h_2}^\varepsilon(t,\sigma)\mathrm{op}_\varepsilon(k_{\varepsilon,R}(\sigma)\Pi_2B_2\Pi_1\vec{V}_1(\sigma))v_1^\varepsilon(\sigma)d\sigma+O(\sqrt{\varepsilon}R^{-1})+O(\varepsilon)+O(R^{-N}).\end{aligned}$$

We then set

$$Q(\sigma)=\mathcal{U}_{h_2}^\varepsilon(t,\sigma)\mathrm{op}_\varepsilon((H-h_1\Pi_2)^{-1}|_{\mathrm{Ran}\,\Pi_2}k_{\varepsilon,R}(\sigma)\Pi_2B_2\Pi_1)\widehat{\vec{V}_1(\sigma)}\mathcal{U}_{h_1}^\varepsilon(\sigma,0)$$

and differentiating

$$\frac{d}{d\sigma}Q(\sigma)=\frac{i}{\varepsilon}\mathcal{U}_{h_2}^\varepsilon(t,\sigma)\widehat{G}(\sigma)\mathcal{U}_{h_1}^\varepsilon(\sigma,0)+O(1)+O(R^{-1}\varepsilon^{-1/2})$$

in $\Sigma_\varepsilon^k(\mathbb{R}^d,\mathbb{C}^N)$, where (using the the equation satisfied by $\vec{V}_1$ and differentiating k_ε^R), we have

$$\begin{aligned}\widehat{G}&=\widehat{h}_2\ \mathrm{op}_\varepsilon\Big((H-h_1\Pi_2)^{-1}|_{\mathrm{Ran}\,\Pi_2}k_{\varepsilon,R}(\sigma)\Pi_2B_2\Pi_1\vec{V}_1(\sigma)\Big)\\&\quad-\mathrm{op}_\varepsilon\left((H-h_1\Pi_2)^{-1}|_{\mathrm{Ran}\,\Pi_2}k_{\varepsilon,R}(\sigma)\Pi_2B_2\Pi_1V_1(\sigma)\right)\widehat{h}_1+O(\varepsilon)\\&=-\mathrm{op}_\varepsilon\Big(k_{\varepsilon,R}(\sigma)(H-h_1\Pi_2)^{-1}|_{\mathrm{Ran}\,\Pi_2}(h_1-h_2)\Pi_2B_2\Pi_1\vec{V}_1(\sigma)\Big)+O(\varepsilon)+O(R^{-1}\sqrt{\varepsilon})\\&=-\mathrm{op}_\varepsilon\Big(k_{\varepsilon,R}(\sigma)\Pi_2B_2\Pi_1\vec{V}_1(\sigma)\Big)+O(\varepsilon)+O(R^{-1}\sqrt{\varepsilon}),\end{aligned}$$

where we have used the identity

$$(H-h_1\Pi_2)^{-1}(h_1-h_2)\Pi_2=\Pi_2. \tag{39}$$

Finally, we obtain in $\Sigma^k_\varepsilon(\mathbb{R}^d)$,

$$(40)\qquad \begin{aligned} A_\varepsilon &= \frac{\varepsilon}{2}\int_s^t \frac{d}{d\sigma}Q(\sigma)\, v_0^\varepsilon\, d\sigma + O(\varepsilon) + O(R^{-1}\sqrt{\varepsilon}) + O(\varepsilon) + O(R^{-N}) \\ &= \frac{\varepsilon}{2}(Q(t)-Q(s))\, v_0^\varepsilon\, d\sigma + O(\varepsilon\delta^{-1}) = O(\varepsilon\delta^{-1}) \end{aligned}$$

since $R^{-1}\sqrt{\varepsilon} = \frac{2}{c}\varepsilon\delta^{-1}$ and by choosing N large enough so that $R^{-N} = O(\varepsilon\delta^{-1})$ □

3.3. **Remarks on systems with gapped eigenvalues.** Note that the proof of Proposition 3.1 can be adapted to prove Theorem 2.3. Besides, this result extends to a more general setting where two blocks of eigenvalues of H are separated than a gap and where h is no longer scalar and has to be replaced by a matrix $H^\flat$ with

$$H = \Pi H^\flat H + (\mathbb{I}-\Pi)H^\perp(\mathbb{I}-\Pi).$$

One can then prove the analogue to Theorem 2.3.

Proposition 3.5. *Assume* $\widehat{\Pi}\psi_0^\varepsilon = \psi_0^\varepsilon + O(\varepsilon)$ *in* $\Sigma^k_\varepsilon(\mathbb{R}^d)$. *Then*

$$\sup_{t\in[0,T]}\left\|\widehat{(\mathbb{I}-\Pi)}\psi^\varepsilon(t)\right\|_{\Sigma^k_\varepsilon(\mathbb{R}^d)} + \sup_{t\in[0,T]}\left\|\widehat{\Pi}\psi^\varepsilon(t) - \phi^\varepsilon(t)\right\|_{\Sigma^k_\varepsilon(\mathbb{R}^d)} \le C\varepsilon,$$

where ϕ^ε *solves*

$$i\varepsilon\partial_t\phi^\varepsilon = \widehat{H^\flat}\phi^\varepsilon,\ \ \phi^\varepsilon(0) = \psi_0^\varepsilon.$$

The proof of this proposition follows the lines of the proof of Theorem 2.3. However, some new difficulties arise because $H^\flat$ is no longer scalar and, thus, one cannot use some commutation relations that we used above in the algebraic Lemma. Setting

$$B^\flat = -2\partial_t\Pi - \{H^\flat,\Pi\} + \{\Pi, H\}\ \text{ and }\ C^\flat = 2\partial_t\Pi - \{\Pi,H\} + \{H^\perp,\Pi\}$$

one then uses the following properties which are enough to run the proof.

Lemma 3.6. (1) *The matrix* $\Pi B^\flat\Pi$ *is skew symmetric.*
(2) *There exists* $Q = (\mathbb{I}-\Pi)Q\Pi$ *such that*

$$(\mathbb{I}-\Pi)C\Pi = [H,Q] = H^\perp Q - QH^\flat$$

and

$$\Pi C\Pi = H^\perp(\Pi\{\Pi,\Pi\}\Pi) - (\Pi\{\Pi,\Pi\}\Pi)H^\flat$$

Proof. (1) One argue as in the proof of Lemma B.1 by using the relation

$$(\Pi\{H^\perp,\Pi\}\Pi)^* = -\Pi\{\Pi,H^\perp\}\Pi = -\Pi\{H^\perp,\Pi\}$$

which comes from the fact thet $\Pi\{H^\perp,\Pi\} = \{\Pi,H^\perp,\Pi\}$. This latter relation can be proved by use of the property

$$(41)\qquad \{A,BC\} - \{AB,C\} = \{A,B\}C - A\{B,C\}.$$

Indeed, taking $A = C = \Pi$ and $B = H^\perp$, one gets

$$(42)\qquad 0 = \{\Pi,H^\perp\}\Pi - \Pi\{H^\perp,\Pi\}$$

whence $\Pi C\Pi = -\Pi\{\Pi, H^\flat\}\Pi$.

