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PROPAGATION OF COHERENT STATES THROUGH CONICAL INTERSECTIONS

CLOTILDE FERMANIAN KAMMERER, STEPHANIE GAMBLE, AND LYSIANNE HARI

ABSTRACT. In this paper, we analyze the propagation of a wave packet through a conical intersection. This question has been addressed for Gaussian wave packets in the 90s by George Hagedorn and we consider here a more general setting. We focus on the case of Schrödinger equation but our methods are general enough to be adapted to systems presenting codimension 2 crossings and to codimension 3 ones with specific geometric conditions. Our main Theorem gives explicit transition formulas for the profiles when passing through a conical crossing point, including precise computation of the transformation of the phase. Its proof is based on a normal form approach combined with the use of superadiabatic projectors and the analysis of their degeneracy close to the crossing.

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1. INTRODUCTION

We consider a system of two Schrödinger equations coupled by a matrix-valued potential

$$(1) \quad i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi^\varepsilon + V(x) \psi^\varepsilon, \quad \psi^\varepsilon|_{t=t_0} = \psi_0^\varepsilon$$

where ψ_0^ε is a bounded family in $L^2(\mathbb{R}^d, \mathbb{C}^2)$, and $V \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C}^{2,2})$ is a self-adjoint matrix that we assume to be subquadratic: $\|\cdot\|_{\mathbb{C}^{2,2}}$ denotes a norm in the space of matrices $\mathbb{C}^{2,2}$, the matrix V satisfies

$$(2) \quad \forall \gamma \in \mathbb{N}^d, \quad |\gamma| \geq 2, \quad \exists c_\gamma > 0, \quad \sup_{x \in \mathbb{R}^d} \|\partial_x^\gamma V(x)\|_{\mathbb{C}^{2,2}} \leq c_\gamma.$$

These assumptions guarantee the existence of solutions to equation (1) in $L^2(\mathbb{R}^d, \mathbb{C}^2)$ or, more generally, in the functional spaces $\Sigma_\varepsilon^k := \Sigma_\varepsilon^k(\mathbb{R}^d, \mathbb{C}^2)$ containing functions $f \in L^2(\mathbb{R}^d, \mathbb{C}^2)$ such that

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

with a uniform control of the norm, with respect to $\varepsilon \in (0, 1]$

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

For simplicity, we denote by Σ^k the sets Σ_ε^k corresponding to $\varepsilon = 1$. The Schwartz space $\mathcal{S}(\mathbb{R}^d)$ then satisfies $\cap_{k \in \mathbb{N}} \Sigma^k = \mathcal{S}(\mathbb{R}^d)$. The initial data that we will consider belong to Σ_ε^k for all $k \in \mathbb{N}$, as explained below.

Let us first detail the assumptions we make on the matrix structure of the potential. As any symmetric matrix, the potential V can be decomposed as the sum of a scalar function and a trace-free matrix: we write

$$(3) \quad V(x) = v(x) \text{Id}_{\mathbb{C}^2} + \begin{pmatrix} w_1(x) & w_2(x) \\ w_2(x) & -w_1(x) \end{pmatrix}$$

and denote by λ_- and λ_+ the eigenvalues of V with $\lambda_- \leq \lambda_+$. We have

$$\lambda_\pm(x) = v(x) \pm |w(x)|, \quad |w(x)| = \sqrt{w_1^2(x) + w_2^2(x)}.$$

We associate with these eigenvalues the scalar Hamiltonians

$$(4) \quad h_\pm(z) = \frac{|\xi|^2}{2} + \lambda_\pm(x), \quad z = (x, \xi).$$

Since V is smooth, the functions v and $w = (w_1, w_2)$ are also smooth and the eigenvalues of V are smooth outside the set Υ of crossing points

$$\Upsilon = \{z = (x, \xi) \in \mathbb{R}^{2d}, h_+(z) = h_-(z)\} = \{z = (x, \xi) \in \mathbb{R}^{2d}, w(x) = 0_{\mathbb{R}^2}\}.$$

We shall also consider the eigenprojectors associated with each of the eigenvalues

$$\Pi_\pm(x) = \frac{1}{2} \left(\text{Id}_{\mathbb{R}^2} \pm \frac{1}{|w(x)|} \begin{pmatrix} w_1(x) & w_2(x) \\ w_2(x) & -w_1(x) \end{pmatrix} \right).$$

Following [23], we will work in the case of conical crossing points by considering the following set of assumptions.

