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ABSTRACT. We analyze the propagation of wave packets through general Hamiltonian systems presenting codimension one eigenvalue crossings. The class of time-dependent Hamiltonians we consider is of general pseudodifferential form with subquadratic growth. It comprises Schrödinger operators with matrix-valued potential, as they occur in quantum molecular dynamics, but also covers matrix-valued models of solid state physics describing the motion of electrons in a crystal. We calculate precisely the non-adiabatic effects of the crossing in terms of a transition operator, whose action on coherent states can be spelled out explicitly.

1. INTRODUCTION

We consider systems of $N \geq 2$ equations of pseudodifferential form

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

where $(\psi^\varepsilon_0)_{\varepsilon>0}$ is a bounded family in $L^2(\mathbb{R}^d, \mathbb{C}^N)$. The Hamiltonian operator

$$\widehat{H}(t) = H(t, x, -i\varepsilon\nabla_x)$$

is the semi-classical Weyl quantization of a time-dependent Hamiltonian

$$H : \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}^{N \times N}, \quad (t, x, \xi) \mapsto H(t, x, \xi),$$

that is a smooth matrix-valued function and satisfies suitable growth conditions guaranteeing a well-defined and unique solution of the system. We denote with a "$\widehat{\cdot}$" the semi-classical Weyl quantization, the definition of which is recalled in Section 2.1. Phase space variables are denoted by $z = (x, \xi) \in \mathbb{R}^{2d}$. The semi-classical parameter $\varepsilon > 0$ is assumed to be small. The initial data are wave packets associated with one of the eigenspaces of the Hamiltonian matrix. That is,

$$(2) \qquad \psi^\varepsilon_0 = \widehat{\vec{V}_0} \, \mathcal{WP}^\varepsilon_{z_0} \varphi_0,$$

where $\vec{V}_0(z)$ is a normalized eigenvector of the matrix $H(t_0, z)$ such that $\vec{V}_0 : \mathbb{R}^{2d} \to \mathbb{C}^N$ is a smooth vector-valued function, and $\mathcal{WP}^\varepsilon_{z_0} \varphi_0$ denotes the wave packet transform of a Schwartz function $\varphi_0 \in \mathcal{S}(\mathbb{R}^d, \mathbb{C})$ for a phase space point $z_0 = (x_0, \xi_0) \in \mathbb{R}^{2d}$,

$$(3) \qquad \mathcal{WP}^\varepsilon_{z_0} \varphi_0(x) = \varepsilon^{-d/4} \, e^{i\xi_0 \cdot (x-x_0)/\varepsilon} \varphi_0\left(\frac{x-x_0}{\sqrt{\varepsilon}}\right).$$

Our aim is to describe the structure of the system's solutions in the case, when eigenvalues of the Hamiltonian matrix $H(t,z)$ coincide for some point $(t,z) \in \mathbb{R} \times \mathbb{R}^{2d}$, while all eigenvalues and eigenvectors retain their smoothness. The literature refers to them as codimension one crossings. In the presence of eigenvalue crossings the key assumption for space-adiabatic theory (the existence of a positive gap between eigenvalues) is violated, and the knowledge of the dynamics associated with one of the eigenvalues is not enough any more. Moreover, in addition to the necessity to include more than one eigenvalue for an effective dynamical description, also the non-adiabatic transitions between the coupled eigenspaces have to be properly resolved. These questions have already been addressed for special systems corresponding to the following physical settings: In his monograph [15, Chapter 5], G. Hagedorn investigated Schrödinger Hamiltonians with matrix-valued potential,

$$(4) \qquad \widehat{H}_S = -\frac{\varepsilon^2}{2}\Delta_x \, \mathbb{I}_{\mathbb{C}^N} + V(x), \quad V \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C}^{N \times N}).$$

More recently, in [40], A. Watson and M. Weinstein studied models arising in solid state physics in the context of Bloch band decompositions,

$$(5) \qquad \widehat{H}_A = A(-i\varepsilon\nabla_x) + W(x)\mathbb{I}_{\mathbb{C}^2}, \quad A \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C}^{N \times N}), \quad W \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C}).$$

In both settings, the eigenvalues of the matrices $V(x)$, $x \in \mathbb{R}^d$, respectively $A(\xi)$, $\xi \in \mathbb{R}^d$, have a codimension one crossing of their eigenvalues.

We develop here a new analytical method which applies for general matrix-valued Hamiltonians with a codimension one crossings of eigenvalues, which might also have multiplicity larger than one. In particular, we give a general and unified computation of the transfer operator which describes the non-adiabatic interactions due to the crossing. The non-adiabatic transition formulae of Corollary 3.9 are explicit and derived in a self-contained and more accessible way than the previous ones in the literature. Due to their explicit form, they can directly be applied to numerical simulations based on thawed Gaussians that are currently investigated in chemical physics, see for example [38] or the recent review [39].

As another byproduct of our method, we also obtain an effortless generalization of the semi-classical Herman–Kluk approximation to the case of systems with eigenvalue gaps (see Corollary 3.5 below). We expect that a refinement of the present error analysis is possible, such that our codimension one result can be extended to the Herman–Kluk framework as well. This is work in progress, which might also contribute to the algorithmical development of superpositions of surface-hopping approximations using frozen (or thawed) Gaussian wave packets in the spirit of [41], see also [25].

We assume that the matrix $H(t,z)$ has a smooth eigenvalue $h_1(t,z)$, the eigenspace of which admits a smooth eigenprojector $\Pi_1(t,z)$, that is,

$$H(t,z)\Pi_1(t,z) = \Pi_1(t,z)H(t,z) = h_1(t,z)\Pi_1(t,z).$$

We shall consider two situations, depending on whether the eigenvalue $h_1(t,z)$ crosses another smooth eigenvalue $h_2(t,z)$ or not. Because we assume the Hamiltonian matrix $H(t,z)$ to be independent of ε, then, in *the gap situation*, the eigenvalue $h_1(t,z)$ is separated

from $h_2(t,z)$ by a gap larger than some fixed positive real number $\delta_0 > 0$ that is of order one with respect to the semi-classical parameter ε. In the second case, *the smooth crossing* case, both eigenvalues are smooth and have smooth eigenprojectors. Note that it is not the case in general since eigenvalues may develop singularities at the crossing; however, we do not consider that situations here. We shall also assume that $H(t,z)$ has no other eigenvalues since one can reduce to that case as soon as 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 gap situation is well understood and corresponds to adiabatic situations that have been studied by several authors (see in particular the lecture notes [36] of S. Teufel or the memoirs[27] of A. Martinez and V. Sordoni and note that the thesis [2] is devoted to wave packets in the adiabatic situation). For avoided crossings, the coupling of the gap and the semi-classical parameter violates the key requirement for adiabatic decoupling. The resulting non-adiabatic dynamics have been studied for wave packets by G. Hagedorn and A. Joye in [16, 17] and for the Wigner function of general initial data in [10]. Smooth crossings have been less studied so far. Some results on the subject focus on the evolution at leading order in ε of quadratic quantities of the wave function for initial data which are not necessarily wave packets (see [21, 7] and the references therein). The main results devoted to wave packet propagation through smooth eigenvalue crossings are the references [15] and [40] mentioned above. There, for the specific Hamiltonian operators (4) and (5), respectively, the authors gave rather explicit descriptions of the propagated wave packet, exhibiting non-adiabatic transitions that occur at the crossing between the two eigenvalues that are of order $\sqrt{\varepsilon}$. As in these contributions, we assume that the crossing set

$$(6) \qquad \Upsilon = \{(t,z) \in \mathbb{R}^{2d+1},\ h_1(t,z) = h_2(t,z)\}$$

of two smooth eigenvalues $h_1(t,z)$ and $h_2(t,z)$ is a codimension one manifold.

Our main result (Theorem 3.8 below) makes the following assumptions for the initial data ψ_0^ε. Let v_0^ε be a wave packet centered in a phase space point z_0, that is,

$$v_0^\varepsilon = \mathcal{WP}_{z_0}^\varepsilon \varphi_0 \quad \text{for some} \quad \varphi_0 \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}).$$

Let $\vec{V}_0(z)$ be a smooth normalized eigenvector of $H(t_0,z)$, that is, $\vec{V}_0 \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^N)$ is a smooth vector-valued function that satisfies in a neighborhood U of z_0,

$$H(t_0,z)\vec{V}_0(z) = h_1(t_0,z)\vec{V}_0(z) \quad \text{for all} \quad z \in U.$$

Then, we define the initial wave packet according to (2). Let $z_1(t)$ denote the classical trajectory associated with the eigenvalue $h_1(t,z)$ initiated in wave packet's core z_0. Let $t^\flat > t_0$ be the first time, when the trajectory $z_1(t)$ meets the crossing set Υ, and let $z_2(t)$ denote the classical trajectory associated with the second eigenvalue $h_2(t,z)$, that is initiated in the crossing point $z_1(t^\flat)$. That is,

$$\dot{z}_1(t) = J\partial_z h_1(t, z_1(t)), \quad z_1(t_0) = z_0,$$
$$\dot{z}_2(t) = J\partial_z h_2(t, z_2(t)), \quad z_2(t^\flat) = z_1(t^\flat).$$

Then, the solution of system (1) satisfies

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

where the profiles of the wave packets

$$\mathcal{WP}^\varepsilon_{z_1(t)}(\varphi_1^0(t) + \sqrt{\varepsilon}\varphi_1^1(t)) \quad \text{and} \quad \mathcal{WP}^\varepsilon_{z_2(t)}\varphi_2(t)$$

are Schwartz functions $\varphi_1^0(t)$, $\varphi_1^1(t)$, and $\varphi_2(t)$, that solve ε-independent PDEs on $[t_0, t^\flat]$ and $[t^\flat, t_0 + T]$, respectively, that are explicitly given in terms of the classical dynamics associated with the eigenvalues $h_1(t, z)$ and $h_2(t, z)$. The profile associated with the second eigenvalue is generated by the leading order profile of the first eigenvalue via

$$\varphi_2(t^\flat) = \mathcal{T}^\flat \varphi_1^0(t^\flat),$$

where the non-adiabatic transfer operator $\mathcal{T}^\flat$ is a metaplectic transform (which implies that the structure of Gaussian states is preserved, see Corollary 3.9). The two 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, that are obtained by parallel transport.

We point out that, in the uniform gap case, an initial datum that is associated with one eigenvalue issues a solution at time t that is associated with the same eigenvalue up to terms of order ε, which is the standard order of the adiabatic approximation, while for smooth crossings a perturbative term of order $\sqrt{\varepsilon}$ associated with the other eigenvalue has to be taken into account for an order ε approximation.

Before giving a more precise statement of the result, we mention that the propagation of wave packets was also studied for nonlinear systems in [4, 18, 19], including situations with avoided crossings [19]. However, nonlinear systems with codimension one crossings have not yet been analysed. We expect that our result can be extended when imposing appropriate assumptions on the nonlinearity.

2. Preliminary results

In this section, we introduce the relevant function spaces for the unitary propagation and also recall some known results on wave packets for scalar evolution equations.

2.1. **Function spaces and quantization.** Let $a \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ be a smooth scalar-, vector- or matrix-valued function with adequate control on the growth of derivatives. Then, the Weyl operator $\widehat{a} = \mathrm{op}_\varepsilon^w(a)$ is defined by

$$\mathrm{op}_\varepsilon^w(a)f(x) := \widehat{a}f(x) := (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} a\left(\frac{x+y}{2}, \xi\right) \mathrm{e}^{i\xi \cdot (x-y)/\varepsilon} f(y)\, dy\, d\xi$$

for all $f \in \mathcal{S}(\mathbb{R}^d)$. According to [31], the unitary propagator $\mathcal{U}_H^\varepsilon(t, t_0)$ associated with the Hamiltonian operator $\widehat{H}(t)$,

$$i\varepsilon\, \partial_t \mathcal{U}_H^\varepsilon(t, t_0) = \widehat{H}(t)\mathcal{U}_H^\varepsilon(t, t_0), \quad \mathcal{U}_H^\varepsilon(t_0, t_0) = \mathbb{I}_{L^2(\mathbb{R}^d)},$$

is well defined when 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.

$$(7) \qquad \forall \alpha \in \mathbb{N}^{2d}, \ |\alpha| \geq 2, \ \exists C_\alpha > 0, \quad \sup_{(t,z) \in \mathbb{R} \times \mathbb{R}^{2d}} \|\partial_z^\alpha H(t, z)\|_{\mathbb{C}^{N \times N}} \leq C_\alpha.$$

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

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

endowed with the norm

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

We note that also with respect to the $\Sigma_\varepsilon^k(\mathbb{R}^d)$ spaces, the unitary propagator $\mathcal{U}_H^\varepsilon(t, t_0)$ is ε-uniformly-bounded in the sense, that for all $T > 0$ there exists $C > 0$ such that

$$\sup_{t \in [t_0, t_0+T]} \|\mathcal{U}_H^\varepsilon(t, t_0)\|_{\mathcal{L}(\Sigma_\varepsilon^k)} \leq C.$$

Remark 2.1. The analysis below could apply to more general settings as long as the classical quantities are well-defined in finite time with some technical improvements that are not discussed here.

2.2. **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 $\varphi \mapsto \mathcal{WP}_z^\varepsilon \varphi$ is a unitary map in $L^2(\mathbb{R}^d)$ which maps continuously Σ_k^1 into Σ_k^ε with a continuous inverse. Other elementary properties of the wave packet transform are listed in Lemma A.1. We shall use the notation

$$(8) \qquad\qquad J = \begin{pmatrix} 0 & \mathbb{I}_{\mathbb{R}^d} \\ -\mathbb{I}_{\mathbb{R}^d} & 0 \end{pmatrix}.$$

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

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

Let $h : \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R}$, $(t, z) \mapsto h(t, z)$ be a smooth function of subquadratic growth(7).We now review the main tools for the semi-classical propagation of wave-packets. We let $z(t) = (q(t), p(t))$ denote the *classical Hamiltonian trajectory* issued from a phase space point z_0 at time t_0, that is defined by the ordinary differential equation

$$\dot{z}(t) = J \partial_z h(t, z(t)), \quad z(t_0) = z_0.$$

The trajectory $z(t) = z(t, t_0, z_0)$ depends on the initial datum and defines via $\Phi_h^{t,t_0}(z_0) = z(t, t_0, z_0)$ the associated *flow map* of the Hamiltonian function h. We will also use the trajectory's *action integral*

$$(9) \qquad S(t, t_0, z_0) = \int_{t_0}^{t} (p(s) \cdot \dot{q}(s) - h(s, z(s))) \, ds,$$

and the Jacobian matrix of the flow map

$$F(t, t_0, z_0) = \partial_z \Phi_h^{t,t_0}(z_0).$$

Note that $F(t, t_0, z_0)$ is a symplectic $2d \times 2d$ matrix, that satisfies the linearized flow equation

$$(10) \qquad \partial_t F(t, t_0, z_0) = J \mathrm{Hess}_z h(t, z(t)) \, F(t, t_0, z_0), \quad F(t_0, t_0, z_0) = \mathbb{I}_{\mathbb{R}^{2d}}.$$

We denote its blocks by

$$(11) \qquad F(t, t_0, z_0) = \begin{pmatrix} A(t, t_0, z_0) & B(t, t_0, z_0) \\ C(t, t_0, z_0) & D(t, t_0, z_0) \end{pmatrix}.$$

In a last step, we define the corresponding unitary evolution operator, the *metaplectic transformation*, that acts on square integrable functions in $L^2(\mathbb{R}^d)$.

Definition 2.2 (Metaplectic transformation). *Let $h : \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R}$ be a smooth function of subquadratic growth (7). Let $t, t_0 \in \mathbb{R}$ and $z_0 \in \mathbb{R}^{2d}$. Let $F(t, t_0, z_0)$ be the solution of the linearized flow equation (10) associated with the Hamiltonian function $h(t)$. Then, we call the unitary operator*

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

that associates with an initial datum φ_0 the solution at time t of the Cauchy problem

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

the metaplectic transformation *associated with the matrix $F(t, t_0, z_0)$.*

Using these three ε-independent building blocks – the classical trajectories, the action integrals, and the metaplectic transformations associated with the linearized flow map – we can approximate the action of the unitary propagator

$$i \varepsilon \partial_t \mathcal{U}_h^\varepsilon(t, t_0) = \mathrm{op}_\varepsilon^w(h(t)) \mathcal{U}_h^\varepsilon(t, t_0), \quad \mathcal{U}_h^\varepsilon(t_0, t_0) = \mathbb{I}_{L^2(\mathbb{R}^d)}$$

on wave packets as follows.

Proposition 2.3. *[6, §4.3]] Consider a smooth scalar Hamiltonian $h(t)$ of subquadratic growth (7). Let $T > 0$, $k \geq 0$, $z_0 \in \mathbb{R}^{2d}$, and $\varphi_0 \in \mathcal{S}(\mathbb{R}^d)$. Then, there exists a positive constant $C > 0$ such that*

$$\sup_{t \in [t_0, t_0+T]} \left\| \mathcal{U}_h^\varepsilon(t, t_0) \mathcal{WP}_{z_0}^\varepsilon \varphi_0 - e^{\frac{i}{\varepsilon} S(t, t_0, z_0)} \mathcal{WP}_{z(t)}^\varepsilon \varphi^\varepsilon(t) \right\|_{\Sigma_\varepsilon^k} \leq C\varepsilon,$$

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

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

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

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

The constant $C = C(T, k, z_0, \varphi_0) > 0$ is independent of ε but depends on derivative bounds of the flow map $\Phi_h^{t,t_0}(z_0)$ for $t \in [t_0, t_0 + T]$ and the Σ_1^{k+3}-norm of the initial profile φ_0.