(2) Finding Q is done by use of the integral relation (19). We choose

$$Q = -\frac{1}{2i\pi}\int_{\mathcal{C}} (H-\zeta)^{-1}(\mathbb{I}-\Pi)C\Pi(H-\zeta)^{-1}d\zeta$$

and observe that

$$\begin{aligned}
[H,Q] &= -\frac{1}{2i\pi}\int_{\mathcal{C}}(H(H-\zeta)^{-1}(\mathbb{I}-\Pi)C\Pi(H-\zeta)^{-1} - (H-\zeta)^{-1}(\mathbb{I}-\Pi)C\Pi(H-\zeta)^{-1}H)d\zeta \\
&= -\frac{1}{2i\pi}\int_{\mathcal{C}}((\mathbb{I}-\Pi)C\Pi(H-\zeta)^{-1} - (H-\zeta)^{-1}(\mathbb{I}-\Pi)C\Pi)d\zeta \\
&= -[(\mathbb{I}-\Pi)C\Pi, \Pi] = (\mathbb{I}-\Pi)C\Pi.
\end{aligned}$$

Besides, and, using again the brackets relation (56) with $A = B = \Pi$ and $C = H^\flat$, we obtain

$$\{\Pi, \Pi H^\flat\} - \{\Pi, H^\flat\} = \{\Pi,\Pi\}H^\flat - \Pi\{\Pi, H^\flat\}$$

whence

$$\Pi\{\Pi, H^\flat\}\Pi = \Pi\{\Pi,\Pi\}H^\flat.$$

We deduce, using again (42),

$$\Pi C\Pi = -\Pi\{\Pi,\Pi\}H^\flat = H^\perp(\Pi\{\Pi,\Pi\}\Pi) - (\Pi\{\Pi,\Pi\}\Pi)H^\flat.$$

□

4. Analysis in the crossing region

4.1. **A priori estimate in the crossing region.** The analysis performed before gives that if $\sqrt{\varepsilon} \ll \delta \leq 1$ and $k \in \mathbb{N}$, there exists a constant $C_k > 0$ such that

$$\sup_{t\in[t_0, t^\flat-\delta]} \|\psi^\varepsilon(t) - \widehat{\vec{V}_1}(t)v^\varepsilon(t)\|_{\Sigma^k_\varepsilon} \leq C_k\frac{\varepsilon}{\delta}.$$

Therefore, using (34), we deduce that there exists $C'_k > 0$ such that

$$\sup_{t\in[t_0, t^\flat+\delta]} \|\psi^\varepsilon(t) - \widehat{\vec{V}_1}(t)v^\varepsilon(t)\|_{\Sigma^k_\varepsilon} \leq C'_k\left(\delta + \frac{\varepsilon}{\delta}\right). \tag{43}$$

In the next section, we improve this estimate to go beyond this δ-approximation.

4.2. **Towards a more precise analysis.** We now want to derive a more precise estimate on $\psi^\varepsilon(t)$. We prove the following result.

Proposition 4.1. *Assume $\sqrt{\varepsilon} \ll \delta \leq 1$. Then, for all $k \in \mathbb{N}$, there exists a constant $C_k > 0$ such that*

$$\left\|\psi^\varepsilon(t^\flat+\delta) - \vec{V}_1\widehat{(t^\flat+\delta)}v_1^\varepsilon(t^\flat+\delta) - \sqrt{\varepsilon}\vec{V}_2\widehat{(t^\flat+\delta)}v_2^\varepsilon(t^\flat+\delta)\right\|_{\Sigma^k_\varepsilon} \leq C_k(\varepsilon + \delta^2 + \varepsilon\delta^{-1}),$$

where $v_1^\varepsilon(t)$ and $v_2^\varepsilon(t)$ are as in Theorem 2.8.

Here again, for proving the proposition, we follow the arguments of the proof of Proposition 3.1 and, with the same notations, we write

$$\psi^\varepsilon(t) = \widehat{\vec{V}_1(t)} v_1^\varepsilon(t) + w_1^\varepsilon(t) + w_2^\varepsilon(t).$$

By equations (34), (33), and in view of the a priori estimate (43) that we have obtained in the preceding subsection, we have

$$\begin{aligned} w_1^\varepsilon(t^\flat+\delta) &= O(\delta^{-1}\varepsilon) + O(\varepsilon) + O(\delta^2), \\ w_2^\varepsilon(t^\flat+\delta) &= O(\delta^{-1}\varepsilon) + O(\varepsilon) + +O(\delta^2) - \frac{i}{2}\int_{t^\flat-\delta}^{t^\flat+\delta} \mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,\sigma)\Pi_2 \widehat{B_2\Pi_1}\vec{V}_1(\sigma) v_1^\varepsilon(\sigma) d\sigma \\ &= -\frac{1}{2}\,\mathrm{e}^{iS^\flat/\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\int_{t^\flat-\delta}^{t^\flat+\delta} \mathcal{U}^\varepsilon_{h_2}(t^\flat,\sigma)\Pi_2\widehat{B_2\Pi_1}\vec{V}_1(\sigma)\mathcal{U}^\varepsilon_{h_1}(\sigma,t^\flat)\mathcal{W}\mathcal{P}_{z^\flat}\varphi_1(t^\flat)d\sigma \\ &\quad + O(\delta^{-1}\varepsilon) + O(\varepsilon) + O(\delta^2) \end{aligned}$$

where we have used

$$v_1^\varepsilon(t^\flat) = \mathrm{e}^{iS^\flat/\varepsilon}\mathcal{W}\mathcal{P}_{z^\flat}\varphi_1(t^\flat) + O(\sqrt{\varepsilon})$$

and $O(\delta\sqrt{\varepsilon}) = O(\delta^2) + O(\varepsilon)$. We recall that $z^\flat = \Phi_{h_1}^{t^\flat,t_0}(z_0)$, $S^\flat = S_1(t^\flat,t_0,z_0)$ and $\varphi_1(t^\flat)$ is associated with φ_0 according to Proposition 2.1. We set

$$A_\varepsilon = -\frac{1}{2}\,\mathrm{e}^{iS^\flat/\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\int_{t^\flat-\delta}^{t^\flat+\delta} \mathcal{U}^\varepsilon_{h_2}(t^\flat,\sigma)\Pi_2\widehat{B_2\Pi_1}\vec{V}_1(\sigma)\mathcal{U}^\varepsilon_{h_1}(\sigma,t^\flat)\mathcal{W}\mathcal{P}_{z^\flat}\varphi_1(t^\flat)d\sigma$$

and we focus in determining the leading order contribution of A_ε.