Assumption 1.1.

(1) *The crossing on Υ is a conical crossing of codimension 2:*

$$\forall q^b \in \Upsilon, \text{Rank } dw(q^b) = 2.$$

(2) *The conical crossing point $z^b = (q^b, p^b)$ is non-degenerate:*

$$E(z^b) := (p^b \cdot \nabla w_1(q^b), p^b \cdot \nabla w_2(q^b)) = dw(q^b) p^b \neq 0_{\mathbb{R}^2}$$

We write $dw(q^b) p^b = r\omega$ with $r > 0$ and $\omega \in \mathbf{S}^1$.

In the notations above, we denote by $dw(q)$ the $2 \times d$ matrix

$$dw(q) = (\partial_{q_j} w_i)_{1 \leq i \leq 2, 1 \leq j \leq d},$$

meaning that, when applied to a vector $p \in \mathbb{R}^d$, one gets a vector $r\omega = dw(q)p \in \mathbb{R}^2$. Note that Point (1) of Assumption 1.1 implies that Υ is a submanifold of \mathbb{R}^d . Then, the points of Υ are said to be conical crossing points because the eigenvalues λ_+ and λ_- develop a conical singularity at

those points. This singularity induces special behaviors of the solution to Equation (1) that has been already studied in the literature (see [23, 12] for example) and that we want to analyze here for wave packets propagation.

The eigenvalues λ_+ and λ_- are also supposed to satisfy a polynomial gap condition at infinity: we assume that there exist constants $c_0, n_0, r_0 > 0$ such that

$$(5) \quad |\lambda_+(x) - \lambda_-(x)| \geq c_0 \langle x \rangle^{-n_0}, \quad \text{when } |w(x)| \geq r_0,$$

where $\langle x \rangle = (1 + |x|^2)^{1/2}$. This gap condition at infinity (5) ensures, that the derivatives of the eigenprojectors $\Pi_{\pm}(x)$ grow at most polynomially : it is proved in [3, Lemma B.2] that for all $\beta \in \mathbb{N}^d$ there exists a constant $C_{\beta} > 0$ such that

$$(6) \quad \|\partial_x^{\beta} \Pi_{\pm}(x)\|_{\mathcal{C}^{2,2}} \leq C_{\beta} \langle x \rangle^{|\beta|(1+n_0)}, \quad \text{when } |w(x)| \geq r_0.$$

We are interested in initial data that are wave packets as studied in [7]. Wave packets are highly localized in position and impulsion, they are associated with a profile $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and a point $z = (q, p) \in \mathbb{R}^{2d}$ of the phase space according to

$$(7) \quad \text{WP}_z^{\varepsilon} \varphi(x) = \varepsilon^{-d/4} e^{\frac{i}{\varepsilon} p \cdot (x-q)} \varphi\left(\frac{x-q}{\sqrt{\varepsilon}}\right).$$

Such families are uniformly bounded in all the spaces Σ_{ε}^k for any $k \in \mathbb{N}$. Note that Hagedorn's wave packets in [23] are built by choosing φ related to Hermite functions. Our set of data contains Hagedorn's ones. With these notations, we shall make the following set of assumptions on the initial data.

Assumption 1.2. *The initial data of the system (1) is given by*

$$\psi_0^{\varepsilon}(x) = \vec{Y}_0 \text{WP}_{z_0}^{\varepsilon} \varphi(x),$$

where $\varphi \in \mathcal{S}(\mathbb{R}^d)$, $z_0 = (q_0, p_0) \in \mathbb{R}^{2d} \setminus \Upsilon$ and $\vec{Y}_0 \in \mathbb{R}^2$ is a normalized eigenvector of the matrix V in q_0 for the minus-mode:

$$V(q_0) \vec{Y}_0 = \lambda_-(q_0) \vec{Y}_0.$$

Note that since \vec{Y}_0 is assumed to be a real-valued normalized eigenvector of $V(q_0)$ with $w(q_0) \neq 0$, one can replace the pair (\vec{Y}_0, φ) by $(-\vec{Y}_0, -\varphi)$ without changing the wave packet.