Let us discuss the especially interesting case of initial Gaussian states. *Gaussian states* are wave packets with complex-valued Gaussian profiles, whose covariance matrix is taken in the Siegel half-space $\mathfrak{S}^+(d)$ of $d \times d$ complex-valued symmetric matrices with positive imaginary part,

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

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

$$(14) \qquad g^\Gamma(x) := c_\Gamma \, e^{\frac{i}{2}\Gamma x \cdot x}, \quad x \in \mathbb{R}^d,$$

where $c_\Gamma = \pi^{-d/4} \det^{1/4}(\operatorname{Im}\Gamma)$ 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 working environment. By Proposition 2.3, the Gaussian states remain Gaussian under the evolution by $\mathcal{U}_h^\varepsilon(t, t_0)$. Indeed, for $\Gamma_0 \in \mathfrak{S}^+(d)$, we have

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

where the width $\Gamma(t, t_0, z_0) \in \mathfrak{S}^+(d)$ and the corresponding normalization $c_{\Gamma(t, t_0, z_0)}$ are determined by the initial width Γ_0 and the Jacobian $F(t, t_0, z_0)$ according to

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

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

The semiclassical wave packets used by G. Hagedorn in [13, 14] are Gaussian wave packets, which are multiplied with a specifically chosen complex-valued polynomial function, that depends on the Gaussian's width matrix. If $A \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C})$ is an arbitrary polynomial function, then $\operatorname{op}_1^w(A)g^{\Gamma_0}$ is the product of a polynomial times a Gaussian, and we can

again describe the action of the metaplectic transformation explictly. Indeed, by Egorov's theorem (which is exact here),

$$\mathcal{M}[F(t,t_0,z_0)](\mathrm{op}_1^w(A)g^{\Gamma_0}) = \mathrm{op}_1^w(A \circ F(t,t_0,z_0))\mathcal{M}[F(t,t_0,z_0)]g^{\Gamma_0}$$
$$= \mathrm{op}_1^w(A \circ F(t,t_0,z_0))g^{\Gamma(t,t_0,z_0)}.$$

In particular, functions that are polynomials times a Gaussian remain of the same form under the evolution, even the polynomial degree is preserved.

3. Precise statement of the results

We now present our main results, that extend the previous theory of wave packet propagation for scalar evolution equations to systems associated with Hamiltonians that have smooth eigenvalues and eigenprojectors.

3.1. **Vector-valued wave packets and parallel transport.** We consider initial data that are vector-valued wave packets associated with a normalized eigenvector of the Hamiltonian matrix $H(t_0, z)$ as given in (2). The evolution of such a function also requires an appropriate evolution of its vector part, which we refer to as *parallel transport*. The following construction generalizes [4, Proposition 1.9], which was inspired by the work of G. Hagedorn, see [15, Proposition 3.1]. Let us denote the complementary orthogonal projector by $\Pi^\perp(t,z) = \mathbb{I}_{\mathbb{C}^N} - \Pi(t,z)$ and assume that

$$(16) \qquad\qquad H(t,z) = h(t,z)\Pi(t,z) + h^\perp(t,z)\Pi^\perp(t,z)$$

with the second eigenvalue given by $h^\perp(t,z) = \mathrm{tr}(H(t,z)) - h(t,z)$. We introduce the auxiliary matrices

$$(17) \qquad\qquad \Omega(t,z) = -\tfrac{1}{2}\big(h(t,z) - h^\perp(t,z)\big)\Pi(t,z)\{\Pi,\Pi\}(t,z)\Pi(t,z),$$

$$(18) \qquad\qquad K(t,z) = \Pi^\perp(t,z)\left(\partial_t\Pi(t,z) + \{h,\Pi\}(t,z)\right)\Pi(t,z),$$

$$(19) \qquad\qquad \Theta(t,z) = i\Omega(t,z) + i(K - K^*)(t,z),$$

that are smooth and satisfy algebraic properties detailed in Lemma B.1 below. In particular, Ω is skew-symmetric and Θ is self-adjoint, $\Omega = -\Omega^*$ and $\Theta = \Theta^*$. We note, that for the Schrödinger and the Bloch Hamiltonian,

$$H_S(z) = \tfrac{1}{2}|\xi|^2\,\mathbb{I}_{\mathbb{C}^N} + V(x) \quad\text{and}\quad H_A(z) = \begin{pmatrix} 0 & \xi_1 + i\xi_2 \\ \xi_1 - i\xi_2 & 0 \end{pmatrix} + W(x)\mathbb{I}_{\mathbb{C}^2},$$

the skew-symmetric Ω-matrix vanishes, that is, $\Omega_S = 0$ and $\Omega_A = 0$. For Dirac Hamiltonians with electromagnetic potential or Hamiltonians that describe acoustic waves in elastic media, the Ω-matrix need not vanish.

Proposition 3.1. *Let $H(t,z)$ be a smooth Hamiltonian with values in the set of self-adjoint $N \times N$ matrices that is of subquadratic growth (7) and has a smooth spectral decomposition (16). We assume that both eigenvalues are of subquadratic growth as well. We consider*

$\vec{V}_0 \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}, \mathbb{C}^N)$ and $z_0 \in \mathbb{R}^{2d}$ such that there exits a neighborhood U of z_0 such that for all $z \in U$

$$\vec{V}_0(z) = \Pi(t_0, z)\vec{V}_0(z) \quad \text{and} \quad \|\vec{V}_0(z)\|_{\mathbb{C}^N} = 1.$$

Then, there exists a smooth normalized vector-valued function $\vec{V}(t, t_0)$ satisfying

$$\vec{V}(t, t_0, z) = \Pi(t, z)\vec{V}(t, t_0, z) \quad \text{for all} \quad z \in \Phi_h^{t,t_0}(U),$$

such that for all $t \in \mathbb{R}$ and $z \in \Phi_h^{t,t_0}(U)$,

(20) $\qquad \partial_t \vec{V}(t, t_0, z) + \{h, \vec{V}\}(t, t_0, z) = -i\Theta(t, z)\vec{V}(t, t_0, z), \quad \vec{V}(t_0, t_0, z) = \vec{V}_0(z).$

Proposition 3.1 is proved in Appendix C. Note that it does not require any gap condition for the eigenvalues. We will use it in the crossing situation, with smooth eigenvalues and eigenprojectors.

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

(21) $\qquad\qquad\qquad \text{dist}\,(h(t, z), \sigma(H(t, z)) \setminus \{h(t, z)\}) > \delta.$

Note that, this gap assumption implies the existence of a Cauchy 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 eigenprojector as $\Pi(t, z) = -\frac{1}{2\pi i} \oint_{\mathcal{C}} (H(t, z) - \zeta)^{-1} d\zeta$, which implies that the projector $\Pi(t, z)$ inherits the smoothness properties of the Hamiltonian $H(t, z)$ in the presence of an eigenvalue gap. However, if the symbol Π is of course of matrix norm 1, its derivatives may grow as $|z|$ goes to infinity and we shall make assumption below (see (24)) in order to guarantee that this growth is at most polynomial. Since the pioneering work of T. Kato [K1], numerous studies have been devoted to this *adiabatic situation* (see for example [28, 29, 36, 27] and references therein). One can derive from these results the following statement of adiabatic decoupling.

Theorem 3.2. *[36, 27, 4]] Let $H(t, z)$ be a smooth Hamiltonian with values in the set of self-adjoint $N \times N$ matrices and $h(t, z)$ a smooth eigenvalue of $H(t, z)$. Assume that both $H(t, z)$ and $h(t, z)$ are of subquadratic growth (7) and that there exists an eigenvalue gap as in Assumption (21). Consider initial data $(\psi_0^\varepsilon)_{\varepsilon > 0}$ that are wave packets as in (2). 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*

$$\sup_{t \in [t_0, t_0 + T]} \left\| \widehat{\Pi^\perp(t)}\psi^\varepsilon(t) \right\|_{L^2(\mathbb{R}^d)} + \left\| \psi^\varepsilon(t) - \widehat{\vec{V}(t)}v^\varepsilon(t) \right\|_{L^2(\mathbb{R}^d)} \leq C\varepsilon$$

where $v^\varepsilon(t) = \mathcal{U}_h^\varepsilon(t, t_0)v_0^\varepsilon$ and $\vec{V}(t)$ is determined by Proposition 3.1. Besides, if there exists $k \in \mathbb{N}$ such that $(\psi_0^\varepsilon)_{\varepsilon > 0}$ is a bounded family in the space Σ_ε^k, then the convergence above holds in Σ_ε^k.

Theorem 3.2 is obtained as an intermediate result in the proof of Proposition 4.1, see Section 4 below. There, we perform a refined analysis of the adiabatic approximation that explicitly accounts for the size of the eigenvalue gap. We note that the estimate of Theorem 3.2 is unchanged, when allowing for perturbations of the initial data that are of order ε in $L^2(\mathbb{R}^d)$ or Σ_ε^k, respectively. We also note, that in general the operator $\widehat{\Pi}(t)$ is *not* a projector, but coincides at order ε with the superadiabatic operators constructed in [27, 36], which are projectors (see also Appendix B).

Remark 3.3. The result of Theorem 3.2 can be generalized by means of superadiabatic projectors, showing that $\psi^\varepsilon(t)$ can be approximated at any order by an asymptotic sum of wave packets. The precise time evolution of coherent states was studied in the adiabatic setting in [2, 27, 33]. These results are obtained via an asymptotic quantum diagonalization, in the spirit of the construction of the superadiabatic projectors of [27, 36].

Theorem 3.2 allows a semi-classical description of the dynamics of an initial wave packet, that is associated with a gapped eigenvalue. The building blocks are the scalar classical quantities introduced in section 2.2 and the parallel transport of eigenvectors given in Proposition 3.1. This is stated in the next Corollary; our aim is to derive a similar description for systems presenting a codimension one crossing.

Corollary 3.4 (Adiabatic wave packet)**.** *In the situation of Theorem 3.2, for any $T > 0$, $k \in \mathbb{N}$, $z_0 \in \mathbb{R}^{2d}$, and $\varphi_0 \in \mathcal{S}(\mathbb{R}^d, \mathbb{C})$, there exists a constant $C > 0$ such*

$$\sup_{t \in [t_0, t_0+T]} \left\| \mathcal{U}_H^\varepsilon(t, t_0) \widehat{\vec{V}_0} \, \mathcal{WP}_{z_0}^\varepsilon \varphi_0 - \mathrm{e}^{iS(t, t_0, z_0)/\varepsilon} \, \widehat{\vec{V}(t, t_0)} \, \mathcal{WP}_{\Phi_h^{t,t_0}(z_0)}^\varepsilon \varphi^\varepsilon(t) \right\|_{\Sigma_\varepsilon^k} \leq C\varepsilon,$$

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

We close this section devoted to gapped systems by formulating another semi-classical consequence of adiabatic theory using the *Herman–Kluk propagator*. This approximate propagator has first been proposed by M. Herman and E. Kluk in [20] for scalar Schrödinger equations and later used as a numerical method for quantum dynamics in the semi-classical regime, see for example [42] or more recently [24, 11] with references therein. The rigorous mathematical analysis of the Herman–Kluk propagator is due to [32, 35]. The starting point of this approximation is the wave packet inversion formula

$$\psi(x) = (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi \rangle g_z^\varepsilon(x) dz$$

that allows to write any square integrable function $\psi \in L^2(\mathbb{R}^d)$ as a continuous superposition of Gaussian wave packets of unit width,

$$g_z^\varepsilon(x) \;=\; \mathcal{WP}_z^\varepsilon(g^{i\mathbb{I}})(x) \;=\; (\pi\varepsilon)^{-d/4} \mathrm{e}^{-|x-q|^2/(2\varepsilon) + ip\cdot(x-q)/\varepsilon}.$$

The semi-classical description of unitary quantum dynamics within the framework of Gaussians of fixed unit width becomes possible due to a reweighting factor, the so-called

Herman–Kluk prefactor,

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

which is solely determined by the blocks of the Jacobian matrix of the classical flow map. The resulting propagator

$$\psi \mapsto \mathcal{I}_h^\varepsilon(t, t_0)\psi = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi \rangle a_h(t, t_0, z) \mathrm{e}^{iS(t, t_0, z)/\varepsilon} g^\varepsilon_{\Phi_h^{t, t_0}(z)} dz$$

provides an order ε approximation to the scalar unitary propagator $\mathcal{U}_h^\varepsilon(t, t_0)$ in operator norm. Combining [35, Proposition 2 and Theorem 2] or [32, Theorem 1.2] with our previous results we obtain a Herman–Kluk approximation for gapped systems.

Corollary 3.5 (Adiabatic Herman–Kluk approximation). *In the situation of Theorem 3.2, for all $T > 0$ there exists a constant $C = C(T) > 0$ such that*

$$\sup_{t \in [t_0, t_0 + T]} \|\mathcal{U}_H^\varepsilon(t, t_0)\psi_0^\varepsilon - \mathcal{I}_H^\varepsilon(t, t_0)\psi_0^\varepsilon\|_{L^2(\mathbb{R}^d)} \le C\varepsilon,$$

where the vector-valued Herman–Kluk propagator is defined by

$$\mathcal{I}_H^\varepsilon(t, t_0)\psi_0^\varepsilon = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, v_0^\varepsilon \rangle \vec{A}(t, t_0, z) \mathrm{e}^{iS(t, t_0, z)/\varepsilon} g^\varepsilon_{\Phi_h^{t, t_0}(z)} dz.$$

The prefactor $\vec{A}(t, t_0, z)$ is given by $\vec{A}(t, t_0, z) = \vec{V}(t, t_0, z) a_h(t, t_0, z)$, where $a_h(t, t_0, z)$ is the Herman–Kluk prefactor associated with the eigenvalue $h(t)$.

Theorem 3.2 formulates adiabatic decoupling for a single eigenvalue that is uniformly separated from the remainder of the spectrum. As it is well-known, adiabatic theory also extends to the situation where a subset of eigenvalues is isolated from the remainder of the spectrum. For this reason, in the next section, we reduce our analysis to the case of matrices with two eigenvalues that coincide on a hypersurface Υ of codimension one and differ away from it. We explicitly describe the dynamics of wave packets through this type of crossings, which is our main result.

3.2. **Main result: propagation of wave packets through codimension one crossings.** We write the Hamiltonian matrix $H(t, z)$ as

$$(22) \qquad H(t, z) = v(t, z)\mathbb{I}_{\mathbb{R}^N} + H_0(t, z), \quad v(t, z) = \frac{1}{N}\mathrm{tr}H(t, z),$$

where $v(t, z)$ is a real number and $H_0(t, z)$ a trace-free self-adjoint $N \times N$ matrix. We assume that $H(t, z)$ has two smooth eigenvalues that cross on a hypersurface Υ. Such a situation is called a *codimension one crossing* (see Hagedorn's classification [15] for example). Let us formulate our assumptions on the crossing set more precisely.

Assumption 3.6 (Codimension one crossing). *Let $H : \mathbb{R}^{2d+1} \to \mathbb{C}^{N \times N}$ be a smooth function with values in the set of self-adjoint $N \times N$ matrices that is of subquadratic growth (7). We assume:*

a) *The matrix $H(t, z)$ has two smooth eigenvalues $h_1(t, z)$ and $h_2(t, z)$ that are of subquadratic growth (7).*

b) *These eigenvalues cross on a hypersurface Υ of $\mathbb{R}^{2d+1}$ and differ outside of Υ. In particular, for any $(t^\flat, z^\flat) \in \Upsilon$ there exists a neighbourhood Ω of $(t^\flat, z^\flat)$ and a smooth scalar function $(t, z) \mapsto f(t, z)$ defined on Ω such that $f(t, z) = 0$ is a local equation of Υ with $d_{t,z} f \neq 0$ on Ω.*

c) *The scalar function $(t, z) \mapsto v(t, z)$ defined by the decomposition (22) satisfies*

$$(23) \qquad\qquad \partial_t f + \{v, f\} \neq 0 \ \text{on} \ \Omega.$$

d) *The crossing is non-degenerate in the sense, that the matrix $H_0(t, z)$ defined by the decomposition (22) satisfies*

$$H_0(t, z) = f(t, z) \tilde{H}_0(t, z) \ \text{on} \ \Omega$$

for some smooth matrix-valued map $(t, z) \mapsto \tilde{H}_0(t, z)$ with $\tilde{H}_0(t, z)$ invertible on Ω. The spectrum of the matrix $\tilde{H}_0(t, z)$ consists of two distinct eigenvalues of constant multiplicity which do not cross on Ω.

e) *The eigenvalues satisfy a polynomial gap condition at infinity, in the sense that there exist constants $c_0, n_0, r_0 > 0$ such that*

$$(24) \qquad\qquad |h_1(t, z) - h_2(t, z)| \geq c_0 \langle z \rangle^{-n_0} \ \text{for all} \ (t, z) \ \text{with} \ |z| \geq r_0,$$

where we denote $\langle z \rangle = (1 + |z|^2)^{1/2}$.

In the above setting, the trace-free smooth matrix $\tilde{H}_0(t, z)$ has non-crossing and thus smooth eigenvalues. The eigenprojectors of $\tilde{H}_0(t, z)$ are smooth and are also those of $H(t, z)$. Note that one can then modify the function f in Ω so that the functions

$$(25) \qquad\qquad h_j(t, z) = v(t, z) - (-1)^j f(t, z), \quad j \in \{1, 2\},$$

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 3.7. Take $N = 2$, $v, f \in \mathcal{C}^\infty(\mathbb{R}^{2d+1}, \mathbb{R})$ and $u \in \mathcal{C}^\infty(\mathbb{R}^{2d+1}, \mathbb{R}^3)$ with $|u(t, z)| = 1$ for all (t, z). Consider the Hamiltonian

$$H(t, z) = v(t, z) \mathrm{Id} + f(t, z) \begin{pmatrix} u_1(t, z) & u_2(t, z) + i u_3(t, z) \\ u_2(t, z) - i u_3(t, z) & -u_1(t, z) \end{pmatrix}.$$

The smooth eigenvalues of H, $h_1 = v + f$ and $h_2 = v - f$, cross on the set $\Upsilon = \{f = 0\}$, and H satisfies Assumption 3.6 as soon as the conditions (23) and (24) hold.

Note that the condition (23) implies the transversality of the classical trajectories to the crossing set Υ. The gap condition at infinity (24) ensures, that the derivatives of the eigenprojectors $\Pi_j(t)$, $j = 1, 2$, grow at most polynomially, in the sense that for all $\beta \in \mathbb{N}_0^{2d}$ there exists a constant $C_\beta > 0$ such that

$$(26) \qquad\qquad \|\partial_z^\beta \Pi_j(t, z)\| \leq C_\beta \langle z \rangle^{|\beta|(1+n_0)} \ \text{for all} \ (t, z) \ \text{with} \ |z| \geq r_0,$$

see [4, Lemma B.2] for a proof of this estimate.