4.2.1. *Egorov semi-classical Theorem.* We use Egorov semiclassical theorem (Theorem 12 in [5]): that is, in Σ^k_ε,

$$\mathcal{U}^\varepsilon_{h_2}(t^\flat,\sigma)\Pi_2\widehat{B_2\Pi_1}\vec{V}_1(\sigma) = \mathrm{op}^w(\Pi_2 B_2\Pi_1\vec{V}_1(\sigma)\circ\Phi_2^{\sigma,t^\flat})\,\mathcal{U}^\varepsilon_{h_2}(t^\flat,\sigma) + O(\varepsilon),$$

Using that $\Phi_j^{\sigma,t^\flat} = \mathbb{I}_{\mathbb{R}^{2d}} + O(|\sigma - t^\flat|)$, we obtain

$$A_\varepsilon = -\frac{1}{2}\,\mathrm{e}^{iS^\flat/\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\Pi_2\widehat{B_2\Pi_1\vec{V}_1}(t^\flat)\int_{t^\flat-\delta}^{t^\flat+\delta}\mathcal{U}^\varepsilon_{h_2}(t^\flat,\sigma)\mathcal{U}^\varepsilon_{h_1}(\sigma,t^\flat)\mathcal{W}\mathcal{P}^\varepsilon_{z^\flat}\varphi_1(t^\flat)d\sigma + O(\varepsilon+\delta^2+\delta^{-1}\varepsilon) \tag{44}$$

By the definition of $\vec{V}_2(t^\flat,z)$, we have

$$-\frac{1}{2}\Pi_2 B_2\Pi_1\vec{V}_1(t^\flat,z) = \gamma(t^\flat,z)\vec{V}_2(t^\flat,z),\quad \gamma(t^\flat,z) = \frac{1}{2}\|\Pi_2 B_2\Pi_1\vec{V}_1(t^\flat,z)\|_{\mathbb{C}^N}.$$

Therefore

$$A_\varepsilon = \mathrm{e}^{iS^\flat/\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\widehat{\gamma\vec{V}_2(t^\flat)}\int_{t^\flat-\delta}^{t^\flat+\delta}\mathcal{U}^\varepsilon_{h_2}(t^\flat,\sigma)\mathcal{U}^\varepsilon_{h_1}(\sigma,t^\flat)\mathcal{W}\mathcal{P}^\varepsilon_{z^\flat}\varphi_1(t^\flat)d\sigma + O(\varepsilon+\delta^2+\delta^{-1}\varepsilon) \tag{45}$$

4.2.2. *Wave packet formulation of propagators.* Now applying successively Proposition 2.1 to the evolutions $\mathcal{U}^\varepsilon_{h_1}$ and $\mathcal{U}^\varepsilon_{h_2}$, with error term $O(\sqrt{\varepsilon})$, we get after a change of variables

(46)

$$A_\varepsilon = \mathrm{e}^{iS^\flat/\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\widehat{\alpha\vec{V}_2(t^\flat)}$$
$$\times \int_{-\delta}^{+\delta} \mathrm{e}^{\frac{i}{\varepsilon}\left(S_1(t^\flat+\sigma,t^\flat,z^\flat)+S_2(t^\flat,t^\flat+\sigma,\Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat))\right)}\mathcal{WP}^\varepsilon_{\zeta(\sigma)}\varphi_1(t^\flat)d\sigma + O(\varepsilon+\delta^2+\delta^{-1}\varepsilon)$$

where

$$\zeta(\sigma) = \Phi_2^{t^\flat,t^\flat+\sigma}\left(\Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat)\right).$$

Since $\zeta(0)=z^\flat$, we set

$$\Phi_2^{t^\flat,t^\flat+\sigma}\left(\Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat)\right) = \zeta(\sigma) = z^\flat + (q(\sigma),p(\sigma)) = z^\flat + \sqrt{\varepsilon}(q_\varepsilon(\sigma),p_\varepsilon(\sigma)), \tag{47}$$

with $(q_\varepsilon(\sigma),p_\varepsilon(\sigma)) = \varepsilon^{-1/2}(q(\sigma),p(\sigma))$, and we write by using (51),

$$\mathcal{WP}^\varepsilon_{\zeta(\sigma)} = \mathrm{e}^{-\frac{i}{\varepsilon}p^\flat\cdot q(\sigma)}\mathcal{WP}^\varepsilon_{z^\flat}\Lambda_\varepsilon^{-1}\mathcal{WP}^\varepsilon_{(q(\sigma),p(\sigma))},$$

whence

$$\mathcal{WP}^\varepsilon_{\zeta(\sigma)}\varphi_1(t^\flat,\cdot) = \mathrm{e}^{-\frac{i}{\varepsilon}p^\flat\cdot q(\sigma)}\mathcal{WP}^\varepsilon_{z^\flat}(\mathrm{e}^{i(y-q_\varepsilon(\sigma))\cdot p_\varepsilon(\sigma)}\varphi_1(t^\flat,y-q_\varepsilon(\sigma)).$$

We are left with

$$A_\varepsilon = \mathrm{e}^{iS^\flat/\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\widehat{\gamma\vec{V}_2(t^\flat)}\mathcal{WP}^\varepsilon_{z^\flat}\,\mathcal{T}^\varepsilon\varphi_1(t^\flat) + O(\varepsilon+\delta^2+\delta^{-1}\varepsilon)$$

where the operator $\mathcal{T}^\varepsilon$ is defined on functions $\varphi\in\mathcal{S}(\mathbb{R}^d)$ by

$$\mathcal{T}^\varepsilon\varphi(y) = \int_{-\delta}^{+\delta}\mathrm{e}^{\frac{i}{\varepsilon}\Lambda(\sigma)}\mathrm{e}^{i(y-q_\varepsilon(\sigma)))\cdot p_\varepsilon(\sigma)}\varphi(y-q_\varepsilon(\sigma))d\sigma$$

with

$$\Lambda(\sigma) = S_1(t^\flat+\sigma,t^\flat,z^\flat) + S_2(t^\flat,t^\flat+\sigma,\Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat)) - q(\sigma)\cdot p^\flat. \tag{48}$$

4.2.3. *The transfer operator.* Proposition 4.1 then comes from the analysis of the operator $\mathcal{T}^\varepsilon$ when ε goes to 0.

Lemma 4.2. *We have*

$$\mathcal{T}^\varepsilon = \sqrt{\varepsilon}\mathcal{T}^\flat + O(\varepsilon+\delta^2), \tag{49}$$

where $\mathcal{T}^\flat = \mathcal{T}_{\mu^\flat,\alpha^\flat,\beta^\flat}$ *with* $\lambda^\flat$ *given by* (28) *and* $(\alpha^\flat,\beta^\flat)$ *by* (29)

Proof. The proof relies on the analysis close to $\sigma=0$ of the phasis $\Lambda(\sigma)$ and of the function $\zeta(\sigma)=(q(\sigma),p(\sigma))$, as stated in Lemma D.1 in Appendix D. Then, to prove the estimate (49) we use that if $\varphi \in \mathcal{S}(\mathbb{R}^d)$, the map $z \mapsto \mathcal{WP}^1_z\varphi$ is locally Lipschitz from $\mathbb{R}^{2d}$ in $\mathcal{S}(\mathbb{R}^d)$. Using $\zeta(0) = 0$ and $\Lambda(0) = \dot\Lambda(0) = 0$, we obtain

$$\mathcal{T}^\varepsilon\varphi(y) = \sqrt{\varepsilon}\int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}} \mathrm{e}^{i(\frac{\ddot\Lambda(0)}{2}-\dot q(0)\cdot\dot p(0))s^2}\mathrm{e}^{isy\cdot\dot p(0)}\varphi(y - s\dot q(0))ds + R^{\varepsilon,\delta}.$$