Wave packets satisfy localization properties that are recalled in Appendix B. In particular, considering a function $\vec{V}_0 \in \mathcal{C}^{\infty}(\mathbb{R}^d, \mathbb{R}^2)$ such that $\vec{V}_0(q_0) = \vec{Y}_0$, we have

$$(8) \quad \psi_0^{\varepsilon}(x) = \vec{V}_0(x) \text{WP}_{z_0}^{\varepsilon} \varphi(x) + \mathcal{O}(\sqrt{\varepsilon})$$

in Σ_{ε}^k for all $k \in \mathbb{N}$. Additionally, we can assume without loss of generality, that $\vec{V}_0(x)$ is an eigenvector of $V(x)$ associated with $\lambda_-(x)$ for all x in a neighborhood Ω of q_0 .

It is well-known (and we provide a detailed exposition of those results below) that, outside the crossing set, such a wave packet propagates along the classical trajectories associated with the mode $\lambda_-(x)$ (see [7]). We aim at precisely describing what happens when a wave packet reaches the crossing set, and passes through it. These results have been announced in [20].

We provide a picture similar to the one involving Gaussian wave packets in [23]: as long as the gap remains large enough on the trajectory, the solution can be approximated by a wave packet with a time dependent profile, an action $S_-(t, t_0, z_0)$ and a time dependent eigenvector $\vec{Y}_-(t)$

$$\psi^{\varepsilon}(t) = \vec{Y}_-(t) e^{\frac{i}{\varepsilon} S_-(t, t_0, z_0)} \text{WP}_{\Phi_-^{t, t_0}}^{\varepsilon}(u_-(t)) + o(1),$$

in Σ_ε^k . Besides, as soon as the gap shrinks, transitions occur on the other mode, leading to the birth of a quite similar wave packet on the other mode. The advantage of considering general wave packets lies in the fact that the transitions generate contributions on each mode that keep the more general structure, while the Gaussian one is not preserved (see [23]).

We use the following ingredients:

- (1) The existence of generalized trajectories that exist despite the conical singularity (see [23, 12, 13]).
- (2) The use of real-valued eigenvectors evaluated along the time-dependent classical trajectories.
- (3) The introduction of a profile equation along a trajectory and the analysis of this profile when the trajectory reaches a crossing point, proving precise estimates on its behavior close to the crossing time. This is performed in Section 1.1.3 and uses ideas from [23, 24].
- (4) The definition of a thin layer close to the crossing point of the trajectory and the reduction to a model problem in this thin layer.

In the next Section 1.1, we introduce the main objects (classical trajectories, actions, eigenvectors and profiles) that characterize the approximate solution, and our result is stated in Section 1.2.

We point out that this transfer has been precisely described in terms of Wigner measures by the results of [13] when one single wave packet reaches a crossing point. However, if two wave packets reach simultaneously a point of the crossing set, the Wigner measure information is not enough and a phase information is needed to describe the Wigner measure of the outgoing wave packets. One of our aim here is to get this phase information.

Even though our results are inspired by those of [23], they differ on several aspects. First, the way we handle the problem is different and easier to generalize to other Hamiltonians. Secondly, the results obtained are more general in terms of the data that are considered. Thirdly, the method we develop also allow to treat data passing close to the crossing set and not exactly through it (see Remark 4.3) and more general Hamiltonian (see Appendix D). The latter point opens the way to further development and proofs of the convergence of numerical methods mixing surface hopping approaches [14, 15, 16, 17, 31] and thawed or frozen Gaussian algorithms (also called Herman-Kluk approximation) as introduced in chemical literature in [26, 27, 28] and studied from a mathematical point of view in [38, 40] (see also [19]).

1.1. The parameters of the approximate solution. The aim of this paper is to give a precise description of how one can approximate solutions to equation (1) in the framework of Assumptions 1.1 and 1.2. This result is presented in the next section and we begin here by introducing the parameters of the wave packets that are involved in the process. We give a description of their centers, profiles and phase factor, which are ε -independent and related with classical quantities.