We associate with each eigenvalue h_j the classical quantities introduced in section 2.2, that we index by j: Φ_j^{t,t_0}, $S_j(t,t_0)$, $F_j(t,t_0)$, etc. We consider initial data at time $t = t_0$ as in (2), where the coherent state is associated with the first eigenvalue h_1 and centered in a phase space point z_0 such that $(t_0, z_0) \notin \Upsilon$, while $z \mapsto \vec{V}_0(z)$ is a smooth map with $\|\vec{V}_0(z)\| = 1$ for all z. We assume that the Hamiltonian trajectory $z_1(t, t_0, z_0) = \Phi_1^{t,t_0}(z_0)$ reaches Υ at time $t = t^\flat$ and point $z = z^\flat$ where (23) holds. Therefore, $f(t, z) = 0$ is a local equation of Υ in a neighborhood Ω of $(t^\flat, z^\flat)$, and the assumption 3.6 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. The same holds for trajectories $\Phi_1^{t,t_0}(z)$ starting from z close enough to z_0.

We associate with $\vec{V}_0(z)$ the time-dependent eigenvector $(\vec{V}_1(t, z))_{t \geq t_0}$ constructed as in Proposition 3.1 for the eigenvalue $h_1(t, z)$ with initial data $\vec{V}_0(z)$ at time t_0. We also consider the time-dependent eigenvector $(\vec{V}_2(t, z))_{t \geq t^\flat}$ constructed for $t \geq t^\flat$ as in Proposition 3.1 for the eigenvalue $h_2(t, z)$ and with initial data at time $t^\flat$ satisfying

$$(27) \qquad \vec{V}_2(t^\flat, z) = -\gamma(t^\flat, z)^{-1} \Pi_2 (\partial_t \Pi_2 + \{v, \Pi_2\}) \vec{V}_1(t^\flat, z)$$

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

Note that the vector $\vec{V}_2(t^\flat, z)$ is in the range of $\Pi_2(t^\flat, z)$. We next introduce a family of transformations, which describes the non-adiabatic effects for a wave packet that passes the crossing. For $(\mu, \alpha, \beta) \in \mathbb{R} \times \mathbb{R}^{2d}$ and $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we set

$$(28) \qquad \mathcal{T}_{\mu,\alpha,\beta} \varphi(y) = \left(\int_{-\infty}^{+\infty} e^{i\mu s^2} e^{is(\beta \cdot y - \alpha \cdot D_y)} ds \right) \varphi(y).$$

By the Baker-Campbell-Hausdorff formula, we have

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

and we deduce the equivalent representation

$$(29) \qquad \mathcal{T}_{\mu,\alpha,\beta} \varphi(y) = \int_{-\infty}^{+\infty} e^{i(\mu - \alpha \cdot \beta / 2)s^2} e^{is\beta \cdot y} \varphi(y - s\alpha) ds.$$

We prove in Proposition E.1 below that this operator maps $\mathcal{S}(\mathbb{R}^d)$ into itself if and 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.

Combining the parallel transport for the eigenvector and the metaplectic transformation for the non-adiabatic transitions, we obtain the following result.

Theorem 3.8 (Propagation through a codimension one crossing). *Let Assumption 3.6 on the Hamiltonian matrix $H(t)$ hold, and assume that the initial data $(\psi_0^\varepsilon)_{\varepsilon>0}$ are wave packets as in (2). 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 $C > 0$ such that for all $t \in [t_0, t^\flat) \cup (t^\flat, t_0 + T]$ and for all $\varepsilon \le [t - t^\flat]^{9/2}$,*

$$\left\| \psi^\varepsilon(t) - \widehat{\vec{V}}_1(t) v_1^\varepsilon(t) - \sqrt{\varepsilon} \mathbf{1}_{t>t^\flat} \widehat{\vec{V}}_2(t) v_2^\varepsilon(t) \right\|_{\Sigma_\varepsilon^k} \le C\,\varepsilon^m,$$

with an exponent $m \ge 5/9$. The components of the approximate solution are

$$v_1^\varepsilon(t) = \mathcal{U}_{h_1}^\varepsilon(t, t_0) v_0^\varepsilon \quad and \quad v_2^\varepsilon(t) = \mathcal{U}_{h_2}^\varepsilon(t, t^\flat) v_2^\varepsilon(t^\flat)$$

with

$$v_2^\varepsilon(t^\flat) = \gamma^\flat \mathrm{e}^{iS^\flat/\varepsilon} \mathcal{W} \mathcal{P}_{z^\flat}^\varepsilon \mathcal{T}^\flat \varphi_1(t^\flat), \tag{30}$$

where $\varphi_1(t) = \mathcal{M}[F_{h_1}(t, t_0, z_0)]\varphi_0$ is the leading order profile of the coherent state $v_1^\varepsilon(t)$ given by Proposition 2.3, and

$$\gamma^\flat = \gamma(t^\flat, z^\flat) = \| \left(\{v, \Pi_2\} + \partial_t \Pi_2 \right) \vec{V}_1(t^\flat, z^\flat) \|_{\mathbb{C}^N}. \tag{31}$$

The transition operator

$$\mathcal{T}^\flat = \mathcal{T}_{\mu^\flat, \alpha^\flat, \beta^\flat} \tag{32}$$

is defined by the parameters

$$\mu^\flat = \tfrac{1}{2} \left(\partial_t f + \{v, f\} \right)(t^\flat, z^\flat) \ \ and \ \ (\alpha^\flat, \beta^\flat) = J d_z f(t^\flat, z^\flat). \tag{33}$$

The constant $C = C(T, k, z_0, \varphi_0) > 0$ is ε-independent but depends on the Hamiltonian $H(t, z)$, the final time T, and on the initial wave packet's center z_0 and profile φ_0.

Note that by Assumption 3.6, $\mu^\flat \neq 0$, which guarantees that $\mathcal{T}^\flat \varphi_1(t^\flat)$ is Schwartz class. Besides, if the Hamiltonian is time-independent, then Assumption 3.6 also implies that $(\alpha^\flat, \beta^\flat) \neq (0, 0)$. The coefficient $\gamma^\flat$ quantitatively describes the distortion of the projector Π_1 during its evolution along the flow generated by $h_1(t)$. In particular, we have

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

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

The proof uses two types of arguments, one of the them applying away from the crossing set Υ, and the other one in a boundary layer of Υ. The boundary layer is taken of size $\delta > 0$, and we have to balance the two estimates: an error of order $\varepsilon \delta^{-2}$ which comes from the adiabatic propagation of wave packets outside the boundary layer, and an additional error of order $\delta \varepsilon^{1/3}$ generated by the passage through the boundary. The choice of $\delta = \varepsilon^{2/9}$ optimizes the combined estimate and yields convergence of order ε^m with $m \ge 5/9$. We also want to emphasize that the method of proof we propose here allows to systematically

avoid the impressive computations, which appear in [15] pages 65 to 72, and are also present in [40] via the reference [46] to which the authors refer therein.

The wave packet that makes the transition to the other eigenspace can be described even more explicitly for the special case that the initial wave packet is a Gaussian state. The following corollary is proved in Proposition E.1.

Corollary 3.9 (Transitions for Gaussian wave packets)**.** *We consider the situation of Theorem 3.8 and in particular the transition operator $\mathcal{T}^\flat$ defined by the parameters $\mu^\flat \neq 0$ and $(\alpha^\flat, \beta^\flat) \in \mathbb{R}^{2d}$.*

(1) *If $v_0^\varepsilon = \mathcal{WP}_{z_0}^\varepsilon(g^{\Gamma_0})$ is a Gaussian state with width matrix $\Gamma_0 \in \mathfrak{S}^+(d)$, then*

$$v_2^\varepsilon(t^\flat) = \gamma^\flat \sqrt{\frac{2\pi}{i\mu^\flat}} \, e^{iS^\flat/\varepsilon} \, \mathcal{WP}_{z^\flat}^\varepsilon(g^{\Gamma^\flat})$$

with $\;\Gamma^\flat = \Gamma_1(t^\flat, t_0, z_0) - \dfrac{(\beta^\flat - \Gamma_1(t^\flat, t_0, z_0)\alpha^\flat) \otimes (\beta^\flat - \Gamma_1(t^\flat, t_0, z_0)\alpha^\flat)}{2\mu^\flat - \alpha^\flat \cdot \beta^\flat + \alpha^\flat \cdot \Gamma_1(t^\flat, t_0, z_0)\alpha^\flat}$

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).

(2) *If $A \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ is a polynomial function and $v_0^\varepsilon = \mathcal{WP}_{z_0}^\varepsilon(\mathrm{op}_1^w(A)g^{\Gamma_0})$, then*

$$v_2^\varepsilon(t^\flat) = \gamma^\flat \sqrt{\frac{2\pi}{i\mu^\flat}} \, e^{iS^\flat/\varepsilon} \, \mathcal{WP}_{z^\flat}^\varepsilon\left(\mathrm{op}_1^w(A^\flat)g^{\Gamma^\flat}\right)$$

with $A^\flat = A \circ \Phi_{\alpha^\flat, \beta^\flat}(-(4\mu^\flat)^{-1})$ where $\Phi_{\alpha^\flat, \beta^\flat}(t)$ is the symplectic $2d \times 2d$ matrix given by

(34)
$$\Phi_{\alpha^\flat, \beta^\flat}(t) = \begin{pmatrix} \mathbb{I} - 2t\beta^\flat \otimes \alpha^\flat & 2t\alpha^\flat \otimes \alpha^\flat, \\ -2t\beta^\flat \otimes \beta^\flat & \mathbb{I} + 2t\alpha^\flat \otimes \beta^\flat \end{pmatrix}.$$

As a concluding remark of this section, we want to emphasize that our results indeed generalize those of [15, 40].

(1) In the Schrödinger example (4), denoting by $E_A(x)$ and $E_B(x)$ the two eigenvalues of the potential matrix $V(x)$ as in [15], one has

$$\alpha_S^\flat = 0, \;\; \beta_S^\flat = \nabla(E_A - E_B)(q^\flat), \;\; \mu_S^\flat = p^\flat \cdot \nabla(E_A - E_B)(q^\flat).$$

These coefficients appear in equation (5.3) of [15]. There, the initial states are Gaussian wave packets that are multiplied with a polynomial function. Thus, the second part of Corollary 3.9 reproduces these results.

(2) For the Bloch example (5), we obtain

$$\alpha_A^\flat = \nabla(E_+ - E_-)(p^\flat), \;\; \beta_A^\flat = 0, \;\; \mu_A^\flat = -\frac{1}{2}\nabla W(q^\flat) \cdot \nabla(E_+ - E_-)(p^\flat),$$

where $E_\pm(\xi)$ are the eigenvalues of $A(\xi)$ as in equation (3.41) of [40]. The result of [40, Theorem 3.20 (via Definition 3.18)] is therefore a special case of ours.

We notice, that for these special examples either one of the coefficients $\alpha^\flat$ or $\beta^\flat$ is 0. This need not be the case for more general Hamiltonians that have position and momentum variables mixed in the matrix part of the Hamiltonian. Actually, for Dirac Hamiltonians with electromagnetic potential (V, A), the function $\xi - A(t, x)$ appears in the coefficients of the matrix. Also for the propagation of acoustical waves in elastic media the Hamiltonian is of the form $\rho(x)\mathbb{I}_{\mathbb{C}^N} - \Gamma(x, \xi)$, where $\rho(x) > 0$ is the density and $\Gamma(x, \xi)$ the elastic tensor.

3.3. **Organization of the paper.** The proof of Theorem 3.8 is decomposed into two steps: an analysis outside the crossing region in Section 4 and an analysis in the crossing region in Section 5, that allows to conclude the proof in Section 5.4, together with the one of Corollary 3.9. 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.

4. 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 3.6 and with an initial datum which is a coherent state as in (2). We focus here on regions where the classical trajectories associated with the coherent state do not touch the crossing set Υ but are close enough. We prove the next adiabatic result.

Proposition 4.1. *Let* $k \in \mathbb{N}$, $\delta = \delta(\varepsilon)$ *be such that* $\sqrt{\varepsilon} \ll \delta \leq 1$. *Let* $f(t, z) = 0$ *be an equation of* Υ *in an open set* $\Omega \subset \mathbb{R} \times \mathbb{R}^{2d}$. *Assume that for* $j \in \{1, 2\}$,

$$u_j^\varepsilon = \mathcal{WP}_{\widetilde{z}_j}^\varepsilon(\widetilde{\varphi}_j),$$

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* $t \in [s_1, s_2]$, $z_j(t) := \Phi_j^{t,s_1}(\widetilde{z}_j) \in \Omega$ *with* $|f(z_j(t))| > c\delta$ *and*

$$\left\| \psi^\varepsilon(s_1) - \widehat{\vec{V}_1(s_1)} u_1^\varepsilon - \widehat{\vec{V}_2(s_1)} u_2^\varepsilon \right\|_{\Sigma_\varepsilon^k} \leq C\varepsilon.$$

Then, there exists $C_k > 0$ *such that for all* $j \in \{1, 2\}$,

$$\sup_{t \in [s_1, s_2]} \left\| \widehat{\Pi}_j \psi^\varepsilon(t) - \widehat{\vec{V}_j(t)} \mathcal{U}_{h_j}^\varepsilon(t, s_1) u_j^\varepsilon \right\|_{\Sigma_\varepsilon^k} \leq C_k \, \varepsilon \, \delta^{-2}.$$

The constant C_k *does not depend on* δ *and* ε.

For fixed δ, that is independent of ε, this Proposition implies Theorem 3.8 for $t \in [0, t^\flat[$. We shall choose later $\delta = \varepsilon^{1/3}$ for obtaining a global a priori estimate in Section 4.2 below. Finally with $\delta = \varepsilon^{2/9}$, we will prove Theorem 3.8 in Section 5.4 by using the Proposition 4.1 for propagation times $t \in [t_0, t^\flat - \delta]$ and $t \in [t^\flat + \delta, t^\flat + T]$ with initial data at times $t = t_0$ and $t = t^\flat + \delta$ respectively.

Remark 4.2. Pushing the construction of superadiabatic projectors of Appendix B, we would obtain that $\psi^\varepsilon(t)$ can be approximated by an asymptotic sum of wave packets up to order $\varepsilon^N \delta^{p(N)}$ for some $p(N) \leq N$ to be computed precisely.

4.1. **Proof of the adiabatic decoupling.** We prove here Proposition 4.1.

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 being symmetric, we can choose equivalently one or the other one. Therefore, without loss of generality, we assume $\psi^\varepsilon(s_1) = \widehat{\vec{V_1}(s_1)}u_1^\varepsilon$, and we focus on

$$\psi_{1,\mathrm{app}}^\varepsilon(t) := \widehat{\vec{V_1}(t)}\mathcal{U}_{h_1}^\varepsilon(t,s_1)u_1^\varepsilon$$

Then, using the parallel transport equation (20) associated with the eigenvalue h_1,

$$i\varepsilon\partial_t\psi_{1,\mathrm{app}}^\varepsilon(t) = \widehat{h_1}\psi_{1,\mathrm{app}}^\varepsilon(t) + \left(\left[\widehat{\vec{V_1}(t)},\widehat{h_1}\right] + i\varepsilon\partial_t\widehat{\vec{V_1}(t)}\right)\mathcal{U}_{h_1}^\varepsilon(t,s_1)u_1^\varepsilon$$

$$(35) \qquad = (\widehat{h_1}\mathrm{Id} + \varepsilon\widehat{\Theta}_1)\psi_{1,\mathrm{app}}^\varepsilon(t) + \varepsilon^2\widehat{r(t)}\mathcal{U}_{h_1}^\varepsilon(t,s_1)u_1^\varepsilon,$$

where the remainder $r(t)$ depends on second order derivatives of h_1 and $\vec{V_1}$. Since u_1^ε is a wave packet with a Schwartz function amplitude, we obtain

$$(36) \qquad i\varepsilon\partial_t\psi_{1,\mathrm{app}}^\varepsilon(t) = (\widehat{h_1}\mathrm{Id} + \varepsilon\widehat{\Theta}_1)\psi_{1,\mathrm{app}}^\varepsilon(t) + O(\varepsilon^2)$$

in Σ_ε^k for all $k \in \mathbb{N}$.

We now use the superadiabatic correctors of Π_1 and Π_2 defined in Definition B.3 that we denote by $\mathbb{P}_1$ and $\mathbb{P}_2$, respectively, and the associated correctors Θ_1 and Θ_2 of the Hamiltonian H. Since $\mathbb{P}_1$ and $\mathbb{P}_2$ are singular on Υ, we use cut-off functions that follow the flows arriving at time s_2 in $\Phi_{h_1}^{s_2,s_1}(\tilde{z}_1)$. We introduce two sets of cut-off functions, one for each mode. Let I an interval containing $[s_1,s_2]$ and for $j \in \{1,2\}$ let the cut-off functions $\chi_j^\delta, \tilde{\chi}_j^\delta \in \mathcal{C}(I,\mathcal{C}_0^\infty(\mathbb{R}^{2d}))$ satisfy as in Lemma B.5:

   (1) For any $t \in I$ and any z in the support of $\chi_j^\delta(t)$ and $\tilde{\chi}_j^\delta(t)$ we have $|f(t,z)| > \delta$.

   (2) The functions χ_j^δ and $\tilde{\chi}_j^\delta$ are identically equal to 1 close to a trajectory $\Phi_j^{t,s_1}(\tilde{z}_1)$ for all $t \in I$ and they satisfy

$$\partial_t\chi_j^\delta + \left\{h_j,\chi^\delta\right\} = 0, \quad \partial_t\tilde{\chi}_j^\delta + \left\{h_j,\tilde{\chi}_j^\delta\right\} = 0.$$

   (3) The functions $\tilde{\chi}_j^\delta$ are supported in $\{\chi_j^\delta = 1\}$.

   (4) Finally, we require $\chi_1^\delta(s_2) = \chi_2^\delta(s_2)$ and $\tilde{\chi}_1^\delta(s_2) = \tilde{\chi}_2^\delta(s_2)$.