We set

$$\mu^\flat = \frac{1}{2}\left(\ddot\Lambda(0) - \dot q(0)\cdot\dot p(0)\right), \quad \alpha^\flat = \dot q(0), \quad \beta^\flat = \dot p(0), \quad L = \beta^\flat\cdot y - \alpha^\flat\cdot D_y \tag{50}$$

and write

$$\mathrm{e}^{i(\frac{\ddot\Lambda(0)}{2}-\dot q(0)\cdot\dot p(0))s^2}\mathrm{e}^{isy\cdot\dot p(0)}\varphi(y - s\dot q(0)) = \mathrm{e}^{i\mu^\flat s^2+isL}\varphi(y).$$

With these notations the remainder $R^{\varepsilon,\delta}$ are sum of terms of the form

$$\Theta_k(y) = (\sqrt{\varepsilon})^{k+1}\int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}} \mathrm{e}^{i\mu^\flat s^2+isL}s^k\theta_k(y,s)ds$$

where $k \in \{1,2,3\}$ and $\theta_k(y,s)$ are smooth bounded functions with bounded derivatives. For estimating semi-norms of the functions $y \mapsto \Theta_k(y)$, we use integration by parts. Indeed,

$$\Theta_k(y) = \left[\frac{(\sqrt{\varepsilon})^{k+1}}{2i\mu^\flat}\mathrm{e}^{i\mu^\flat s^2+isL}s^{k-1}\theta_k(y,s)\right]_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}} - \frac{(\sqrt{\varepsilon})^{k+1}}{2i\mu^\flat}\int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}} \mathrm{e}^{i\mu^\flat s^2}\frac{d}{ds}\left(\mathrm{e}^{isL}s^{k-1}\theta_k(y,s)\right)ds.$$

Since e^{iLs} is a bounded operator in Σ^k_ε, we obtain

$$R^{\varepsilon,\delta} = O(\varepsilon) + O(\delta^2) \text{ in } \Sigma^k_\varepsilon,$$

which gives (28) and (29) in view of (59) and (61). $\square$

4.3. **Proof of Theorem 2.8 and Corollary 2.9.** Theorem 2.8 comes from Propositions 3.1 and 4.1 with the adequate choice of $\delta = \varepsilon^{1/3}$. Corollary 2.9 comes from Theorem 2.8 and Point (3) of Proposition E.1.

Appendix A. The wave packet transform

We discuss here useful properties of the wave-packet transform. We define the Weyl translation operator T^ε

$$\widehat{T}^\varepsilon(z) = \mathrm{e}^{\frac{i}{\varepsilon}(p\cdot\widehat{x}-q\cdot\widehat{\xi})}, \quad z = (q,p) \in \mathbb{R}^{2d},$$

the semi-classical scaling operator Λ_ε

$$\Lambda_\varepsilon\varphi(x) = \varepsilon^{-d/4}\varphi\left(\frac{x}{\sqrt{\varepsilon}}\right), \qquad \varphi \in \mathcal{S}(\mathbb{R}^d),$$

and we denote by $a_{\varepsilon,z} \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ the function $a_{\varepsilon,z}(w) = a(\sqrt{\varepsilon}w + z)$, $w \in \mathbb{R}^{2d}$.

Lemma A.1. *The wave packet transform satisfies for all points $z, z' \in \mathbb{R}^{2d}$ and all smooth functions $a \in \mathcal{C}^\infty(\mathbb{R}^{2d})$*

$$\mathcal{WP}^\varepsilon_z = \mathrm{e}^{-\frac{i}{2\varepsilon}p\cdot q}\,\hat{T}^\varepsilon(z)\,\Lambda_\varepsilon,$$

$$\mathcal{WP}^\varepsilon_{z+z'} = \mathrm{e}^{-\frac{i}{\varepsilon}p\cdot q'}\,\mathcal{WP}^\varepsilon_z\,\Lambda_\varepsilon^{-1}\mathcal{WP}^\varepsilon_{z'}, \tag{51}$$

$$\mathrm{op}^w_\varepsilon(a)\mathcal{WP}^\varepsilon_z = \mathcal{WP}^\varepsilon_z\,\mathrm{op}^w_1(a_{\varepsilon,z}), \tag{52}$$

Remark A.2. The property (52) induces a strong localisation property of wave packets. Let $\chi \in \mathcal{C}^\infty_0(\mathbb{R}^d)$ such that $\chi = 1$ close 0 and $0 \le \chi \le 1$ and define for $R > 0$, $\chi_R(y) = \chi(R^{-1}y)$. Then, for $\varphi \in \mathcal{S}(\mathbb{R}^d)$, $N \in \mathbb{N}$, $k \in \mathbb{N}$, and in Σ^k_ε,

$$\begin{aligned}\mathcal{WP}^\varepsilon_0(\varphi) &= \mathcal{WP}^\varepsilon_0(\widehat{\chi}_R\varphi) + \mathcal{WP}^\varepsilon_0((\widehat{1-\chi_R}\varphi) = \mathcal{WP}^\varepsilon_0(\widehat{\chi}_R\varphi) + O(R^{-N})\\ &= \widehat{\chi_{R\sqrt{\varepsilon}}}\mathcal{WP}^\varepsilon_0(\phi) + O(R^{-N}).\end{aligned} \tag{53}$$

Proof. We consider $\varphi \in \mathcal{S}(\mathbb{R}^d)$. Then $\widehat{T}^\varepsilon(z)\varphi$ is the solution at time $t = 1$ of the initial value problem

$$i\varepsilon\partial_t\psi = (q\cdot\widehat{\xi} - p\cdot\widehat{x})\psi, \qquad \psi(0) = \varphi.$$

The explicit form of this solution

$$\psi(t,x) = \mathrm{e}^{-\frac{i}{2\varepsilon}t^2 q\cdot p}\,\mathrm{e}^{\frac{i}{\varepsilon}tp\cdot x}\varphi(x - tq)$$

implies for the action of the Weyl translation that

$$\widehat{T}^\varepsilon(z)\varphi(x) = \mathrm{e}^{-\frac{i}{2\varepsilon}q\cdot p}\,\mathrm{e}^{\frac{i}{\varepsilon}p\cdot x}\varphi(x-q).$$

This yields

$$\mathrm{e}^{-\frac{i}{2\varepsilon}p\cdot q}\,\hat{T}^\varepsilon(z)\,\Lambda_\varepsilon\varphi(x) = \varepsilon^{-d/4}\,\mathrm{e}^{-\frac{i}{\varepsilon}p\cdot q}\,\mathrm{e}^{\frac{i}{\varepsilon}p\cdot x}\varphi(\tfrac{x-q}{\sqrt{\varepsilon}}) = \mathcal{WP}^\varepsilon_z\varphi(x).$$

For the commutation property we compute

$$\begin{aligned}\mathrm{e}^{-\frac{i}{\varepsilon}p\cdot q'}\mathcal{WP}^\varepsilon_z\Lambda_\varepsilon^{-1}\mathcal{WP}^\varepsilon_{z'}\varphi(x) &= \mathrm{e}^{-\frac{i}{\varepsilon}p\cdot q'}\mathcal{WP}^\varepsilon_z\mathrm{e}^{\frac{i}{\varepsilon}p'\cdot(\sqrt{\varepsilon}x-q')}\varphi\Big(\tfrac{\sqrt{\varepsilon}x-q'}{\sqrt{\varepsilon}}\Big)\\ &= \mathrm{e}^{-\frac{i}{\varepsilon}p\cdot q'}\varepsilon^{-d/4}\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)}\mathrm{e}^{\frac{i}{\varepsilon}p'\cdot(x-q-q')}\varphi\Big(\tfrac{x-q-q'}{\sqrt{\varepsilon}}\Big)\\ &= \mathcal{WP}^\varepsilon_{z+z'}\varphi(x).\end{aligned}$$