We set for $t \in [s_1,s_2]$

$$w_1^\varepsilon(t) = \widehat{\tilde{\chi}_1^\delta}(\widehat{\chi_1^\delta\Pi_1^\varepsilon}\psi^\varepsilon(t) - \psi_{1,\mathrm{app}}^\varepsilon(t)), \quad w_2^\varepsilon(t) = \widehat{\tilde{\chi}_2^\delta}\widehat{\chi_2^\delta\Pi_2^\varepsilon}\psi^\varepsilon(t),$$

where $\quad \Pi_j^\varepsilon(t,z) = \Pi_j(t,z) + \varepsilon\mathbb{P}_j(t,z), \quad \forall z \in \mathbb{R}^{2d}\setminus\Upsilon, \quad t \in I, \quad j \in \{1,2\}.$

Then, as a consequence of (36) and of Lemma B.5, we have for $j \in \{1,2\}$ and in Σ_ε^k,

$$i\varepsilon\partial_tw_j^\varepsilon(t) = (\hat{h}_j + \varepsilon\widehat{\Theta}_j)w_j^\varepsilon(t) + O(\varepsilon^2\delta^{-2}).$$

For the initial data at time $t = s_1$, we have in Σ_ε^k,

$$w_1^\varepsilon(s_1) = \widehat{\widetilde{\chi}_1^\delta}\big(\widehat{\chi_1^\delta \Pi_1^\varepsilon} \widehat{V_1} - \widehat{V_1}\big) u_1^\varepsilon = O(\varepsilon \delta^{-1}), \quad w_2^\varepsilon(s_1) = \widehat{\widetilde{\chi}_2^\delta} \, \widehat{\chi_2^\delta \Pi_2^\varepsilon} \, \widehat{V_1} u_1^\varepsilon = O(\varepsilon \delta^{-1}).$$

We deduce that for any $k \in \mathbb{N}$, $j \in \{1, 2\}$ and $t \in [s_1, s_2]$, we have in Σ_ε^k, $w_j^\varepsilon(t) = O(\varepsilon \delta^{-2})$. When $t = s_2$, we have

$$w_1^\varepsilon(s_2) + w_2^\varepsilon(s_2) = \widehat{\widetilde{\chi}_1^\delta} \left(\mathrm{op}_\varepsilon(\chi_1^\delta(\Pi_1^\varepsilon + \Pi_2^\varepsilon)) \psi^\varepsilon(s_2) - \psi_{1,\mathrm{app}}^\varepsilon(s_2) \right)$$

$$= \widehat{\widetilde{\chi}_1^\delta}(\psi^\varepsilon(s_2) - \psi_{1,\mathrm{app}}^\varepsilon(s_2)) + O(\varepsilon \delta^{-1})$$

and thus $\widehat{\widetilde{\chi}_1^\delta}(s_2) \psi^\varepsilon(s_2) = \widehat{\widetilde{\chi}_1^\delta}(s_2) \psi_{1,\mathrm{app}}^\varepsilon(s_2) + O(\varepsilon \delta^{-2})$. Because of the localisation of the wave packet $\psi_{1,\mathrm{app}}^\varepsilon(s_2)$, as stated in Remark A.2, we have in Σ_ε^k for any $N \in \mathbb{N}$,

$$\widehat{\widetilde{\chi}_1^\delta}(s_2) \psi_{1,\mathrm{app}}^\varepsilon(s_2) = \psi_{1,\mathrm{app}}^\varepsilon(s_2) + O(\varepsilon^{N/2} \delta^{-N}).$$

Hence, choosing $N = 2$, we obtain

$$\widehat{\widetilde{\chi}_1^\delta}(s_2) \psi^\varepsilon(s_2) = \psi_{1,\mathrm{app}}^\varepsilon(s_2) + O(\varepsilon \delta^{-2}),$$

and it only remains to study $(1 - \widehat{\widetilde{\chi}_1^\delta}(s_2)) \psi^\varepsilon(s_2)$. Before that, some remarks are in order. Note that the arguments developed above do not depend on the choice of s_2 and could have been developed for any $s \in [s_1, s_2]$. They are also independent of the choices of the functions χ_j^δ and $\widetilde{\chi}_j^\delta$ as long as they satisfy the properties stated above. Therefore, we have actually obtained a more general result, namely that for any function θ supported in $\{|f| > \delta\}$ and equal to 1 close to $\Phi_1^{t,s_1}(\widetilde{z}_1)$, we have for $t \in [s_1, s_2]$,

$$(37) \qquad\qquad \widehat{\theta} \psi^\varepsilon(t) = \widehat{\theta} \psi_{1,\mathrm{app}}^\varepsilon(t) + O(\varepsilon \delta^{-2}).$$

We can now study $(1 - \widehat{\widetilde{\chi}_1^\delta}(s_2)) \psi^\varepsilon(s_2)$. We set for $s \in [s_1, s_2]$, $w^\varepsilon(s) = (1 - \widehat{\widetilde{\chi}_1^\delta}(s)) \psi^\varepsilon(s)$. We have

$$i\varepsilon \partial_s w^\varepsilon(s) = \widehat{H}(s) w^\varepsilon(s) - \left[\widehat{\widetilde{\chi}_1^\delta}(s), \widehat{H}(s) \right] \psi^\varepsilon(s) - i\varepsilon \partial_s \widehat{\widetilde{\chi}_1^\delta}(s) \psi^\varepsilon(s)$$

$$= \widehat{H}(s) w^\varepsilon(s) - \varepsilon \widehat{r_\delta^\varepsilon}(s) \psi^\varepsilon(s) + O(\varepsilon^2 \delta^{-2})$$

where $r_\delta^\varepsilon(s)$ depends linearly on $d\widetilde{\chi}_1^\delta(s)$, and thus is compactly supported close to the trajectory $\Phi_1^{t,s_1}(\widetilde{z}_1)$ and equal to 0 very close to it. Therefore, by (37) and Remark A.2,

$$\varepsilon \widehat{r_\delta^\varepsilon(s)} \psi^\varepsilon(s) = \varepsilon \widehat{r_\delta^\varepsilon(s)} \psi_{1,\mathrm{app}}^\varepsilon(s) = O(\varepsilon^{N/2+1} \delta^{-N-1})$$

for any $N \in \mathbb{N}$. Choosing $N = 1$, we deduce $w^\varepsilon(s_2) = O(\varepsilon \delta^{-2})$. $\qquad\square$

4.2. **A global a priori estimate.** In this section, we prove the following a priori estimate.

Lemma 4.3. *Let $k \in \mathbb{N}$ and $T > 0$ such that $[t_0, t^\flat]$ is strictly included in $[t_0, t_0 + T]$. Then there exists a constant $C_k > 0$ such that*

$$\tag{38} \sup_{t \in [t_0, t_0+T]} \|\psi^\varepsilon(t) - \widehat{\vec{V_1}}(t) v_1^\varepsilon(t)\|_{\Sigma_\varepsilon^k} \le C_k \, \varepsilon^{1/3},$$

where $v_1^\varepsilon(t) = \mathcal{U}_{h_1}^\varepsilon(t, t_0) v_0^\varepsilon$ for all $t \in [t_0, t_0 + T]$.

In the next section, we shall improve this estimate to go beyond this approximation and exhibits elements of order $\sqrt{\varepsilon}$. However, we shall use this a priori estimate, together with elements developed in this section.

Proof. Of course, in view of the results of the preceding section, we choose $\delta > 0$ and we focus on the time interval $[t^\flat - \delta, t^\flat + \delta]$, taking into account that for times $t \in [t_0, t^\flat - \delta]$, we have

$$\|\psi^\varepsilon(t) - \widehat{\vec{V_1}}(t) v_1^\varepsilon(t)\|_{\Sigma_\varepsilon^k} \le C_k \, \varepsilon \delta^{-2}$$

for some constant $C_k > 0$, and that for $t \in [t^\flat + \delta, t_0 + T]$ we can use the same kind of transport estimate since the trajectory does not meet again the crossing set. It is thus enough to pass from $t^\flat - \delta$ to $t^\flat + \delta$ and analyze $\psi^\varepsilon(t^\flat + \delta)$. Between the times $t^\flat - \delta$ and $t^\flat + \delta$, we cannot use the super-adiabatic corrections to the projectors Π_1 and Π_2, because they become singular when the eigenvalue gap closes. We thus simply work with the projectors Π_1 and Π_2. We define the families $w^\varepsilon(t) = (w_1^\varepsilon(t), w_2^\varepsilon(t))$ by

$$\tag{39} w_1^\varepsilon = \widehat{\Pi}_1 \psi^\varepsilon - \widehat{\vec{V_1}} v_1^\varepsilon, \quad w_2^\varepsilon = \widehat{\Pi}_2 \psi^\varepsilon.$$

Since $\psi^\varepsilon(t)$ and $\widehat{\vec{V_1}} v_1^\varepsilon(t)$ are in all spaces $\Sigma_\varepsilon^\ell(\mathbb{R}^d)$ for $\ell \in \mathbb{N}$ and $t \in [t_0, t_0 + T]$, the same is true for $w_1^\varepsilon(t)$ and $w_2^\varepsilon(t)$. We now use our former observations, that is, the evolution equation (35) for the approximate wave packet and the relation (52) of Appendix B, which gives that $w^\varepsilon(t)$ satisfies the following system:

$$\begin{cases} i\varepsilon \partial_t w_1^\varepsilon & = \widehat{h}_1 w_1^\varepsilon + i\varepsilon f_1^\varepsilon, \\ i\varepsilon \partial_t w_2^\varepsilon & = \widehat{h}_2 w_2^\varepsilon + \frac{i\varepsilon}{2} \widehat{B_2 \Pi_1} \vec{V_1} v_1 + i\varepsilon f_2^\varepsilon \end{cases}$$

with

$$\tag{40} f_1^\varepsilon = -i\widehat{\Theta}_1 w_1^\varepsilon + \tfrac{1}{2} \widehat{B_1 \Pi_2} w_2^\varepsilon + \varepsilon r_1^\varepsilon \quad \text{and} \quad f_2^\varepsilon = -i\widehat{\Theta}_2 w_2^\varepsilon + \tfrac{1}{2} \widehat{B_2 \Pi_1} w_1^\varepsilon + \varepsilon r_2^\varepsilon.$$

The matrices B_1 and B_2 are defined according to

$$B_j = -2\partial_t \Pi_j - \{h_j, \Pi_j\} + \{\Pi_j, H\}, \qquad j = 1, 2,$$

and the sequences $(r_1^\varepsilon(t))_{\varepsilon > 0}$ and $(r_2^\varepsilon(t))_{\varepsilon > 0}$ are uniformly bounded in $\Sigma_\varepsilon^k(\mathbb{R}^d)$ due to the polynomial growth estimate (26) for the eigenprojectors. We immediately deduce that for

all $t \in [t_0, t_0 + T]$,

$$(41) \quad \begin{aligned} w_1^\varepsilon(t) &= \mathcal{U}_{h_1}^\varepsilon(t, t^\flat - \delta) w_1^\varepsilon(t^\flat - \delta) + \int_{t^\flat - \delta}^t \mathcal{U}_{h_1}^\varepsilon(t, \sigma) f_1^\varepsilon(\sigma) d\sigma, \\ w_2^\varepsilon(t) &= \mathcal{U}_{h_2}^\varepsilon(t, t^\flat - \delta) w_2^\varepsilon(t^\flat - \delta) + \int_{t^\flat - \delta}^t \mathcal{U}_{h_2}^\varepsilon(t, \sigma) f_2^\varepsilon(\sigma) d\sigma \\ &\quad + \frac{1}{2} \int_{t^\flat - \delta}^t \mathcal{U}_{h_2}^\varepsilon(t, \sigma) \widehat{B_2 \Pi_1} \widehat{\vec{V}_1}(\sigma) v_1^\varepsilon(\sigma) d\sigma. \end{aligned}$$

Therefore, in $\Sigma_\varepsilon^k(\mathbb{R}^d)$, for all times $t \in [t^\flat - \delta, t^\flat + \delta]$ and $j \in \{1, 2\}$, $w_j^\varepsilon(t) = O(\varepsilon \delta^{-2}) + O(\delta)$. Choosing $\delta = \varepsilon^{1/3}$, we obtain that $w_j^\varepsilon(t) = O(\varepsilon^{1/3})$. □

5. ANALYSIS IN THE CROSSING REGION

We now want to pass through the crossing and derive a more precise estimate on the function $\psi^\varepsilon(t^\flat + \delta)$. We prove the following result.

Proposition 5.1. *Assume $\sqrt{\varepsilon} \ll \delta \ll \varepsilon^{1/3}$. Then, for all $k \in \mathbb{N}$, there exists a constant $C_k > 0$ such that*

$$\left\| \psi^\varepsilon(t^\flat + \delta) - \widehat{\vec{V}_1}(t^\flat + \delta) v_1^\varepsilon(t^\flat + \delta) - \sqrt{\varepsilon} \widehat{\vec{V}_2}(t^\flat + \delta) v_2^\varepsilon(t^\flat + \delta) \right\|_{\Sigma_\varepsilon^k} \leq C_k(\varepsilon \delta^{-2} + \varepsilon^{1/3} \delta),$$

where $v_1^\varepsilon(t) = \mathcal{U}_{h_1}^\varepsilon(t, t_0) v_0^\varepsilon$ and $v_2^\varepsilon(t) = \mathcal{U}_{h_2}^\varepsilon(t, t^\flat) v_2^\varepsilon(t^\flat)$ are as in Theorem 3.8.

Proof. We split the proof in several steps. In Lemma 5.2 we use the a priori estimate of Lemma 4.3 to simplify the approximation of $\psi^\varepsilon(t^\flat + \delta)$ and exhibit the contribution of order $\sqrt{\varepsilon}$ according to

$$\psi^\varepsilon(t^\flat + \delta) = \widehat{\vec{V}_1}(t^\flat + \delta) v_1^\varepsilon(t^\flat + \delta) + e^{iS^\flat/\varepsilon} \mathcal{U}_{h_2}^\varepsilon(t^\flat + \delta, t^\flat) A_\varepsilon + O(\varepsilon \delta^{-2}) + O(\varepsilon^{1/3} \delta).$$

Then, we carefully analyze the contribution A_ε and construct a preliminary transfer operator $\mathcal{T}^\varepsilon$ satisfying

$$A_\varepsilon = \mathcal{W} \mathcal{P}_{z^\flat}^\varepsilon \mathcal{T}^\varepsilon \varphi_1(t^\flat) + O(\sqrt{\varepsilon} \delta),$$

see Lemma 5.3. As the third step, Lemma 5.5 establishes the relation to the transfer operator $\mathcal{T}^\flat$ according to

$$\mathcal{T}^\varepsilon = \sqrt{\varepsilon} \, \mathcal{Q}^\varepsilon(0) \mathcal{T}^\flat + O(\sqrt{\varepsilon} \delta) + O(\varepsilon \delta^{-1})$$

with $\mathcal{Q}^\varepsilon(0) = \mathrm{op}_1^w((\gamma \vec{V}_2)(t^\flat, z^\flat + \sqrt{\varepsilon} \bullet))$. The wave packet relation (49) in combination with symbolic calculus implies for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$ that

$$\begin{aligned} \mathcal{W} \mathcal{P}_{z^\flat}^\varepsilon \mathcal{Q}^\varepsilon(0) \varphi &= \widehat{\gamma \vec{V}_2}(t^\flat) \mathcal{W} \mathcal{P}_{z^\flat}^\varepsilon \varphi \\ &= \widehat{\vec{V}_2}(t^\flat) \widehat{\gamma}(t^\flat) \mathcal{W} \mathcal{P}_{z^\flat}^\varepsilon \varphi + O(\varepsilon) = \widehat{\vec{V}_2}(t^\flat) \gamma^\flat \mathcal{W} \mathcal{P}_{z^\flat}^\varepsilon \varphi + O(\sqrt{\varepsilon}). \end{aligned}$$

Hence, we have proven that

$$e^{iS^\flat/\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\,A_\varepsilon$$

$$= \sqrt{\varepsilon}\,\gamma^\flat\, e^{iS^\flat/\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\widehat{\vec{V_2}}(t^\flat)\mathcal{W}\mathcal{P}^\varepsilon_{z^\flat}\mathcal{T}^\flat\varphi_1(t^\flat) + O(\varepsilon\delta^{-2}) + O(\varepsilon^{1/3}\delta)$$

$$= \sqrt{\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\,\widehat{\vec{V_2}}(t^\flat)v^\varepsilon_2(t^\flat) + O(\varepsilon\delta^{-2}) + O(\varepsilon^{1/3}\delta).$$

It remains to analyze the function $\omega(t) = \vec{V_2}(t)\mathcal{U}^\varepsilon_{h_2}(t,t^\flat) - \mathcal{U}^\varepsilon_{h_2}(t,t^\flat)\vec{V_2}(t^\flat)$. An analogous calculation to the one at the beginning of the proof of Proposition 4.1 yields that

$$i\varepsilon\partial_t\omega = \widehat{h}_2\omega + O(\varepsilon).$$

Since $\omega(t^\flat) = 0$, the Duhamel principle implies that $\omega(t^\flat+\delta) = O(\delta)$ and

$$e^{iS^\flat/\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\,A_\varepsilon = \sqrt{\varepsilon}\,\widehat{\vec{V_2}}(t^\flat+\delta)\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\,v^\varepsilon_2(t^\flat) + O(\varepsilon\delta^{-2}) + O(\varepsilon^{1/3}\delta).$$

$\square$

5.1. Using the a priori estimate.
We start describing the part of the wave packet that has been transferred at the crossing and identify its main contribution.

Lemma 5.2. *Let $k \in \mathbb{N}$. With the assumptions of Proposition 5.1, we have in $\Sigma^k_\varepsilon(\mathbb{R}^d)$,*

$$\psi^\varepsilon(t^\flat+\delta) = \widehat{\vec{V_1}}(t^\flat+\delta)v^\varepsilon_1(t^\flat+\delta) + e^{iS^\flat/\varepsilon}\,\mathcal{U}^\varepsilon_{h_2}(t^\flat+\delta,t^\flat)\,A_\varepsilon + O(\varepsilon\delta^{-2}) + O(\varepsilon^{1/3}\delta)$$

(42)
$$with \;\; A_\varepsilon = \int_{t^\flat-\delta}^{t^\flat+\delta}\mathcal{U}^\varepsilon_{h_2}(t^\flat,\sigma)\gamma\widehat{\vec{V_2}}(\sigma)\mathcal{U}^\varepsilon_{h_1}(\sigma,t^\flat)\mathcal{W}\mathcal{P}_{z^\flat}\varphi_1(t^\flat)d\sigma,$$

where the eigenvector $\vec{V_2}$ is defined in (27) and the Schwartz function $\varphi_1(t^\flat)$ is associated with the profile φ_0 of the initial wave packet according to Proposition 2.3.

Proof. We again analyse the functions $w^\varepsilon_1(t)$ and $w^\varepsilon_2(t)$ introduced in (39), that are of order $\varepsilon\delta^{-2}$ at time $t = t^\flat - \delta$. By the a priori estimate of Lemma 4.3, the remainder terms $f^\varepsilon_1(t)$ and $f^\varepsilon_2(t)$, which appear in (40), are of order $\varepsilon^{1/3}$. Therefore, the relation (41) gives for all times $t \in [t^\flat-\delta, t^\flat+\delta]$ and in $\Sigma^k_\varepsilon(\mathbb{R}^d)$,

$$w^\varepsilon_1(t) = O(\varepsilon\delta^{-2}) + O(\delta\varepsilon^{1/3}),$$

$$w^\varepsilon_2(t) = O(\varepsilon\delta^{-2}) + O(\delta\varepsilon^{1/3}) + \frac{1}{2}\int_{t^\flat-\delta}^t\mathcal{U}^\varepsilon_{h_2}(t,\sigma)\widehat{B_2\Pi_1}\widehat{\vec{V_1}}(\sigma)v^\varepsilon_1(\sigma)d\sigma.$$

At this stage of the proof, we write $B_2\Pi_1 = \Pi_1 B_2\Pi_1 + \Pi_2 B_2\Pi_1$ and take advantage of $\Pi_1 B_2\Pi_1 = (h_2 - h_1)\Pi_1\{\Pi_1, \Pi_1\}\Pi_1$ (see Lemma B.1) to write

$$\int_{t^\flat-\delta}^t \mathcal{U}_{h_2}^\varepsilon(t,\sigma)\widehat{\Pi_1 B_2\Pi_1}\widehat{\vec{V}_1}(\sigma)\mathcal{U}_{h_1}^\varepsilon(\sigma, t^\flat-\delta)v_1^\varepsilon(t^\flat-\delta)d\sigma$$

$$= i\varepsilon\int_{t^\flat-\delta}^t \frac{d}{d\sigma}\left(\mathcal{U}_{h_2}^\varepsilon(t,\sigma)\,\mathrm{op}_\varepsilon^w\left(\Pi_1\{\Pi_1,\Pi_1\}\Pi_1\vec{V}_1(\sigma)\right)\mathcal{U}_{h_1}^\varepsilon(\sigma, t^\flat-\delta)\right)v_1^\varepsilon(t^\flat-\delta)\,d\sigma + \varepsilon\rho^\varepsilon(t)$$

$$= \varepsilon\tilde{\rho}^\varepsilon(t),$$

where both families $(\rho^\varepsilon(t))_{\varepsilon>0}$ and $(\tilde{\rho}^\varepsilon(t))_{\varepsilon>0}$ are uniformly bounded in $\Sigma_\varepsilon^k(\mathbb{R}^d)$. Therefore,

$$\int_{t^\flat-\delta}^t \mathcal{U}_{h_2}^\varepsilon(t,\sigma)\widehat{B_2\Pi_1}\widehat{\vec{V}_1}(\sigma)v_1^\varepsilon(\sigma)d\sigma = \int_{t^\flat-\delta}^t \mathcal{U}_{h_2}^\varepsilon(t,\sigma)\widehat{\Pi_2 B_2\Pi_1}\widehat{\vec{V}_1}(\sigma)v_1^\varepsilon(\sigma)d\sigma + O(\varepsilon).$$

By Lemma B.1 and the definition of the eigenvector $\vec{V}_2$ (see (27))

$$\tfrac{1}{2}\Pi_2 B_2\vec{V}_1 = \Pi_2(-\partial_t\Pi_2 - \{v,\Pi_2\})\vec{V}_1 = \gamma\vec{V}_2.$$

According to Proposition 2.3, we have for the wave packet

$$v_1^\varepsilon(\sigma) = \mathcal{U}_{h_1}(\sigma, t^\flat)v_1^\varepsilon(t^\flat) = \mathcal{U}_{h_1}(\sigma, t^\flat)e^{iS^\flat/\varepsilon}\mathcal{WP}_{z^\flat}\varphi_1(t^\flat) + O(\varepsilon).$$

Therefore,

$$\frac{1}{2}\int_{t^\flat-\delta}^t \mathcal{U}_{h_2}^\varepsilon(t,\sigma)\widehat{B_2\Pi_1}\widehat{\vec{V}_1}(\sigma)v_1^\varepsilon(\sigma)d\sigma$$

$$= e^{iS^\flat/\varepsilon}\mathcal{U}_{h_2}^\varepsilon(t,t^\flat)\int_{t^\flat-\delta}^t \mathcal{U}_{h_2}^\varepsilon(t^\flat,\sigma)\widehat{\gamma\vec{V}_2}(\sigma)\mathcal{U}_{h_1}(\sigma, t^\flat)\mathcal{WP}_{z^\flat}\varphi_1(t^\flat)d\sigma + O(\varepsilon),$$

and, in terms of the function A_ε is defined in (42), we are left at time $t = t^\flat + \delta$ with

$$w_1^\varepsilon(t^\flat + \delta) = O(\varepsilon\delta^{-2}) + O(\delta\varepsilon^{1/3}),$$

$$w_2^\varepsilon(t^\flat + \delta) = e^{iS^\flat/\varepsilon}\mathcal{U}_{h_2}^\varepsilon(t^\flat + \delta, t^\flat)\,A_\varepsilon + O(\varepsilon\delta^{-2}) + O(\delta\varepsilon^{1/3}).$$

<div style="text-align: right;">□</div>

5.2. Constructing the transfer operator.
Next, we relate the transition term A_ε to an integral operator that is defined in terms of the crossing parameters $\mu^\flat$ and $(\alpha^\flat, \beta^\flat)$ introduced in Theorem 3.8.

Lemma 5.3. *Let $k \in \mathbb{N}$. With the assumptions of Proposition 5.1, there exist*

- *a smooth real-valued map $\sigma \mapsto \Lambda(\sigma)$ with $\Lambda(0) = 0$, $\dot{\Lambda}(0) = 0$, $\ddot{\Lambda}(0) = 2\mu^\flat + \alpha^\flat \cdot \beta^\flat$,*
- *a smooth vector-valued map $\sigma \mapsto z(\sigma) = (q(\sigma), p(\sigma))$ with $z(0) = 0$, $\dot{z}(0) = (\alpha^\flat, \beta^\flat)$,*
- *a smooth map $\sigma \mapsto \mathcal{Q}^\varepsilon(\sigma)$ of operators, that map Schwartz functions to Schwartz functions, with $\mathcal{Q}^\varepsilon(0) = \mathrm{op}_1^w(\gamma\vec{V}_2(t^\flat, z^\flat + \sqrt{\varepsilon}\bullet))$,*

such that the transition quantity A_ε defined in Lemma 5.2 satisfies

$$(43) \qquad A_\varepsilon = \mathcal{WP}^\varepsilon_{z^\flat} \mathcal{T}^\varepsilon \varphi_1(t^\flat) + O(\sqrt{\varepsilon}\delta)$$

in $\Sigma^k_\varepsilon(\mathbb{R}^d)$ for the integral operator $\mathcal{T}^\varepsilon$ defined by

$$\mathcal{T}^\varepsilon \varphi(y) = \int_{-\delta}^{+\delta} e^{\frac{i}{\varepsilon}\Lambda(\sigma)} \mathcal{Q}^\varepsilon(\sigma) e^{ip_\varepsilon(\sigma)\cdot(y-q_\varepsilon(\sigma))} \varphi(y - q_\varepsilon(\sigma))\, d\sigma, \quad \varphi \in \mathcal{S}(\mathbb{R}^d),$$

where we have used the scaling notation $z_\varepsilon(\sigma) = z(\sigma)/\sqrt{\varepsilon}$.

Proof. We use Egorov's semi-classical theorem [6, Theorem 12] and obtain that in $\Sigma^k_\varepsilon(\mathbb{R}^d)$,

$$\mathcal{U}^\varepsilon_{h_2}(t^\flat, \sigma) \widehat{\gamma \vec{V}_2}(\sigma) f = \mathrm{op}^w_\varepsilon((\gamma \vec{V}_2)(\sigma) \circ \Phi^{\sigma,t^\flat}_2) \mathcal{U}^\varepsilon_{h_2}(t^\flat, \sigma) f + O(\varepsilon)$$

for all $f \in \bigcap_{\ell \geq k} \Sigma^\ell_\varepsilon(\mathbb{R}^d)$. Hence,

$$A_\varepsilon = \int_{t^\flat - \delta}^{t^\flat + \delta} \mathrm{op}^w_\varepsilon((\gamma \vec{V}_2)(\sigma) \circ \Phi^{\sigma,t^\flat}_2) \mathcal{U}^\varepsilon_{h_2}(t^\flat, \sigma) \mathcal{U}^\varepsilon_{h_1}(\sigma, t^\flat) \mathcal{WP}^\varepsilon_{z^\flat} \varphi_1(t^\flat) d\sigma + O(\delta\varepsilon).$$

We set $\vec{Q}_2(\sigma) = (\gamma \vec{V}_2)(t^\flat + \sigma) \circ \Phi^{\sigma+t^\flat,t^\flat}_2$, and note that $\vec{Q}_2(0) = (\gamma \vec{V}_2)(t^\flat)$. We get after a change of variables

$$A_\varepsilon = \int_{-\delta}^{\delta} \widehat{\vec{Q}_2}(\sigma) \mathcal{U}^\varepsilon_{h_2}(t^\flat, t^\flat + \sigma) \mathcal{U}^\varepsilon_{h_1}(t^\flat + \sigma, t^\flat) \mathcal{WP}^\varepsilon_{z^\flat} \varphi_1(t^\flat) d\sigma + O(\delta\varepsilon).$$

Now we apply successively Proposition 2.3 to the evolutions $\mathcal{U}^\varepsilon_{h_1}$ and $\mathcal{U}^\varepsilon_{h_2}$ without encorporating the first amplitude correction, that is, for a basic approximation of order $\sqrt{\varepsilon}$. We obtain

$$\mathcal{U}^\varepsilon_{h_2}(t^\flat, t^\flat + \sigma) \mathcal{U}^\varepsilon_{h_1}(t^\flat + \sigma, t^\flat) \mathcal{WP}^\varepsilon_{z^\flat} \varphi_1(t^\flat) = e^{\frac{i}{\varepsilon}S(\sigma)} \mathcal{WP}^\varepsilon_{\zeta(\sigma)} \mathcal{M}(\sigma) \varphi_1(t^\flat) + O(\sqrt{\varepsilon}),$$

where we denoted the combined center, phase and metaplectic transform by

$$\zeta(\sigma) = \Phi^{t^\flat, t^\flat+\sigma}_2\big(\Phi^{t^\flat+\sigma,t^\flat}_1(z^\flat)\big),$$

$$S(\sigma) = S_1(t^\flat + \sigma, t^\flat, z^\flat) + S_2(t^\flat, t^\flat + \sigma, \Phi^{t^\flat+\sigma,t^\flat}_1(z^\flat)),$$

$$\mathcal{M}(\sigma) = \mathcal{M}[F_2(t^\flat, t^\flat + \sigma, \Phi^{t^\flat+\sigma,t^\flat}_1(z^\flat))] \, \mathcal{M}[F_1(t^\flat + \sigma, t^\flat, z^\flat)].$$

This implies

$$A_\varepsilon = \int_{-\delta}^{+\delta} \widehat{\vec{Q}_2}(\sigma) e^{\frac{i}{\varepsilon}S(\sigma)} \mathcal{WP}^\varepsilon_{\zeta(\sigma)} \mathcal{M}(\sigma) \varphi_1(t^\flat) d\sigma + O(\delta\sqrt{\varepsilon}).$$

We observe that

$$\zeta(0) = z^\flat, \quad S(0) = 0, \quad \mathcal{M}(0) = \mathbb{I},$$

and write $\zeta(\sigma) = z^\flat + z(\sigma)$ with $z(0) = 0$. By Lemma D.1,

$$\dot{z}(0) = (\alpha^\flat, \beta^\flat), \quad \dot{S}(0) = p^\flat \cdot \alpha^\flat.$$

Moreover, using the group and translation properties of the wave packet transform (48) and (47), we have

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

$$= \mathrm{e}^{-\frac{i}{\varepsilon}p^\flat \cdot q(\sigma)}\mathrm{e}^{-\frac{i}{2\varepsilon}p(\sigma)\cdot q(\sigma)}\mathcal{WP}^\varepsilon_{z^\flat}\Lambda_\varepsilon^{-1}\widehat{T}^\varepsilon(z(\sigma))\Lambda_\varepsilon$$

$$= \mathrm{e}^{-\frac{i}{\varepsilon}p^\flat \cdot q(\sigma)}\mathrm{e}^{-\frac{i}{2\varepsilon}p(\sigma)\cdot q(\sigma)}\mathcal{WP}^\varepsilon_{z^\flat}\widehat{T}^1(z_\varepsilon(\sigma)),$$

By the translation properties of the metaplectic transform [6, Section 3.3], we have

$$\widehat{T}^1(z_\varepsilon(\sigma))\mathcal{M}(\sigma) = \mathcal{M}(\sigma)\widehat{T}^1(\widetilde{z}_\varepsilon(\sigma))$$

with new center

$$\widetilde{z}(\sigma) = F_1(t^\flat + \sigma, t^\flat, z^\flat)^{-1}F_2(t^\flat, t^\flat + \sigma, \Phi_1^{t^\flat+\sigma,t^\flat}(z^\flat))^{-1}z(\sigma)$$

We observe that

$$\widetilde{z}(0) = z(0) = 0, \quad \dot{\widetilde{z}}(0) = \dot{z}(0) = (\alpha^\flat, \beta^\flat).$$

Moreover, in view of the relation (49),

$$\widehat{\vec{Q}_2}(\sigma)\mathcal{WP}^\varepsilon_{\zeta(\sigma)}\mathcal{M}(\sigma) = \mathrm{e}^{-\frac{i}{\varepsilon}p^\flat \cdot q(\sigma)}\mathrm{e}^{-\frac{i}{2\varepsilon}p(\sigma)\cdot q(\sigma)}\widehat{\vec{Q}_2}(\sigma)\mathcal{WP}^\varepsilon_{z^\flat}\mathcal{M}(\sigma)\widehat{T}^1(\widetilde{z}_\varepsilon(\sigma))$$

$$= \mathrm{e}^{-\frac{i}{\varepsilon}p^\flat \cdot q(\sigma)}\mathrm{e}^{-\frac{i}{2\varepsilon}p(\sigma)\cdot q(\sigma)}\mathcal{WP}^\varepsilon_{z^\flat}\mathrm{op}_1^w(\vec{Q}_2(\sigma, z^\flat + \sqrt{\varepsilon}\bullet))\mathcal{M}(\sigma)\widehat{T}^1(\widetilde{z}_\varepsilon(\sigma)).$$

Since

$$\widehat{T}^1(\widetilde{z}_\varepsilon(\sigma))\varphi_1(t^\flat, y) = \mathrm{e}^{\frac{i}{2}\widetilde{q}_\varepsilon(\sigma)\cdot\widetilde{p}_\varepsilon(\sigma)}\mathrm{e}^{i\widetilde{p}_\varepsilon(\sigma)\cdot(y-\widetilde{q}_\varepsilon(\sigma))}\varphi_1(t^\flat, y - \widetilde{q}_\varepsilon(\sigma)),$$

we may introduce the phase $\widetilde{\Lambda}(\sigma)$ and the operator $\mathcal{Q}^\varepsilon(\sigma)$ acccording to

$$\widetilde{\Lambda}(\sigma) = S(\sigma) - p^\flat \cdot q(\sigma) - p(\sigma) \cdot q(\sigma) + \widetilde{p}(\sigma) \cdot \widetilde{q}(\sigma),$$

(44) $$\mathcal{Q}^\varepsilon(\sigma) = \mathrm{op}_1^w(\vec{Q}_2(\sigma, z^\flat + \sqrt{\varepsilon}\bullet))\mathcal{M}(\sigma),$$

to obtain the approximation

$$A_\varepsilon = \mathcal{WP}^\varepsilon_{z^\flat}\int_{-\delta}^{+\delta}\mathrm{e}^{\frac{i}{\varepsilon}\widetilde{\Lambda}(\sigma)}\mathcal{Q}^\varepsilon(\sigma)\mathrm{e}^{i\widetilde{p}_\varepsilon(\sigma)\cdot(y-\widetilde{q}_\varepsilon(\sigma))}\varphi_1(t^\flat, y - \widetilde{q}_\varepsilon(\sigma))\,d\sigma + O(\delta\sqrt{\varepsilon}).$$

We clearly have $\widetilde{\Lambda}(0) = \dot{\widetilde{\Lambda}}(0) = 0$ and $\mathcal{Q}^\varepsilon(0) = \mathrm{op}_1^w((\gamma\vec{V}_2)(t^\flat, z^\flat + \sqrt{\varepsilon}\bullet))$, whereas, by Lemma D.1,

$$\ddot{\widetilde{\Lambda}}(0) = \ddot{S}(0) - p^\flat \cdot \ddot{q}(0) = 2\mu^\flat + \alpha^\flat \cdot \beta^\flat.$$

$\square$

Remark 5.4. Note that the first step of the proof of Lemma 5.3 can be performed at any order in ε with a remainder of the form $O(\delta\varepsilon^N)$: pushing the Egorov theorem at higher order, we obtain

$$A_\varepsilon = \int_{t^\flat-\delta}^{t^\flat+\delta}\widehat{\vec{Q}_2^{\varepsilon,N}}(\sigma)\mathcal{U}^\varepsilon_{h_2}(t^\flat, \sigma)\mathcal{U}^\varepsilon_{h_1}(\sigma, t^\flat)\mathcal{WP}^\varepsilon_{z^\flat}\varphi_1(t^\flat)d\sigma + O(\delta\varepsilon^{N+1})$$

$$\text{with } \vec{Q}_2^{\varepsilon,N} = \vec{Q}_2 + \varepsilon\vec{Q}_2^{(1)} + \cdots + \varepsilon^N\vec{Q}_2^{(N)}.$$

Similarly, also Proposition 2.3 can be generalized at any order in ε, which then implies

$$A_\varepsilon = \mathcal{W}\mathcal{P}_{z^\flat}^\varepsilon \, \mathcal{T}^{\varepsilon,N}\varphi_1^\varepsilon(t^\flat) + O(\varepsilon^{N/2+1}\delta)$$

where $\varphi_1^\varepsilon = \varphi_1 + \sqrt{\varepsilon}\varphi_1^{(1)} + \cdots + \varepsilon^{N/2}\varphi_1^{(N)}$ and

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

for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$. The phase function $\Lambda(\sigma)$ and the phase space center $z(\sigma)$ stay the same as in Lemma 5.3, while the operator $\mathcal{Q}^{\varepsilon,N}(\sigma)$ is associated with $\vec{Q}_2^{\varepsilon,N}(\sigma)$ according to (44) by selecting terms up to order $\varepsilon^{N/2}$ in its definition.