Moreover,

$$\begin{aligned}&\mathcal{WP}^\varepsilon_z\,\mathrm{op}^w_1(a_{\varepsilon,z})\varphi(x)\\ &= \varepsilon^{-d/4}\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)}(2\pi)^{-d}\int_{\mathbb{R}^{2d}} a\Big(\tfrac{\sqrt{\varepsilon}}{2}\Big(\tfrac{x-q}{\sqrt{\varepsilon}}+y\Big)+q, \sqrt{\varepsilon}\xi+p\Big))\mathrm{e}^{i\xi\cdot((x-q)/\sqrt{\varepsilon}-y)}\varphi(y)\,dy\,d\xi\\ &= \varepsilon^{-d/4}\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)}(2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} a\big(\tfrac{1}{2}(x+y')+q,\xi'\big)\,\mathrm{e}^{\frac{i}{\varepsilon}(\xi'-p)\cdot(x-y')}\varphi\Big(\tfrac{y'-q}{\sqrt{\varepsilon}}\Big)\,dy'\,d\xi'\\ &= \mathrm{op}^w_\varepsilon(a)\,\mathcal{WP}^\varepsilon_z\varphi(x).\end{aligned}$$

□

Appendix B. Algebraic properties of the eigenprojectors

We thus consider a smooth eigenvalue $h(t,z)$ of a matrix-valued Hamiltonian $H(t,z)$, associated with a smooth eigenprojector $\Pi(t,z)$, and, without restricting the generality of the result, we assume that $h(t,z)\neq 0$. We emphasize that we just assume smoothness of the projector and make no gap assumption.

Lemma B.1. *We assume that h is a smooth eigenvalue of H and Π is a smooth eigenprojector associated with h. Then, the matrix*

$$B \;=\; -2\partial_t\Pi - \{h,\Pi\} + \{\Pi,H\} \tag{54}$$

has the following properties:

(1) *The matrix*

$$\Omega = \Pi B\Pi = \Pi\{\Pi,H\}\Pi$$

is skew-symmetric. Besides, if H has only two eigenvalues h and $h^\perp = \mathrm{tr}(H)-h$ (i.e. $H = h\Pi + h^\perp(\mathbb{I}-\Pi)$), then

$$(\mathbb{I}-\Pi)B(\mathbb{I}-\Pi) = (h-h^\perp)(\mathbb{I}-\Pi)\{\Pi,\Pi\}(\mathbb{I}-\Pi). \tag{55}$$

(2) *The off-diagonal part of $B(t)\Pi(t)$ satisfies*

$$(\mathbb{I}-\Pi)B\Pi = (\mathbb{I}-\Pi)\left(\{\Pi,h\}-2\partial_t\Pi\right)\Pi \;\; \textit{and} \;\; \Pi B(\mathbb{I}-\Pi) = \Pi\left(\{\Pi,h\}-2\partial_t\Pi\right)(\mathbb{I}-\Pi).$$

Proof. For notational simplicity, we suppress the time dependence, once noticed that $\partial_t\Pi(t)$ is off-diagonal. We will twice use the relation

$$\{A,BC\} - \{AB,C\} = \{A,B\}C - A\{B,C\}. \tag{56}$$

We first apply it to $A=C=\Pi$ and $B = H(\mathbb{I}-\Pi)$. We obtain

$$0 = \{\Pi, H(\mathbb{I}-\Pi)\}\Pi - \Pi\{H(\mathbb{I}-\Pi),\Pi\},$$

whence

$$\Pi\{\Pi,H(\mathbb{I}-\Pi)\}\Pi = \Pi\{H(\mathbb{I}-\Pi),\Pi\}\Pi$$

and

$$(\mathbb{I}-\Pi)\{\Pi,H(\mathbb{I}-\Pi)\}\Pi = 0. \tag{57}$$

In particular, we have

$$\Pi\{\Pi,H\}\Pi = \Pi\{H,\Pi\}\Pi.$$

Proving (1): Since $\{\Pi,h\}$ is off-diagonal, $\Pi B\Pi = \Pi\{\Pi,H\}\Pi = \Omega$ and

$$\Omega^* = \Pi\{\Pi,H\}^*\Pi = -\Pi\{H,\Pi\}\Pi = -\Omega.$$

Besides, when H has two eigenvalues, we have

$$\begin{aligned}(\mathbb{I}-\Pi)B(\mathbb{I}-\Pi) &= (\mathbb{I}-\Pi)\{\Pi,H\}(\mathbb{I}-\Pi)\\ &= h(\mathbb{I}-\Pi)\{\Pi,\Pi\}(\mathbb{I}-\Pi) + h^\perp(\mathbb{I}-\Pi)\{\Pi,(\mathbb{I}-\Pi)\}\Pi\\ &= (h-h^\perp)(\mathbb{I}-\Pi)\{\Pi,\Pi\}(\mathbb{I}-\Pi).\end{aligned}$$

Proving (2): We write

$$\{\Pi, H\} = \{\Pi, h\}\Pi + h\{\Pi, \Pi\} + \{\Pi, H(\mathbb{I} - \Pi)\}.$$

We now apply the relation (56) to $A = B = C = \Pi$ and we obtain

$$0 = \{\Pi, \Pi\}\Pi - \Pi\{\Pi, \Pi\},$$

whence

$$(\mathbb{I} - \Pi)\{\Pi, \Pi\}\Pi = \Pi\{\Pi, \Pi\}(\mathbb{I} - \Pi) = 0.$$

Altogether with (57), we have proven

$$(\mathbb{I} - \Pi)\{\Pi, H\}\Pi = (\mathbb{I} - \Pi)\{\Pi, h\}\Pi$$

and $(\mathbb{I} - \Pi)B\Pi = 2(\mathbb{I} - \Pi)\{\Pi, h\}\Pi$. □

Appendix C. Parallel transport

We prove here Proposition 2.2 that provides the time-dependent eigenvector $\vec{V}(t, z)$ defined by parallel transport.