5.3. The transfer operator.
Consider the family of operators

$$\mathcal{T}^\varepsilon\varphi(y) \;\; = \;\; \int_{-\delta}^{+\delta} e^{\frac{i}{\varepsilon}\Lambda(\sigma)} \mathcal{Q}^\varepsilon(\sigma) e^{i(y-q_\varepsilon(\sigma)))\cdot p_\varepsilon(\sigma)}\varphi(y - q_\varepsilon(\sigma))d\sigma, \quad \varphi \in \mathcal{S}(\mathbb{R}^d),$$

as introduced in Lemma 5.3. We next describe such an operator $\mathcal{T}^\varepsilon$, when ε goes to 0.

Lemma 5.5. *Let $k \in \mathbb{N}$. If $\sqrt{\varepsilon} \ll \delta \ll 1$, then for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$,*

$$(45) \qquad\qquad \mathcal{T}^\varepsilon\varphi = \sqrt{\varepsilon}\, \mathcal{Q}^\varepsilon(0)\mathcal{T}^\flat\varphi + O(\sqrt{\varepsilon}\delta) + O(\varepsilon\delta^{-1})$$

in $\Sigma_\varepsilon^k(\mathbb{R}^d)$ with $\mathcal{T}^\flat = \displaystyle\int_{-\infty}^{+\infty} e^{i\mu^\flat s^2} e^{is(\beta^\flat \cdot y - \alpha^\flat \cdot D_y)}\, ds$

Proof. The proof relies on the analysis of the integrand close to $\sigma = 0$. We write

$$\mathcal{T}^\varepsilon = \sqrt{\varepsilon}\int_{-\delta/\sqrt{\varepsilon}}^{+\delta/\sqrt{\varepsilon}} e^{\frac{i}{\varepsilon}\Lambda(\sqrt{\varepsilon}s) - \frac{i}{2}q_\varepsilon(s\sqrt{\varepsilon})\cdot p_\varepsilon(s\sqrt{\varepsilon})} \mathcal{Q}^\varepsilon(s\sqrt{\varepsilon}) e^{iL^\varepsilon(s)}ds$$

where $L^\varepsilon(s) := p_\varepsilon(s\sqrt{\varepsilon}) \cdot y - p_\varepsilon(s\sqrt{\varepsilon})D_y$ defines a family of self-adjoint operators $s \mapsto L^\varepsilon(s)$ mappping $\mathcal{S}(\mathbb{R}^d)$ into itself. Recall that the functions $s \mapsto p_\varepsilon(s\sqrt{\varepsilon})$ and $s \mapsto q_\varepsilon(s\sqrt{\varepsilon})$ are uniformly bounded with respect to ε, and that $q(0) = p(0) = 0$, while

$$(46) \qquad\qquad \mu^\flat = \frac{1}{2}\left(\ddot{\Lambda}(0) - \dot{q}(0)\cdot\dot{p}(0)\right), \quad \alpha^\flat = \dot{q}(0), \quad \beta^\flat = \dot{p}(0).$$

We set $L = \beta^\flat \cdot y - \alpha^\flat \cdot D_y$. Using Taylor expansion in $s = 0$, we obtain

$$\Lambda(\sqrt{\varepsilon}s) - \frac{i}{2}q_\varepsilon(s\sqrt{\varepsilon}) \cdot p_\varepsilon(s\sqrt{\varepsilon}) = \mu^\flat s^2 + \sqrt{\varepsilon}s^3 f_1(s\sqrt{\varepsilon})$$

with $\sigma \mapsto f_1(\sigma)$ bounded, together with its derivatives, for $\sigma \in [t_0, t_0+T]$. In the following, the notation f_j will denote functions that have the same property. We also have

$$L^\varepsilon(s) = sL + \sqrt{\varepsilon}s^2 L_1^\varepsilon(s\sqrt{\varepsilon})$$

where the family of operator $\sigma \mapsto L_1^\varepsilon(\sigma)$ maps $\mathcal{S}(\mathbb{R}^d)$ into itself, for $\sigma \in [t_0, t_0 + T]$. Besides, the commutator $[L, L_1(s\sqrt{\varepsilon})]$ is a scalar, and we set

$$\frac{1}{2}[L, L_1(s\sqrt{\varepsilon})] = f_2(s\sqrt{\varepsilon})$$

with the notation we have just introduced. Therefore, by Baker-Campbell-Hausdorff formula

$$e^{iL^\varepsilon(s)} = e^{isL}e^{is^2\sqrt{\varepsilon}L_1(s\sqrt{\varepsilon})}e^{i\sqrt{\varepsilon}s^3 f_2(s\sqrt{\varepsilon})}.$$

Besides,

$$e^{i\sqrt{\varepsilon}s^2 L_1(s\sqrt{\varepsilon})} = \mathrm{Id} + \sqrt{\varepsilon}s^2 \Theta(s\sqrt{\varepsilon})$$

where the operator-valued map $\sigma \mapsto \Theta(\sigma)$ is smooth and such that for all $\sigma \in [t_0, t_0 + T]$, the operator $\Theta(\sigma)$ and its derivatives maps $\mathcal{S}(\mathbb{R}^d)$ into itself. Setting $f_3 = f_1 + f_2$, we deduce that $\mathcal{T}^\varepsilon$ writes

$$\mathcal{T}^\varepsilon = \sqrt{\varepsilon} \int_{-\delta/\sqrt{\varepsilon}}^{+\delta/\sqrt{\varepsilon}} e^{i\mu^\flat s^2 + \sqrt{\varepsilon}s^3 f_3(s\sqrt{\varepsilon})} \mathcal{Q}^\varepsilon(s\sqrt{\varepsilon})e^{isL}ds + R^{\varepsilon,\delta}$$

$$\text{with } R^{\varepsilon,\delta} = \varepsilon \int_{-\delta/\sqrt{\varepsilon}}^{+\delta/\sqrt{\varepsilon}} e^{i\mu^\flat s^2 + \sqrt{\varepsilon}s^3 f_3(s\sqrt{\varepsilon})} \mathcal{Q}(s\sqrt{\varepsilon})e^{isL}s^2 \Theta^\varepsilon(s\sqrt{\varepsilon})ds.$$

Let us analyze $R^{\varepsilon,\delta}$. For this, we perform an integration by parts. Indeed,

$$\partial_s(\mu^\flat s^2 + \sqrt{\varepsilon}s^3 f_3(s\sqrt{\varepsilon})) = 2\mu^\flat s(1 + s\sqrt{\varepsilon}f_4(s\sqrt{\varepsilon}))$$

for some smooth bounded function f_4 with bounded derivatives. Moreover, since δ is small, we have $1 + s\sqrt{\varepsilon}f_4(s\sqrt{\varepsilon}) > 1/2$ for all $s \in]-\delta/\sqrt{\varepsilon}, +\delta/\sqrt{\varepsilon}[$. Therefore, we can write

$$R^{\varepsilon,\delta} = \left[\frac{\varepsilon s}{2i\mu^\flat(1 + s\sqrt{\varepsilon}f_4(s\sqrt{\varepsilon}))} e^{i\mu^\flat s^2 + i\sqrt{\varepsilon}s^3 f_3(s\sqrt{\varepsilon})} \mathcal{Q}^\varepsilon(s\sqrt{\varepsilon})e^{isL} \right]_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}}$$

$$- \frac{\varepsilon}{2i\mu^\flat} \int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}} e^{i\mu^\flat s^2 + i\sqrt{\varepsilon}s^3 f_3(s\sqrt{\varepsilon})} \frac{d}{ds}\left(\frac{s}{1 + s\sqrt{\varepsilon}f_4(s\sqrt{\varepsilon})} \mathcal{Q}^\varepsilon(s\sqrt{\varepsilon})e^{isL} \right) ds,$$

where $\mu^\flat \neq 0$ by the transversality condition (23). We deduce that for all $k \in \mathbb{N}$ and $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we have in $\Sigma_\varepsilon^k(\mathbb{R}^d)$ that $R^{\varepsilon,\delta}\varphi = O(\sqrt{\varepsilon}\delta) + R_1^{\varepsilon,\delta}\varphi$ with

$$R_1^{\varepsilon,\delta}\varphi = -\frac{\varepsilon}{2i\mu^\flat} \int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}} e^{i\mu^\flat s^2 + i\sqrt{\varepsilon}s^3 f_3(s\sqrt{\varepsilon})} \left(\frac{s}{1 + s\sqrt{\varepsilon}f_4(s\sqrt{\varepsilon})} \mathcal{Q}^\varepsilon(s\sqrt{\varepsilon})e^{isL}L\varphi \right) ds.$$

We then need another integration by parts to obtain that $R_1^{\varepsilon,\delta}\varphi = O(\sqrt{\varepsilon}\delta)$. Note that this additional integration by parts is required by the presence of a s without a coefficient $\sqrt{\varepsilon}$

in the integrand. We write

$$
R_1^{\varepsilon,\delta}\varphi = -\frac{\varepsilon}{(2i\mu^\flat)^2}\left[\mathrm{e}^{i\mu^\flat s^2 + i\sqrt{\varepsilon}s^3 f_3(s\sqrt{\varepsilon})}\left(\frac{1}{(1+s\sqrt{\varepsilon}f_4(s\sqrt{\varepsilon}))^2}\mathcal{Q}^\varepsilon(s\sqrt{\varepsilon})\mathrm{e}^{isL}L\varphi\right)\right]_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}}
$$
$$
+ \frac{\varepsilon}{(2i\mu^\flat)^2}\int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}}\mathrm{e}^{i\mu^\flat s^2 + i\sqrt{\varepsilon}s^3 f_3(s\sqrt{\varepsilon})}\frac{d}{ds}\left(\frac{1}{(1+s\sqrt{\varepsilon}f_4(s\sqrt{\varepsilon}))^2}\mathcal{Q}^\varepsilon(s\sqrt{\varepsilon})\mathrm{e}^{isL}L\varphi\right)ds
$$
$$
= O(\delta\sqrt{\varepsilon})
$$

Therefore, we are left with

$$
\mathcal{T}^\varepsilon = \sqrt{\varepsilon}\int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}}\mathrm{e}^{i\mu^\flat s^2 + i\sqrt{\varepsilon}s^3 f_3(s\sqrt{\varepsilon})}\mathcal{Q}^\varepsilon(s\sqrt{\varepsilon})\mathrm{e}^{isL}\,ds + O(\sqrt{\varepsilon}\delta).
$$

In the positive part of the integral, we perform the change of variable

$$
z = s(1 + \sqrt{\varepsilon}sf_3(s\sqrt{\varepsilon})/\mu^\flat)^{1/2}
$$

and observe that $s = z(1 + \sqrt{\varepsilon}zg_1(z\sqrt{\varepsilon}))$ and $\partial_s z = 1 + \sqrt{\varepsilon}zg_2(z\sqrt{\varepsilon})$ for some smooth bounded functions g_1 and g_2 with bounded derivatives. Note, that here again, we have used that $s\sqrt{\varepsilon}$ is small in the domain of the integral. Besides, there exists a family of operator $\widetilde{\mathcal{Q}}^\varepsilon(z)$ such that $\mathcal{Q}^\varepsilon(s\sqrt{\varepsilon}) = \widetilde{\mathcal{Q}}^\varepsilon(z\sqrt{\varepsilon})$ with $\widetilde{\mathcal{Q}}^\varepsilon(0) = \mathcal{Q}^\varepsilon(0)$. We deduce that there exists a bounded function of δ denoted by $b(\delta)$ such that

$$
\mathcal{T}^\varepsilon = \sqrt{\varepsilon}\int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}b(\delta)}\mathrm{e}^{i\mu^\flat z^2}\widetilde{\mathcal{Q}}^\varepsilon(z\sqrt{\varepsilon})\mathrm{e}^{iz(1+\sqrt{\varepsilon}zg_1(z\sqrt{\varepsilon}))L}\frac{dz}{1+\sqrt{\varepsilon}zg_2(z\sqrt{\varepsilon})}.
$$

A Taylor expansion allows to write

$$
\widetilde{\mathcal{Q}}^\varepsilon(z\sqrt{\varepsilon})\mathrm{e}^{iz(1+\sqrt{\varepsilon}zg_1(z\sqrt{\varepsilon}))L}\frac{1}{1+\sqrt{\varepsilon}zg_2(z\sqrt{\varepsilon})} = \widetilde{\mathcal{Q}}^\varepsilon(0) + \sqrt{\varepsilon}z(\widetilde{\mathcal{Q}}_1^\varepsilon(z\sqrt{\varepsilon}) + z\widetilde{\mathcal{Q}}_2^\varepsilon(z\sqrt{\varepsilon}))
$$
$$
= \mathcal{Q}^\varepsilon(0) + \sqrt{\varepsilon}z(\widetilde{\mathcal{Q}}_1^\varepsilon(z\sqrt{\varepsilon}) + z\widetilde{\mathcal{Q}}_2^\varepsilon(z\sqrt{\varepsilon}))
$$

for some smooth operator-valued maps $z \mapsto \widetilde{\mathcal{Q}}_j^\varepsilon(z\sqrt{\varepsilon})$ mapping $\mathcal{S}(\mathbb{R}^d)$ into itself, such that for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$ the family $(\widetilde{\mathcal{Q}}_j^\varepsilon(z\sqrt{\varepsilon})\varphi)_{\varepsilon>0}$ is bounded in $\Sigma_\varepsilon^k(\mathbb{R}^d)$. We obtain

$$
\mathcal{T}^\varepsilon = \sqrt{\varepsilon}\,\mathcal{Q}^\varepsilon(0)\int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}b(\delta)}\mathrm{e}^{i\mu^\flat z^2}\mathrm{e}^{izL}dz + \tilde{R}^{\varepsilon,\delta}
$$
$$
\text{with } \tilde{R}^{\varepsilon,\delta} = \varepsilon\int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}b(\delta)}z\,\mathrm{e}^{i\mu^\flat z^2}(\widetilde{\mathcal{Q}}_1^\varepsilon(z\sqrt{\varepsilon}) + z\widetilde{\mathcal{Q}}_2^\varepsilon(z\sqrt{\varepsilon}))\,dz.
$$

Arguing by integration by parts as previously, we obtain

$$\tilde{R}^{\varepsilon,\delta} = \varepsilon \left[\frac{1}{2i\mu^\flat} \mathrm{e}^{i\mu^\flat z^2} (\widetilde{\mathcal{Q}}_1^\varepsilon(z\sqrt{\varepsilon}) + z\widetilde{\mathcal{Q}}_2^\varepsilon(z\sqrt{\varepsilon})) \right]_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}b(\delta)}$$

$$- \frac{\varepsilon}{2i\mu^\flat} \int_{-\frac{\delta}{\sqrt{\varepsilon}}}^{+\frac{\delta}{\sqrt{\varepsilon}}b(\delta)} \mathrm{e}^{i\mu^\flat z^2} \frac{d}{dz}(\widetilde{\mathcal{Q}}_1^\varepsilon(z\sqrt{\varepsilon}) + z\widetilde{\mathcal{Q}}_2^\varepsilon(z\sqrt{\varepsilon}))\, dz = O(\sqrt{\varepsilon}\delta).$$

We deduce $\mathcal{T}^\varepsilon = \sqrt{\varepsilon}\, \mathcal{Q}^\varepsilon(0) \displaystyle\int_{-\frac{\delta}{\sqrt{\varepsilon}}b(\delta)}^{+\frac{\delta}{\sqrt{\varepsilon}}b(\delta)} \mathrm{e}^{i\mu^\flat s^2} \mathrm{e}^{isL}\, ds + O(\sqrt{\varepsilon}\delta)$ and it remains to pass to infin-

ity in the domain of the integral. For this, we set $m_\varepsilon = \frac{\delta}{\sqrt{\varepsilon}}b(\delta)$ and consider for $\varphi \in \mathcal{S}(\mathbb{R}^d)$,

$$\mathcal{G}_0^\varepsilon \varphi = \int_{m_\varepsilon}^{+\infty} \mathrm{e}^{i\mu^\flat s^2} \mathrm{e}^{isL} \varphi\, ds.$$

We make two successive integration by parts. We write in $\Sigma_k(\mathbb{R}^d)$,

$$\mathcal{G}_0^\varepsilon \varphi = \left[(2is\mu^\flat)^{-1} \mathrm{e}^{i\mu^\flat s^2} \mathrm{e}^{isL} \varphi \right]_{m_\varepsilon}^{+\infty} - \int_{m_\varepsilon}^{+\infty} \mathrm{e}^{i\mu^\flat s^2} \frac{d}{ds} \left(\frac{\mathrm{e}^{isL}\varphi}{2is\mu^\flat} \right) ds$$

$$= O(m_\varepsilon^{-1})\|\varphi\|_{\Sigma^k} - \int_{m_\varepsilon}^{+\infty} \mathrm{e}^{i\mu^\flat s^2} \frac{i\mathrm{e}^{isL} L\varphi}{2is\mu^\flat} ds + \int_{m_\varepsilon}^{+\infty} \mathrm{e}^{i\mu^\flat s^2} \frac{\mathrm{e}^{isL}\varphi}{2i\mu^\flat s^2} ds$$

$$= O(m_\varepsilon^{-1})\|\varphi\|_{\Sigma^k} - \left[(2is\mu^\flat)^{-2} \mathrm{e}^{i\mu^\flat s^2} i\mathrm{e}^{isL} L\varphi \right]_{m_\varepsilon}^{+\infty} + \int_{m_\varepsilon}^{+\infty} \mathrm{e}^{i\mu^\flat s^2} \frac{d}{ds} \left(\frac{i\mathrm{e}^{isL} L\varphi}{(2is\mu^\flat)^2} \right) ds$$

$$= O(m_\varepsilon^{-1}) \left(\|\varphi\|_{\Sigma^k} + \|L\varphi\|_{\Sigma^k} + \|L^2\varphi\|_{\Sigma^k} \right).$$

We deduce that $\mathcal{T}^\varepsilon = \sqrt{\varepsilon}\, \mathcal{Q}^\varepsilon(0) \displaystyle\int_{-\infty}^{+\infty} \mathrm{e}^{i\mu^\flat s^2} \mathrm{e}^{isL}\, ds + O(\sqrt{\varepsilon}\delta) + O(\varepsilon\delta^{-1})$. $\qquad\square$

Remark 5.6. Note that the previous remainder terms could again by transformed by integration by parts. This implies that $\mathcal{T}^\varepsilon \varphi$ has an asymptotic expansion in $\sqrt{\varepsilon}$ and δ at any order and each term of the expansion is a Schwartz function.

5.4. **Proof of Theorem 3.8 and Corollary 3.9.** We now complete the proof of Theorem 3.8. We choose $\delta = \varepsilon^{2/9}$, and ε is small enough so that $\varepsilon \leq |t - t^\flat|^{9/2}$. Then, one has $|t - t^\flat| \geq \delta$. If $t \in [t_0, t^\flat - \delta]$, then Proposition 4.1 gives the result. If $t \in [t^\flat + \delta, t_0 + T]$, then one combines Proposition 4.1 between times $s_1 = t^\flat + \delta$ and $s_2 = t$ with Proposition 5.1. In summary, we obtain an error estimate of order $\varepsilon\delta^{-2} = \varepsilon^{1/3}\delta = \varepsilon^{5/9}$.

Corollary 3.9 comes from Theorem 3.8 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 $\widehat{T}^\varepsilon$

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

the semi-classical scaling operator Λ_ε

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

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 $a \in \mathcal{C}^\infty(\mathbb{R}^{2d})$*

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

(48) $$\mathcal{WP}_{z+z'}^\varepsilon = \mathrm{e}^{-\frac{i}{\varepsilon}p\cdot q'}\, \mathcal{WP}_z^\varepsilon\, \Lambda_\varepsilon^{-1} \mathcal{WP}_{z'}^\varepsilon,$$

(49) $$\mathrm{op}_\varepsilon^w(a)\mathcal{WP}_z^\varepsilon = \mathcal{WP}_z^\varepsilon\, \mathrm{op}_1^w(a_{\varepsilon,z}),$$

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

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

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

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

This yields

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

For the commutation property we compute

$$\mathrm{e}^{-\frac{i}{\varepsilon}p\cdot q'}\mathcal{WP}_z^\varepsilon\Lambda_\varepsilon^{-1}\mathcal{WP}_{z'}^\varepsilon\varphi(x) = \mathrm{e}^{-\frac{i}{\varepsilon}p\cdot q'}\mathcal{WP}_z^\varepsilon \mathrm{e}^{\frac{i}{\varepsilon}p'\cdot(\sqrt{\varepsilon}x - q')}\varphi\left(\tfrac{\sqrt{\varepsilon}x - q'}{\sqrt{\varepsilon}}\right)$$

$$= \mathrm{e}^{-\frac{i}{\varepsilon}p\cdot q'}\varepsilon^{-d/4}\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)}\mathrm{e}^{\frac{i}{\varepsilon}p'\cdot(x-q-q')}\varphi\left(\tfrac{x-q-q'}{\sqrt{\varepsilon}}\right) = \mathcal{WP}_{z+z'}^\varepsilon\varphi(x).$$

Moreover,

$$\mathcal{WP}_z^\varepsilon\, \mathrm{op}_1^w(a_{\varepsilon,z})\varphi(x)$$

$$= \varepsilon^{-d/4}\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)}(2\pi)^{-d}\int_{\mathbb{R}^{2d}} a\left(\tfrac{\sqrt{\varepsilon}}{2}\left(\tfrac{x-q}{\sqrt{\varepsilon}} + y\right) + q, \sqrt{\varepsilon}\xi + p\right)\mathrm{e}^{i\xi\cdot((x-q)/\sqrt{\varepsilon}-y)}\varphi(y)\,dy\,d\xi$$

$$= \varepsilon^{-d/4}\mathrm{e}^{\frac{i}{\varepsilon}p\cdot(x-q)}(2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} a\left(\tfrac{1}{2}(x + y') + q, \xi'\right)\mathrm{e}^{\frac{i}{\varepsilon}(\xi'-p)\cdot(x-y')}\varphi\left(\tfrac{y'-q}{\sqrt{\varepsilon}}\right)\,dy'\,d\xi'$$

$$= \mathrm{op}_\varepsilon^w(a)\, \mathcal{WP}_z^\varepsilon\varphi(x).$$

$\square$

The intertwining property (49), that relates the wave packet transform with Weyl quantization, allows to describe the localisation properties of wave packets as follows.

Remark A.2 (Localisation on scale $\sqrt{\varepsilon}$). Let $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^{2d})$ be a cut-off function such that $\chi = 1$ close to 0 and $0 \le \chi \le 1$. Define for $R > 0$, $\chi_R(z) = \chi(R^{-1}z)$ for all $z \in \mathbb{R}^{2d}$. Then, for any $k, N \in \mathbb{N}$ and any Schwartz function $\varphi \in \mathcal{S}(\mathbb{R}^d)$

$$\|\mathrm{op}_1^w(1 - \chi_R)\varphi\|_{\Sigma_1^k} \le CR^{-N},$$

where the constant $C > 0$ depends on k, N and the norm of φ in Σ_1^{k+N}. Decomposing a wave packet as

$$\mathcal{WP}_0^\varepsilon \varphi = \mathcal{WP}_0^\varepsilon \, \mathrm{op}_1^w(\chi_R)\varphi + \mathcal{WP}_0^\varepsilon \, \mathrm{op}_1^w(1 - \chi_R)\varphi,$$

the combination of the above estimate with equation (49) and the continuity of the wave packet transform as a mapping from Σ_1^k to Σ_ε^k yields

$$(50) \qquad \left\| \mathcal{WP}_0^\varepsilon \varphi - \mathrm{op}_\varepsilon^w(\chi_{R\sqrt{\varepsilon}})\mathcal{WP}_0^\varepsilon \varphi \right\|_{\Sigma_\varepsilon^k} \le CR^{-N}.$$

Appendix B. Algebraic properties of the eigenprojectors

We consider a smooth eigenvalue $h(t, z)$ of a matrix-valued Hamiltonian $H(t, z)$, associated with a smooth eigenprojector $\Pi(t, z)$ so that $H = h\Pi + h^\perp \Pi^\perp$. We emphasize that, in this section, we just assume smoothness of the projector and make no gap assumption. Let us project the solution of the Hamiltonian system (1) to the eigenspace and consider the function $\tilde{w}^\varepsilon(t) = \widehat{\Pi}\psi^\varepsilon(t)$. We have

$$i\varepsilon \partial_t \tilde{w}^\varepsilon(t) = \left(i\varepsilon \widehat{\partial_t \Pi} + \widehat{\Pi}\widehat{H} \right) \psi^\varepsilon(t),$$

and by symbolic calculus

$$\widehat{\Pi}\widehat{H} = \widehat{h\Pi} + \frac{\varepsilon}{2i}\widehat{\{\Pi, H\}} + O(\varepsilon^2) = \widehat{h\Pi} - \frac{\varepsilon}{2i}\widehat{\{h, \Pi\}} + \frac{\varepsilon}{2i}\widehat{\{\Pi, H\}} + O(\varepsilon^2),$$

where the order ε^2 remainder will be given a precise meaning in Lemma B.2 and Lemma B.5 below. Therefore, if we introduce the matrix

$$(51) \qquad B = -2\partial_t \Pi - \{h, \Pi\} + \{\Pi, H\},$$

then we may write

$$i\varepsilon \partial_t \tilde{w}^\varepsilon(t) = \widehat{h}\tilde{w}^\varepsilon(t) + \frac{\varepsilon}{2i}\widehat{B}\psi^\varepsilon(t) + O(\varepsilon^2).$$

Let us examine the algebraic properties of the first order contribution B in more detail.

Lemma B.1. *Consider a Hermitian matrix $H = h\Pi + h^\perp\Pi^\perp$ with eigenvalues $h, h^\perp$ and corresponding eigenprojectors $\Pi, \Pi^\perp$. Then, the matrix $\{\Pi, \Pi\}$ is skew-symmetric and diagonal,*

$$\Pi^\perp\{\Pi, \Pi\}\Pi = \Pi^\perp\{\Pi, \Pi\}\Pi = 0.$$

The matrix B defined in (51) satisfies

$$B\Pi = -2(\Omega + K) = 2i\Theta\Pi \;\; and \;\; \Pi^\perp B \Pi^\perp = (h - h^\perp)\Pi^\perp\{\Pi, \Pi\}\Pi^\perp,$$

where the matrices Ω, K, and Θ have been introduced in (17), (18), and (19). Moreover, the matrix Ω is skew-symmetric and Θ self-adjoint.

Proof. We use the relation $\{\mathcal{A}, \mathcal{BC}\} - \{\mathcal{AB}, \mathcal{C}\} = \{\mathcal{A}, \mathcal{B}\}\mathcal{C} - \mathcal{A}\{\mathcal{B}, \mathcal{C}\}.$ and apply it to $\mathcal{A} = \mathcal{B} = \mathcal{C} = \Pi$. Since $\Pi^2 = \Pi$, we obtain $0 = \{\Pi, \Pi\}\Pi - \Pi\{\Pi, \Pi\}$ and therefore

$$\Pi^\perp\{\Pi, \Pi\}\Pi = \Pi\{\Pi, \Pi\}\Pi^\perp = 0.$$

Besides, by the definition of the Poisson bracket, we have $\{\Pi, \Pi\}^* = -\{\Pi, \Pi\}$, so that $\{\Pi, \Pi\}$ and $\Omega = -\frac{1}{2}(h - h^\perp)\Pi\{\Pi, \Pi\}\Pi$ are skew-symmetric. In view of

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

$$\{h, \Pi\} = \{h, \Pi\}\Pi + \{h, \Pi\}\Pi^\perp,$$

we obtain that

$$B = -2\partial_t\Pi - \{h, \Pi\} + \{\Pi, H\}$$
$$= -2\partial_t\Pi + (h - h^\perp)\{\Pi, \Pi\} - 2\{h, \Pi\}\Pi - \{h + h^\perp, \Pi\}\Pi^\perp.$$

Hence,

$$B\Pi = -2\Pi^\perp(\partial_t\Pi + \{h, \Pi\})\Pi + (h - h^\perp)\Pi\{\Pi, \Pi\}\Pi = -2(K + \Omega)$$

$$\text{and } \Pi^\perp B\Pi^\perp = (h - h^\perp)\Pi^\perp\{\Pi, \Pi\}\Pi^\perp.$$

The matrix $\Theta = i\Omega + i(K - K^*)$ is hermitian, since $\Theta^* = -i\Omega^* - i(K^* - K) = \Theta$. It also satisfies $2i\Theta\Pi = 2i(i\Omega + iK)\Pi = B\Pi$. $\qquad\square$

Decomposing the matrix $B = B\Pi + B\Pi^\perp$, we may view the contribution associated with the projector Π as an effective dynamical correction to the eigenvalue h. We obtain the following:

Lemma B.2. *Let $H = h\Pi + h^\perp\Pi^\perp$ be a smooth matrix-valued Hamiltonian with smooth eigenvalues $h, h^\perp$ and smooth eigenprojectors $\Pi, \Pi^\perp$. Then, there exists a smooth matrix-valued symbol R^ε such that*

$$(52) \qquad \widehat{\Pi}(i\varepsilon\partial_t - \widehat{H}) = (i\varepsilon\partial_t - \widehat{h} - \varepsilon\widehat{\Theta})\widehat{\Pi} + \frac{\varepsilon}{2i}\widehat{B\Pi^\perp}\widehat{\Pi}^\perp + \varepsilon^2\widehat{R}^\varepsilon,$$

where the matrices B and Θ have been defined in (51) and (19), respectively. If the Hamiltonian and its eigenvalues are of subquadratic growth (7), while the projectors grow at most polynomially (26), then for all $k \in \mathbb{N}$ there exist $C_k > 0$ and $\ell \in \mathbb{N}$ such that

$$\sup_{t\in[t_0, t_0+T]} \|\widehat{R}^\varepsilon(t)\varphi\|_{\Sigma_\varepsilon^k} \le C_k\|\varphi\|_{\Sigma_\varepsilon^\ell} \quad \forall\varphi \in \Sigma_\varepsilon^k(\mathbb{R}^d).$$

Proof. We write

$$\widehat{\Pi}(i\varepsilon\partial_t - \widehat{H}) = (i\varepsilon\partial_t - \widehat{h})\widehat{\Pi} - i\varepsilon\widehat{\partial_t\Pi} + \widehat{h}\widehat{\Pi} - \widehat{\Pi}\widehat{H}.$$

The symbolic calculus gives

$$\widehat{h}\widehat{\Pi} - \widehat{\Pi}\widehat{H} = \frac{\varepsilon}{2i}(\{h, \Pi\} - \{\Pi, H\}) + \varepsilon^2 R^\varepsilon,$$

where the remainder $\widehat{R}^\varepsilon(t)$ satisfies the claimed estimate due to the growth assumptions on the symbols h, H and Π. In view of Lemma B.1, we have

$$-i\partial_t\Pi + \frac{1}{2i}\left(\{h,\Pi\} - \{\Pi,H\}\right) = \Theta\Pi + \frac{1}{2i}B\Pi^\perp,$$

which concludes our proof. $\square$

We note that for the projected solution $\tilde{w}^\varepsilon(t) = \widehat{\Pi}\psi^\varepsilon(t)$, equation (52) implies an evolution equation of the form

$$i\varepsilon\partial_t\tilde{w}^\varepsilon(t) = (\widehat{h} + \varepsilon\widehat{\Theta})\tilde{w}^\varepsilon(t) - \frac{\varepsilon}{2i}\widehat{B\Pi^\perp}\widehat{\Pi}^\perp\psi^\varepsilon(t) + O(\varepsilon^2).$$

In a next step we use the matrix B for introducing the first order super-adiabatic correction of the eigenprojector Π, following ideas from [34, 9, 2, 27, 28, 29, 36].

Definition B.3. *We assume that H is a smooth Hermitian matrix that has two smooth eigenvalues h and $h^\perp$ and smooth eigenprojectors Π and $\Pi^\perp$, that is, $H = h\Pi + h^\perp\Pi^\perp$. The first super-adiabatic corrector of Π is the hermitian matrix $\mathbb{P} = \mathbb{P}^*$ defined by*

$$\Pi\mathbb{P}\Pi^\perp = \frac{i}{h - h^\perp}\Pi\left(\partial_t\Pi + \frac{1}{2}\{h + h^\perp,\Pi\}\right)\Pi^\perp,$$

$$\Pi^\perp\mathbb{P}\Pi = -\frac{i}{h - h^\perp}\Pi^\perp\left(\partial_t\Pi + \frac{1}{2}\{h + h^\perp,\Pi\}\right)\Pi,$$

$$\Pi\mathbb{P}\Pi = -\frac{1}{2i}\Pi\{\Pi,\Pi\}\Pi, \qquad \Pi^\perp\mathbb{P}\Pi^\perp = \frac{1}{2i}\Pi^\perp\{\Pi,\Pi\}\Pi^\perp.$$

Note that one has $\mathbb{P}\Pi^\perp = \frac{1}{2i}(h - h^\perp)^{-1}B\Pi^\perp$ and $\mathbb{P}\Pi = -\frac{1}{2i}(h - h^\perp)^{-1}B\Pi$.

Note that the diagonal part of the matrix $\mathbb{P}$ is smooth, while the off-diagonal part of $\mathbb{P}$ is singular on the crossing set $\Upsilon = \{f = 0\}$. Besides, for all $\beta \in \mathbb{N}^{2d}$ and $R > 0$,

$$(53) \qquad \exists C_{\beta,R} > 0, \quad \forall z \in B(0,R) \cap \{f(t,z) > \delta\}, \quad \forall t \in \mathbb{R}, \quad \|\partial_z^\beta\mathbb{P}(t,z)\| \le C_{\beta,R}\,\delta^{|\beta|+1}.$$

The main interest in the corrector $\mathbb{P}$ comes from the following relations:

Lemma B.4. *With the assumptions of Definition B.3, the corrector matrix $\mathbb{P}$ satisfies*

$$(54) \qquad [H,\mathbb{P}] = i\partial_t\Pi - \frac{1}{2i}(\{H,\Pi\} - \{\Pi,H\}) \quad and \quad \mathbb{P}\Pi + \Pi\mathbb{P} = \mathbb{P} - \frac{1}{2i}\{\Pi,\Pi\},$$

as well as

$$i\partial_t\Pi + \mathbb{P}(H - h) + \frac{1}{2i}\{\Pi, H + h\} = \Theta\Pi \quad and \quad i(\partial_t\Pi + \{h,\Pi\}) = [\Theta,\Pi],$$

where the matrix Θ is given by (19).