Proof. We consider the solution $\vec{V}(t, z)$ of the parallel transport equation and set $Y(t, z) = \vec{V}(t, \Phi_h^{t,t_0}(z))$. We observe that $Y(t, z)$ solves the equation

$$\begin{aligned} \partial_t Y(t, z) &= \partial_t \vec{V}(t, \Phi_h^{t,t_0}(z)) + Jdh(\Phi_h^{t,t_0}(z))V(t, \Phi_h^{t,t_0}(z)) \\ &= \Omega(t, \Phi_h^{t,t_0}(z))Y(t, z) + K(t, \Phi_h^{t,t_0}(z))Y(t, z). \end{aligned} \tag{58}$$

In particular,

$$(\mathbb{I} - \Pi(t, \Phi_h^{t,t_0}(z)))\ \partial_t Y(t, z) = K(t, \Phi_h^{t,t_0}(z))Y(t, z).$$

We now start proving that for $z \in U_{z_0}$

$$\Pi(t, \Phi_h^{t,t_0}(z))Y(t, z) = Y(t, z),$$

or equivalently that

$$Z(t, z) = (\mathbb{I} - \Pi(t, \Phi_h^{t,t_0}(z)))Y(t, z)$$

is constant and equal to 0. We compute

$$\begin{aligned} \partial_t Z(t, z) &= \Big(-\partial_t \Pi(t, \Phi_h^{t,t_0}(z)) - Jdh(\Phi_h^{t,t_0}(z))\Pi(t, \Phi_h^{t,t_0}(z)) + K(t, \Phi_h^{t,t_0}(z))\Big)\, Y(t, z) \\ &= -\Pi(t, \Phi_h^{t,t_0}(z)) \Big(\partial_t \Pi(t, \Phi_h^{t,t_0}(z)) + \mathcal{X}(\Phi_h^{t,t_0}(z))\Pi(t, \Phi_h^{t,t_0}(z))\Big)\, Z(t, z), \end{aligned}$$

where we have used that all derivatives of the projector are off-diagonal. In particular, $\partial_t Z(t, z)$ is an element of the range of $\Pi(t, \Phi_h^{t,t_0}(z))$ and thus orthogonal to $Z(t, z)$. Hence, its norm is constant, $Z(t, z) = 0$ and $Y(t, z) \in \operatorname{Ran} \Pi(t, \Phi^{t,t_0}(z))$.

Besides, we have for any $z \in \mathbb{R}^{2d}$

$$\partial_t Y(t, z) \cdot Y(t, z) = \Omega(t, \Phi_h^{t,t_0}(z))Y(t, z) \cdot Y(t, z) + K(t, \Phi_h^{t,t_0}(z))Y(t, z) \cdot Y(t, z) = 0,$$

because

$$\Omega(t, z)^* = -\Omega(t, z) \text{ and } K(t, z) = (\mathbb{I} - \Pi(t, z))K(t, z).$$

Therefore, $|Y(t, z)| = 1$. □

Appendix D. The phasis $\Lambda(\sigma)$ and the function $\zeta(\sigma)$

Lemma D.1. *Let* Λ *be defined in* (48) *and* ζ *in* (47)*. We have*

$$\zeta(0) = (q(0), p(0)) = z^\flat, \ \ \dot\zeta(0) = (\dot q(0), \dot p(0)) = J\partial_z(h_1 - h_2)(t^\flat, z^\flat) \tag{59}$$

$$\Lambda(0) = \dot\Lambda(0) = 0, \tag{60}$$

$$\ddot\Lambda(0) = \partial_t(h_2 - h_1) - \partial_q h_2 \cdot \partial_p(h_2 - h_1) + \partial_p h_1 \cdot \partial_q(h_2 - h_1) \tag{61}$$

In particular, setting $\mu^\flat = \frac{1}{2}(\ddot\Lambda(0) - \dot p(0) \cdot \dot q(0))$ as in (50), we have

$$\begin{aligned}
\mu^\flat &= \frac{1}{2}(\ddot\Lambda(0) - \dot p(0) \cdot \dot q(0)) \\
&= \frac{1}{2}\left(\partial_t(h_2 - h_1) - \partial_q h_2 \cdot \partial_p(h_2 - h_1) + \partial_p h_1 \cdot \partial_q(h_2 - h_1) + \partial_p(h_2 - h_1) \cdot \partial_q(h_2 - h_1)\right) \\
&= \frac{1}{2}\left(\partial_t(h_2 - h_1) - \partial_q h_1 \cdot \partial_p(h_2 - h_1) + \partial_p h_1 \cdot \partial_q(h_2 - h_1)\right) \\
&= \frac{1}{2}\left(\partial_t(h_2 - h_1) + \left\{\frac{h_1 + h_2}{2}, h_2 - h_1\right\}\right)
\end{aligned}$$

which yields (28).

Proof. We begin with the function ζ and we compute the Taylor expansion at the order 2 for $(q(\sigma), p(\sigma)) = \zeta(\sigma) - z^\flat$ at $\sigma = 0$. Let be $h = h_1, h_2$. We have :

$$\begin{aligned}
\Phi_h^{t,t_0}(z) &= z + (t - t_0)J\partial_z h(t_0, z) + \frac{(t - t_0)^2}{2}\left(J\partial^2_{t,z} h(t_0, z) + J\partial^2_{z,z} h(t_0, z) J\partial_z h(t_0, z)\right) \\
&\quad + O(|t - t_0|^3).
\end{aligned} \tag{62}$$

Applying this formula, we obtain (omitting the argument $(t^\flat, z^\flat)$ in the functions h_1, h_2 and their derivatives)

$$\begin{aligned}
\Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat) &= z^\flat + \sigma J\partial_z h_1 + \frac{\sigma^2}{2}\left(J\partial^2_{t,z} h_1 + J\partial^2_{z,z} h_1 J\partial_z h_1\right) + O(|\sigma|^3), \\
\zeta(t) &= \Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat) - \sigma J\partial_z h_2(t^\flat + \sigma, \Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat)) \\
&\quad + \frac{\sigma^2}{2}\left(J\partial^2_{t,z} h_2 + J\partial^2_{z,z} h_2 J\partial_z h_2\right) + O(|\sigma|^3).
\end{aligned}$$

We deduce

$$\begin{aligned}
\zeta(t) &= z^\flat + \sigma J\partial_z(h_1 - h_2) + O(|\sigma|^3) \\
&\quad + \frac{\sigma^2}{2}\left(J\partial^2_{t,z}(h_1 - h_2) + J\partial^2_{z,z}(h_1 - h_2) J\partial_z h_1 + J\partial^2_{z,z} h_2 J\partial_z(h_2 - h_1)\right),
\end{aligned}$$

and, for further use, the relation

$$-p^\flat \dot q(0) = - p^\flat \cdot \partial_q (h_1 - h_2), \tag{63}$$

$$-p^\flat \cdot \ddot q(0) = - p^\flat \cdot (\partial^2_{t,p}(h_1-h_2) + \partial^2_{z,p}(h_1-h_2)J\partial_z h_1 + \partial^2_{z,p} h_2 J \partial_z (h_2 - h_1)) \tag{64}$$

We continue with the function Λ (defined in (48)) and we use Taylor expansion of the actions for general Hamiltonian h. In view of (11) and (62), we have (omitting the argument (t_0, z_0) in the terms of the form $\partial^\alpha h(t_0,z_0)$)

$$\begin{aligned} S(t,t_0,z_0) &= \int_{t_0}^t (p_0 - (s-t_0)\partial_q h)\cdot(\partial_p h + (s-t_0)(\partial^2_{t,p} h + \partial^2_{z,p} h J \partial_z h))ds \\ &\quad - \int_{t_0}^t (h + (s-t_0)\partial_t h) ds + O((t-t_0)^3) \\ &= (p_0 \cdot \partial_p h - h)(t-t_0) - \frac{(t-t_0)^2}{2}(\partial_t h + \partial_q h \cdot \partial_p h - p_0 \cdot (\partial^2_{t,p} h + \partial^2_{z,p} h J \partial_z h)) \\ &\quad + O((t-t_0)^3). \end{aligned}$$