Proof. Since H is acting as a scalar on $\mathrm{Ran}\Pi$ and $\mathrm{Ran}\Pi^\perp$, we have

$$[H,\mathbb{P}] = [H, \Pi\mathbb{P}\Pi^\perp + \Pi^\perp\mathbb{P}\Pi] = (h - h^\perp)\Pi\mathbb{P}\Pi^\perp + (h^\perp - h)\Pi^\perp\mathbb{P}\Pi$$
$$= i(\partial_t\Pi + \tfrac{1}{2}\{h + h^\perp,\Pi\}).$$

Since
$$\{H, \Pi\} - \{\Pi, H\} = \Pi\{h, \Pi\} + \Pi^\perp\{h^\perp, \Pi\} - \{\Pi, h\}\Pi - \{\Pi, h^\perp\}\Pi^\perp = \{h + h^\perp, \Pi\},$$

we have proven the first equation. For the second equation, we calculate
$$\mathbb{P}\Pi + \Pi\mathbb{P} = 2\Pi\mathbb{P}\Pi + \Pi^\perp\mathbb{P}\Pi + \Pi\mathbb{P}\Pi^\perp = \mathbb{P} + \Pi\mathbb{P}\Pi - \Pi^\perp\mathbb{P}\Pi^\perp = \mathbb{P} - \tfrac{1}{2i}\{\Pi, \Pi\},$$

where we have used that $\{\Pi, \Pi\}$ is diagonal. For the first relation with Θ, we write $H - h = (h^\perp - h)\Pi^\perp$ and obtain

$$\mathbb{P}(H - h) = (h^\perp - h)\mathbb{P}\Pi^\perp = -\frac{1}{2i}B\Pi^\perp.$$

Therefore, by Lemma B.1,

$$i\partial_t\Pi + \mathbb{P}(H - h) + \frac{1}{2i}\{\Pi, H + h\} = \frac{1}{2i}B - \frac{1}{2i}B\Pi^\perp = \Theta\Pi.$$

For the commutator of Θ and Π, we have

$$[\Theta, \Pi] = i[\Omega, \Pi] + i[K, \Pi] - i[K^*, \Pi]$$

$$= i\Pi^\perp(\partial_t\Pi + \{h, \Pi\})\Pi + i\Pi^\perp(\partial_t\Pi + \{h, \Pi\})\Pi = i(\partial_t\Pi + \{h, \Pi\}).$$

$$\square$$

If the crossing set Υ were empty and all the symbols in consideration were bounded, the relations of Lemma B.4 would imply that setting $\Pi^\varepsilon = \Pi + \varepsilon\mathbb{P}$, then $\widehat{\Pi^\varepsilon}$ would be "better" than $\widehat{\Pi}$ in terms of being an eigenprojector of $\widehat{H}$: in $\mathcal{L}(L^2(\mathbb{R}^d))$,

$$\widehat{\Pi^\varepsilon}\widehat{\Pi^\varepsilon} = \widehat{\Pi^\varepsilon} + O(\varepsilon^2) \quad \text{and} \quad \widehat{\Pi^\varepsilon}(-i\varepsilon\partial_t + \widehat{H}) = (-i\varepsilon\partial_t + \widehat{h} + \varepsilon\widehat{\Theta})\widehat{\Pi^\varepsilon} + O(\varepsilon^2),$$

while the estimate would be only $O(\varepsilon)$ when using the uncorrected $\widehat{\Pi}$. However, because the symbols we consider are smooth only outside Υ, we need to use cut-off functions to correctly state such properties.

Lemma B.5. *Let I be an interval of $\mathbb{R}$ and $\chi^\delta, \tilde{\chi}^\delta \in \mathcal{C}(I, \mathcal{C}_0^\infty(\mathbb{R}^{2d}))$ be two cut-off functions that satisfy:*

(1) *For any $t \in I$ and z in the support of $\chi^\delta(t)$ and $\tilde{\chi}^\delta(t)$ we have $|(h - h^\perp)(t, z)| > \delta$.*

(2) *The functions χ^δ and $\tilde{\chi}^\delta$ satisfy*
$$\partial_t\chi^\delta + \left\{h, \chi^\delta\right\} = 0, \ \ \partial_t\tilde{\chi}^\delta + \left\{h, \tilde{\chi}^\delta\right\} = 0.$$

(3) *The functions $\tilde{\chi}^\delta$ are supported in $\{\chi^\delta = 1\}$.*

Let $k \in \mathbb{N}$. Then, we have for all $t \in I$ in Σ_ε^k,

$$\widehat{\tilde{\chi}^\delta}\left(-i\varepsilon\partial_t + (\hat{h} + \varepsilon\widehat{\Theta})\right)\widehat{\chi^\delta\Pi^\varepsilon} = \widehat{\tilde{\chi}^\delta}\widehat{\chi^\delta\Pi^\varepsilon}(-i\varepsilon\partial_t + \widehat{H}) + O(\varepsilon^2\delta^{-2}).$$

In particular, the function $w^\varepsilon(t) = \widehat{\tilde{\chi}^\delta}\widehat{\chi^\delta\Pi^\varepsilon}\psi^\varepsilon(t)$ satisfies for all $t \in I$ in Σ_ε^k,

$$i\varepsilon\partial_t w^\varepsilon(t) = (\hat{h} + \varepsilon\widehat{\Theta})w^\varepsilon(t) + O(\varepsilon^2\delta^{-2}).$$

Proof. We write

$$\widehat{\chi^\delta \Pi^\varepsilon}(-i\varepsilon\partial_t + \widehat{H}) = \mathrm{op}_\varepsilon(\chi^\delta h\Pi) + \varepsilon\mathrm{op}_\varepsilon(\chi^\delta \mathbb{P}H + \frac{1}{2i}\{\chi^\delta\Pi, H\}) - \widehat{\chi^\delta\Pi^\varepsilon}(i\varepsilon\partial_t) + \varepsilon^2 \widehat{R^\delta(t)},$$

where the remainder $R^\delta(t)$ depends on first order derivatives of $\chi^\delta\mathbb{P}$ and H as well as second order derivatives of $\chi^\delta\Pi$ and H. Hence, $\widehat{R^\delta}(t) = O(\delta^{-2})$. Next, we write

$$\mathrm{op}_\varepsilon(\chi^\delta h\Pi) - \widehat{\chi^\delta\Pi^\varepsilon}(i\varepsilon\partial_t) = \mathrm{op}_\varepsilon(h)\mathrm{op}_\varepsilon(\chi^\delta\Pi) - \frac{\varepsilon}{2i}\mathrm{op}_\varepsilon(\{h, \chi^\delta\Pi\})$$

$$- (i\varepsilon\partial_t)\widehat{\chi^\delta\Pi^\varepsilon} + i\varepsilon\mathrm{op}_\varepsilon(\partial_t(\chi^\delta\Pi^\varepsilon)) + \varepsilon^2 \widehat{\rho_2^\delta(t)},$$

where $\rho_2^\delta(t)$ depends linearly on second derivatives of $\chi^\delta\Pi$ and h. By Lemma B.4, one part of the first order contributions can be combined according to

$$i\partial_t\Pi + \mathbb{P}(H - h) + \frac{1}{2i}\{\Pi, H + h\} = \Theta\Pi.$$

All this implies

$$\widehat{\chi^\delta\Pi^\varepsilon}(-i\varepsilon\partial_t + \widehat{H}) = (-i\varepsilon\partial_t + \mathrm{op}_\varepsilon(h + \varepsilon\Theta))\mathrm{op}_\varepsilon(\chi^\delta\Pi^\varepsilon)$$

$$+ \varepsilon\mathrm{op}_\varepsilon(\rho_1^\delta(t)) + \varepsilon^2\mathrm{op}_\varepsilon(\rho_2^\delta(t) + R^\delta(t)),$$

where the remainder is given by

$$\rho_2^\delta(t) = \Pi(i\partial_t\chi^\delta + \frac{1}{2i}\{\chi^\delta, H + h\})$$

$$= \Pi(i\partial_t\chi^\delta + \frac{1}{i}\{\chi^\delta, h\} + \frac{1}{2i}(h - h^\perp)\{\chi^\delta, \Pi\})$$

$$= \frac{1}{2i}(h - h^\perp)\Pi\{\chi^\delta, \Pi\}\Pi^\perp,$$

since $\partial_t\chi^\delta + \{h, \chi^\delta\} = 0$. We note that $\rho_1^\delta(t)$ and $\rho_2^\delta(t)$ are smooth symbols, depending linearly on derivatives of χ^δ and thus are 0 on the support of $\tilde{\chi}^\delta$. The latter observation implies the first result. For the function $w^\varepsilon(t)$ we then have

$$(i\varepsilon\partial_t - \hat{h} - \varepsilon\widehat{\Theta})w^\varepsilon(t)$$

$$= \widehat{\tilde{\chi}^\delta}(i\varepsilon\partial_t - \hat{h} - \varepsilon\widehat{\Theta})\widehat{\chi^\delta\Pi^\varepsilon}\psi^\varepsilon(t) + [(i\varepsilon\partial_t - \hat{h} - \varepsilon\widehat{\Theta}), \widehat{\tilde{\chi}^\delta}]\widehat{\chi^\delta\Pi^\varepsilon}\psi^\varepsilon(t)$$

$$= \widehat{\tilde{\chi}^\delta}\widehat{\chi^\delta\Pi^\varepsilon}(i\varepsilon\partial_t - \widehat{H})\psi^\varepsilon(t) + [(i\varepsilon\partial_t - \hat{h} - \varepsilon\widehat{\Theta}), \widehat{\tilde{\chi}^\delta}]\widehat{\chi^\delta\Pi^\varepsilon}\psi^\varepsilon(t) + \varepsilon^2\widehat{R^\delta(t)}.$$

Moreover, since $\partial_t\tilde{\chi}^\delta + \{h, \tilde{\chi}^\delta\} = 0$, we have

$$[(i\varepsilon\partial_t - \hat{h} - \varepsilon\widehat{\Theta}), \widehat{\tilde{\chi}^\delta}] = \varepsilon^3\widehat{r_3^\delta(t)} + \varepsilon^2\widehat{r_1^\delta(t)},$$

where the first part of the remainder $r_3^\delta(t)$ depends on third derivatives of h and $\tilde{\chi}^\delta$, while the second part $r_1^\delta(t)$ depends on first derivatives of Θ and $\tilde{\chi}^\delta$. Since $\delta \gg \sqrt{\varepsilon}$, we have

$$[(i\varepsilon\partial_t - \hat{h} - \varepsilon\widehat{\Theta}), \widehat{\tilde{\chi}^\delta}] = O(\varepsilon^2\delta^{-1}).$$

Using $(i\varepsilon\partial_t - \widehat{H})\psi^\varepsilon(t) = 0$, we obtain the equation for $w^\varepsilon(t)$. $\qquad\square$

Appendix C. Parallel transport

We prove here Proposition 3.1 that provides the time-dependent eigenvector $\vec{V}(t,z)$ defined by parallel transport. We adapt the proof of [4, Proposition C.1] to account for the matrix $\Omega(t,z)$, noting that we only require that $\Omega(t,z)$ is a skew-symmetric matrix mapping into the range of $\Pi(t,z)$.

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

$$
\begin{aligned}
\partial_t Y(t,z) &= \partial_t \vec{V}(t,\Phi_h^{t,t_0}(z)) + J\partial_z h(\Phi_h^{t,t_0}(z))V(t,\Phi_h^{t,t_0}(z)) \\
&= \Omega(t,\Phi_h^{t,t_0}(z))Y(t,z) + K(t,\Phi_h^{t,t_0}(z))Y(t,z).
\end{aligned}
$$
(55)

In particular, since $\Omega(t,z)$ maps into the range of $\Pi(t,z)$,

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

We now start proving that for $z \in U$, $\Pi(t,\Phi_h^{t,t_0}(z))Y(t,z) = Y(t,z)$, or equivalently that

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

is constant and equal to 0. We compute

$$
\partial_t Z(t,z) = \left(-\partial_t \Pi(t,\Phi_h^{t,t_0}(z)) - J\partial_z h(\Phi_h^{t,t_0}(z))\partial_z \Pi(t,\Phi_h^{t,t_0}(z)) + K(t,\Phi_h^{t,t_0}(z)) \right) Y(t,z).
$$

We recall that $K = (\mathbb{I} - \Pi)(\partial_t \Pi + \{h,\Pi\})\Pi$. Since all derivatives of the projector are off-diagonal, we have

$$
-\partial_t \Pi - \{h,\Pi\} + K = -\Pi\left(\partial_t \Pi + \{h,\Pi\}\right)\Pi^\perp
$$

and therefore

$$
\partial_t Z(t,z) = -\Pi(t,\Phi_h^{t,t_0}(z))\left(\partial_t \Pi(t,\Phi_h^{t,t_0}(z)) + J\partial_z h(\Phi_h^{t,t_0}(z))\partial_z \Pi(t,\Phi_h^{t,t_0}(z)) \right) Z(t,z).
$$

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 $Y(t,z) \in \operatorname{Ran}\Pi(t,\Phi_h^{t,t_0}(z))$.

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

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

Therefore, $\|Y(t,z)\|_{\mathbb{C}^N} = 1$. $\qquad\square$

Remark C.1 (Polynomial growth of the eigenvector). The above proof shows that the time-evolution of $Y(t,z) = \vec{V}(t,\Phi_h^{t,t_0}(z))$ is generated by a norm-conserving evolution operator, that is, $Y(t) = \mathcal{L}(t,t_0)Y(t_0)$. This observation allows to literally repeat the inductive argument in the proof of [4, Proposition C.1] for inferring from a polynomial bound on the

projector $\Pi(t, z)$ a polynomial bound for the eigenvector $\vec{V}(t, z)$. Indeed, if (26) holds for $\Pi(t, z)$, then for all $T > 0$ and $\beta \in \mathbb{N}_0^{2d+1}$ there exists a constant $c_{\beta,T} > 0$ such that

$$\sup_{t \in [t_0, t_0+T], |z| \geq r_0} \|\partial_{t,z}^{\beta} \vec{V}(t, z)\| \leq c_{\beta,T} \langle z \rangle^{|\beta|(1+n_0)}.$$

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

Lemma D.1. *Let Λ and ζ be defined as*

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

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

We have

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

(58) $$\Lambda(0) = \dot{\Lambda}(0) = 0,$$

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

In particular, we have

$$\frac{1}{2}(\ddot{\Lambda}(0) - \dot{p}(0) \cdot \dot{q}(0))$$

$$= \frac{1}{2}\left(\partial_t(h_2 - h_1) - \partial_q h_2 \cdot \partial_p(h_2 - h_1) + \partial_p h_1 \cdot \partial_q(h_2 - h_1) + \partial_p(h_2 - h_1) \cdot \partial_q(h_2 - h_1)\right)$$

$$= \frac{1}{2}\left(\partial_t(h_2 - h_1) - \partial_q h_1 \cdot \partial_p(h_2 - h_1) + \partial_p h_1 \cdot \partial_q(h_2 - h_1)\right)$$

$$= \frac{1}{2}\left(\partial_t(h_2 - h_1) + \left\{\frac{h_1 + h_2}{2}, h_2 - h_1\right\}\right)$$

which yields that (46) is consistent with (33).

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 :

(60)

$$\Phi_h^{t,t_0}(z) = z + (t - t_0)J\partial_z h(t_0, z) + \frac{(t - t_0)^2}{2}\left(J\partial_{t,z}^2 h(t_0, z) + J\partial_{z,z}^2 h(t_0, z)J\partial_z h(t_0, z)\right)$$
$$+ O(|t - t_0|^3).$$

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

$$\Phi_1^{t^\flat + \sigma, t^\flat}(z^\flat) = z^\flat + \sigma J\partial_z h_1 + \frac{\sigma^2}{2}\left(J\partial_{t,z}^2 h_1 + J\partial_{z,z}^2 h_1 J\partial_z h_1\right) + O(|\sigma|^3),$$

$$\zeta(t) = \Phi_1^{t^\flat + \sigma, t^\flat}(z^\flat) - \sigma J\partial_z h_2(t^\flat + \sigma, \Phi_1^{t^\flat + \sigma, t^\flat}(z^\flat)) + \frac{\sigma^2}{2}\left(J\partial_{t,z}^2 h_2 + J\partial_{z,z}^2 h_2 J\partial_z h_2\right) + O(|\sigma|^3).$$

We deduce

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

and, for further use, the relation

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

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

We continue with the function Λ (defined in (56)) and we use Taylor expansion of the actions for general Hamiltonian h. In view of (9) and (60), we have (omitting the argument (t_0, z_0) in the terms of the form $\partial^\alpha h(t_0, z_0)$)

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

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 $(t^\flat, z^\flat)$)

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

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

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

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

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

As a consequence,

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

Combining with (62), 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 (59).

$\square$

APPENDIX E. THE OPERATORS $\mathcal{T}_{\mu,\alpha,\beta}$

We study here the operators $\mathcal{T}_{\mu,\alpha,\beta}$ that are defined in (28) for $(\mu, \alpha, \beta) \in \mathbb{R}^{2d+1}$. An explicit computation gives the following useful connection with the Fourier transform

(63) $$\mathcal{F}\mathcal{T}_{\mu,\alpha,\beta} = \mathcal{T}_{\mu+\alpha\cdot\beta,\beta,-\alpha}\mathcal{F}.$$

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:

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

(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*

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

where $\Phi_{\alpha,\beta}$ satisfies (34) *and*

(65)
$$\Gamma_{\mu,\alpha,\beta,\Gamma} = \Gamma - \frac{(\beta - \Gamma\alpha) \otimes (\beta - \Gamma\alpha)}{2\mu - \alpha \cdot \beta + \alpha \cdot \Gamma\alpha}.$$

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 (29) and (28). Indeed, when $\mu \neq 0$, equation (64) is an application of relation (28) 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:

(66)
$$\int_{-\infty}^{+\infty} e^{is^2\mu} e^{is\tau} ds = \sqrt{\frac{2\pi}{i\mu}}\,e^{\frac{\tau^2}{4i\mu}}, \quad \text{with } \arg(i\mu) \in\,]-\pi,\pi[.$$

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

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

Similar formulas can be obtained when $\beta \neq 0$ using (63). Let us first assume $\alpha \cdot \beta = 0$.

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

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

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

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 [6], 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 (34). 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

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

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 (65). 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 (66) 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 (65). $\qquad\square$

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LAMA, UMR CNRS 8050, Université Paris EST, 61, avenue du Général de Gaulle, 94010 Créteil Cedex, France
  E-mail address: Clotilde.Fermanian@u-pec.fr

Zentrum Mathematik - M8 Technische Universität München 85747 Garching bei München, Germany
  E-mail address: classer@ma.tum.de

Laboratoire de mathématiques Jean Leray UMR 6629 du CNRS Université de Nantes 2, rue de la Houssinière 44322 Nantes Cedex 3, France
  E-mail address: didier.robert@univ-nantes.fr