We first apply the formula with $h = h_1$, $t = t^\flat + \sigma$, $t = t^\flat$ and $z = z^\flat$, which gives (when the arguments of the functions are omitted, they are fixed to $(t^\flat, z^\flat)$)

$$\begin{aligned} S_1(t^\flat + \sigma, t^\flat, z^\flat) = &\,\sigma(p\cdot \partial_p h_1 - h_1) \\ &- \frac{\sigma^2}{2}(\partial_t h_1 + \partial_q h_1 \cdot \partial_p h_1 - p\cdot(\partial^2_{t,p} h_1 + \partial^2_{z,p} h_1 J \partial_z h_1)) + O(\sigma^3). \end{aligned}$$

We now use the same formula with $h = h_2$, $t = t^\flat$, $t_0 = t^\flat + \sigma$, $z_0 = \Phi_1^{t^\flat+\sigma, t^\flat}(z^\flat)$. We obtain

$$\begin{aligned} &S_2(t^\flat, t^\flat+\sigma, \Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat)) = \\ &\qquad -\sigma(p_1(t^\flat+\sigma, t^\flat, z^\flat)\cdot \partial_p h_2(t^\flat+\sigma, \Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat)) - h_2(t^\flat + \sigma, \Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat))) \\ &\qquad - \frac{\sigma^2}{2}(\partial_t h_2 + \partial_q h_2 \cdot \partial_p h_2 - p\cdot(\partial^2_{t,p} h_2 + \partial^2_{z,p} h_2 J \partial_z h_2)) + O(\sigma^3) \end{aligned}$$

Note that the treatment of the term of order σ has to be performed carefully in the case of $S_2(t^\flat, t^\flat+\sigma, \Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat))$. We obtain

$$\begin{aligned} S_2(t^\flat, t^\flat+\sigma, \Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat)) &= -\sigma(p\cdot\partial_p h_2 - h_2) \\ &\quad - \sigma^2(-\partial_t h_2 - \partial_q h_2 \cdot \partial_p h_1 + p\cdot(\partial^2_{t,p} h_2 + \partial^2_{z,p} h_2 J \partial_z h_2)) \\ &\quad - \frac{\sigma^2}{2}(\partial_t h_2 + \partial_q h_2 \cdot \partial_p h_2 - p \cdot (\partial^2_{t,p} h_2 + \partial^2_{z,p} h_2 J \partial_z h_1)) + O(\sigma^3) \\ &= (p\cdot \partial_p h_2 - h_2)\sigma \\ &\quad + \frac{\sigma^2}{2}(\partial_t h_2 + \partial_q h_2 \cdot \partial_p(2h_1 - h_2) - p\cdot(\partial^2_{t,p} h_2 + \partial^2_{z,p} h_2 J \partial_z (2h_2 - h_1) \\ &\quad + O(\sigma^3) \end{aligned}$$

As a consequence,

$$S_1(t^\flat+\sigma,t^\flat,z^\flat)+S_2(t^\flat,t^\flat+\sigma,\Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat)) = \sigma\, p\cdot\partial_p(h_1-h_2)+\frac{\sigma^2}{2}(\partial_t(h_2-h_1)$$
$$-\partial_q h_2\cdot\partial_p(h_2-h_1)+\partial_p h_1\cdot\partial_q(h_2-h_1)$$
$$+p\cdot(\partial^2_{t,p}(h_1-h_2)+\partial^2_{z,p}(h_1-h_2)J\partial_z h_1+\partial^2_{z,p}h_2 J\partial_z(h_1-h_2)))+O(\sigma^3).$$

Combining with (64), we obtain

$$\Lambda(\sigma)=\frac{\sigma^2}{2}(\partial_t(h_2-h_1)-\partial_q h_2\cdot\partial_p(h_2-h_1)+\partial_p h_1\cdot\partial_q(h_2-h_1))+O(\sigma^3),$$

whence (61).

□

Appendix E. The operators $\mathcal{T}_{\mu,\alpha,\beta}$

We study here the operators $\mathcal{T}_{\mu,\alpha,\beta}$ that are defined in (24) for $(\mu,\alpha,\beta)\in\mathbb{R}^{2d+1}$. An explicit computation gives the following useful connection with the Fourier transform

$$\mathcal{F}\mathcal{T}_{\mu,\alpha,\beta}=\mathcal{T}_{\mu+\alpha\cdot\beta,\beta,-\alpha}\mathcal{F}. \tag{65}$$

The next proposition sums up the main information that we will use about these operators.

Proposition E.1. *Let* $(\mu,\alpha,\beta)\in\mathbb{R}^{2d+1}$.

1. *The operator* $\mathcal{T}_{\mu,\alpha,\beta}$ *maps* $\mathcal{S}(\mathbb{R}^d)$ *into itself if and only if* $\mu\neq 0$.
2. *Moreover, if* $\mu\neq 0$, $\mathcal{T}_{\mu,\alpha,\beta}$ *is a metaplectic transformation in the Hilbert space* $L^2(\mathbb{R}^d)$ *multiplied by a complex number:*

$$\mathcal{T}_{\mu,\alpha,\beta}=\sqrt{\frac{2\pi}{i\mu}}\,\mathrm{e}^{\frac{i}{4\mu}(\beta\cdot y-\alpha\cdot D_y)^2}. \tag{66}$$

3. *If* $\mu\neq 0$, $\Gamma\in\mathfrak{S}^+(d)$ *and* $A\in\mathcal{C}^\infty(\mathbb{R}^{2d})$ *is a polynomial function then there exists* $\Gamma_{\mu,\alpha,\beta,\Gamma}\in\mathfrak{S}^+(d)$ *such that*

$$\mathcal{T}_{\mu,\alpha,\beta}(\mathrm{op}_1^w(A)g^\Gamma)=\sqrt{\frac{2\pi}{i\mu}}\mathrm{op}_1^w(A\circ\Phi_{\alpha,\beta}(-(4\mu)^{-1})g^{\Gamma_{\mu,\alpha,\beta,\Gamma}}$$

with

$$\Gamma_{\mu,\alpha,\beta,\Gamma}=\Gamma-\frac{(\beta-\Gamma\alpha)\otimes(\beta-\Gamma\alpha)}{2\mu-\alpha\cdot\beta+\alpha\cdot\Gamma\alpha}. \tag{67}$$

and $\Phi_{\alpha,\beta}$ *satisfying* (31).

Remark E.2. The matrix $\Gamma_{\mu,\alpha,\beta,\Gamma}$ is in $\mathfrak{S}^+(d)$ since $g^{\Gamma_{\mu,\alpha,\beta,\Gamma}}$ is proved to be Schwartz class. It is also important to notice that $2\mu-\alpha\cdot\beta+\alpha\cdot\Gamma\alpha$ is non zero because its imaginary part is non zero.

Proof. Point (1) is linked with Point (2) and comes from the formula (25) and(24). Indeed, when $\mu \neq 0$, equation (66) is an application of relation (24) and of functional calculus on the self-adjoint operator $(\beta \cdot y - \alpha \cdot D_y)^2$ and the Fourier-transform formula of complex Gaussian functions:

$$\int_{-\infty}^{+\infty} \mathrm{e}^{is^2\mu}\mathrm{e}^{is\tau}ds = \sqrt{\frac{2\pi}{i\mu}}\mathrm{e}^{\frac{\tau^2}{4i\mu}}, \text{ with } \arg(i\mu) \in]-\pi,\pi[. \tag{68}$$

It remains to analyze the case where $\mu = 0$. The computations are different whether $\alpha \cdot \beta = 0$ or not. We assume $\alpha \neq 0$ and we set

$$\hat{\alpha} = \frac{\alpha}{|\alpha|}, \;\; y = (y \cdot \hat{\alpha})\hat{\alpha} + y_\perp.$$

Similar formulas can be obtained when $\beta \neq 0$ using (65). Let us first assume $\alpha \cdot \beta = 0$.

$$\begin{aligned}
\mathcal{T}_{0,\alpha,\beta} &= \int \mathrm{e}^{is\beta\cdot y_\perp}\varphi(y\cdot\hat{\alpha}\hat{\alpha} - s\alpha + y_\perp)ds \\
&= |\alpha|^{-1}\int \mathrm{e}^{i|\alpha|^{-1}(y\cdot\hat{\alpha}-\sigma)(\beta\cdot y_\perp)}\varphi(\sigma\hat{\alpha}+y_\perp)d\sigma \\
&= |\alpha|^{-1}\mathrm{e}^{i|\alpha|^{-1}(y\cdot\hat{\alpha})(\beta\cdot y_\perp)}\mathcal{F}_\alpha\varphi\left(\frac{\beta\cdot y_\perp}{|\alpha|}, y_\perp\right)
\end{aligned}$$

where $\varphi \in \mathcal{S}(\mathbb{R}^d)$, $y_\perp = y - \hat{\alpha}\cdot y\hat{\alpha}$ and $\mathcal{F}_\alpha$ is the partial Fourier transform in the direction α. In the case where $\alpha \cdot \beta \neq 0$, we write

$$\begin{aligned}
\mathcal{T}_{0,\alpha,\beta} &= (2\pi)^{-1}\int_{\mathbb{R}^2} \mathrm{e}^{-is^2\frac{\alpha\cdot\beta}{2}+is\beta\cdot y+i\eta(y\cdot\alpha-s)}\mathcal{F}_\alpha\varphi(\eta,y_\perp)d\eta ds \\
&= \sqrt{\frac{i}{\pi\beta\cdot\alpha}}\int \mathrm{e}^{i\frac{(\beta\cdot y-\eta)^2}{2\alpha\cdot\beta}+i\eta y\cdot\alpha}\mathcal{F}_\alpha\varphi(\eta,y_\perp)d\eta \\
&= \sqrt{\frac{i}{\pi\beta\cdot\alpha}}\mathrm{e}^{i\frac{(\beta\cdot y)^2}{2\beta\cdot\alpha}}\int \mathrm{e}^{-i\eta\frac{\beta_\perp\cdot y_\perp}{\beta\cdot\alpha}}e^{i\frac{\eta^2}{2\beta\cdot\alpha}}\mathcal{F}_\alpha\varphi(\eta,y_\perp)d\eta \\
&= \sqrt{\frac{i}{\pi\beta\cdot\alpha}}\mathrm{e}^{i\frac{(\beta\cdot y)^2}{2\beta\cdot\alpha}}\int \mathrm{e}^{-i\eta\frac{\beta_\perp\cdot y_\perp}{\beta\cdot\alpha}}\mathcal{F}_\alpha\left(e^{i\frac{(D_y\cdot\hat{\alpha})^2}{2\beta\cdot\alpha}}\varphi\right)(\eta,y_\perp)d\eta \\
&= \sqrt{\frac{4i\pi}{\beta\cdot\alpha}}\mathrm{e}^{i\frac{(\beta\cdot y)^2}{2\beta\cdot\alpha}}e^{i\frac{(D_y\cdot\hat{\alpha})^2}{2\beta\cdot\alpha}}\varphi\left(-\frac{\beta_\perp\cdot y_\perp}{\beta\cdot\alpha}+y_\perp\right)
\end{aligned}$$

This concludes the proof of Points (1) and (2).

Point (3) derives from the formulation of $\mathcal{T}_{\mu,\alpha,\beta}$ as a metaplectic transform. We use general results concerning the action of a metaplectic transformation on Gaussian g^Γ (for details see [5], Chapter 3). With the quadratic Hamiltonian $K(y,\eta) = (\beta\cdot y - \alpha\cdot\eta)^2$, one associates the linear flow $\Phi_{\alpha,\beta}(t) = (\Phi_{ij}(t))_{1\leq i,j\leq 2}$ (in a $d\times d$ block form) given by (31).

Besides, the Egorov theorem and the propagation of gaussian are both exact: we have

$$\mathrm{e}^{-it\hat{K}}(\mathrm{op}_1^w(A)g^\Gamma) = \mathrm{op}_1^w(A\circ\Phi_{\alpha,\beta}(t))\mathrm{e}^{-it\hat{K}}g^\Gamma = (\mathrm{op}_1^w(A\circ\Phi_{\alpha,\beta}(t))g^{\Gamma_t}$$

where the matrix $\Gamma_t \in \mathfrak{S}^+(d)$ is given by

$$\Gamma_t = (\Phi_{21}(t)+\Phi_{22}(t)\Gamma)(\Phi_{11}(t)+\Phi_{12}(t)\Gamma)^{-1},\;\; c_{\Gamma_t} = \det{}^{-1/2}(A(t)+B(t)\Gamma),$$

where We deduce that if $\mu\neq 0$,

$$\mathcal{T}_{\mu,\alpha,\beta}g^\Gamma = \sqrt{\frac{2\pi}{i\mu}}\mathrm{e}^{\frac{i}{4\mu}\hat{K}}g^\Gamma = \sqrt{\frac{2\pi}{i\mu}}g^{\Gamma_{-(4\mu)^{-1}}}.$$

This induces the existence of the matrix $\Gamma_{\mu,\alpha,\beta,\Gamma}\in\mathfrak{S}^+(d)$ of Point (2) of the Proposition. It remains to prove the formula (67). We use that if $\varphi = g_\Gamma$, we have

$$\mathcal{T}_{\mu,\alpha,\beta}g^\Gamma(y) = c_\Gamma\int_{-\infty}^{+\infty}\mathrm{e}^{is^2(\mu-\alpha\cdot\beta/2)}\mathrm{e}^{is\beta\cdot y}\mathrm{e}^{\frac{i}{2}(y-s\alpha)\cdot(\Gamma(y-s\alpha))}ds.$$

Applying again (68) we get,

$$\mathcal{T}_{\mu,\alpha,\beta}g^\Gamma(y) = c_\Gamma\sqrt{\frac{\pi}{2\mu-\alpha\cdot\beta+\alpha\cdot\Gamma\alpha}}\;\mathrm{e}^{\frac{i}{2}\left(y\cdot\Gamma y-\frac{(y\cdot(\beta-\Gamma\alpha))^2}{2\mu-\alpha\cdot\beta+\alpha\cdot\Gamma\alpha}\right)},$$

which gives (67). □

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