1.1.1. Classical trajectories and actions. For $(t_0, z_0) \in \mathbb{R} \times (\mathbb{R}^{2d} \setminus \Upsilon)$ we consider the classical trajectory $(q_\pm(t), p_\pm(t))$ issued from $z_0 = (q_0, p_0)$ at time t_0 , and defined by the ordinary differential equation

$$\dot{q}_\pm(t) = p_\pm(t), \quad \dot{p}_\pm(t) = -\nabla \lambda_\pm(q_\pm(t))$$

with

$$q_\pm(t_0) = q_0 \quad \text{and} \quad p_\pm(t_0) = p_0.$$

The associated flow map is then denoted by $\Phi_\pm^{t, t_0}(z_0) = (q_\pm(t), p_\pm(t))$ and we have

$$(9) \quad \partial_t \Phi_\pm^{t, t_0} = J \nabla_z h_\pm \circ \Phi_\pm^{t, t_0}, \quad \Phi_\pm^{t_0, t_0} = \mathbf{1}_{\mathbb{R}^{2d}},$$

where

$$(10) \quad J = \begin{pmatrix} 0 & \text{Id}_{\mathbb{R}^d} \\ -\text{Id}_{\mathbb{R}^d} & 0 \end{pmatrix}$$

and the Hamiltonians h_{\pm} are defined in (4). It will be convenient in the following to denote by $\{f, g\}$ the Poisson bracket of two functions $f, g \in \mathcal{C}^{\infty}(\mathbb{R}^{2d})$, that might be scalar-, vector- or matrix-valued as soon as the product fg makes sense:

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

Of course, since $w(q_0) \neq 0_{\mathbb{R}^2}$, the existence of these Hamiltonian trajectories is guaranteed by Cauchy-Lipschitz theorem, as long as they do not reach Υ . Moreover, one can prove that there exist trajectories passing through $z^b = (q^b, p^b) \in \Upsilon$ that are piecewise smooth, as soon as Assumptions 1.1 hold at point (q^b, p^b) . We point out that we will make the convenient abuse of notations of saying indistinctly that $z = (q, p) \in \Upsilon$ or $q \in \Upsilon$.

Proposition 1.3. *[13], Proposition 1] Let $z^b \in \Upsilon$ satisfying Assumptions 1.1, the notations of which we use. Then, there exist two continuous maps*

$$t \mapsto \Phi_{\pm}^{t, t^b}(z^b) = (q_{\pm}(t), p_{\pm}(t))$$

defined in a neighborhood of t^b and which satisfy (9) for $t \neq t^b$ with moreover $\Phi_{\pm}^{t^b, t^b}(z^b) = z^b$. Besides, we have for all $t \sim t^b$

$$(11) \quad w(q_{\pm}(t)) = (t - t^b)r\omega + \mathcal{O}((t - t^b)^2).$$

We shall call *generalized trajectories* these continuous maps passing through points $z^b \in \Upsilon$ satisfying Assumptions 1.1. We associate with $\Phi_{\pm}^{t, t_0}(z_0) = (q_{\pm}(t), p_{\pm}(t))$ the action integral

$$(12) \quad S_{\pm}(t, t_0, z_0) = \int_{t_0}^t (p_{\pm}(s) \cdot \dot{q}_{\pm}(s) - h_{\pm}(z_{\pm}(s))) ds.$$

We analyze in Section 2.1 the behavior of both these generalized trajectories and their actions close to a crossing point.

1.1.2. *Real-valued time-dependent eigenvectors along the trajectory.* We introduce the matrix-valued function $B_{\pm} \in \mathcal{C}^{\infty}(\mathbb{R}^{2d} \setminus \Upsilon)$ defined by

$$(13) \quad B_{\pm}(x, \xi) = \pm \Pi_{\mp}(x) \xi \cdot \nabla_x \Pi_{\pm}(x) \Pi_{\pm}(x) = \mp \Pi_{\mp}(x) \xi \cdot \nabla_x \Pi_{-}(x) \Pi_{\pm}(x) = -B_{\mp}(x, \xi)^*.$$

Proposition 1.4. *Let $(t_0, z_0) \in \mathbb{R}^{2d+1}$ be such that the trajectory $\Phi_{-}^{t, t_0} = (q_{-}(t), p_{-}(t))$ reaches Υ at time $t^b > t_0$ and point $z^b = \Phi_{-}^{t^b, t_0}(z_0)$ satisfying Assumption 1.1. Let \vec{Y}_0 such that $\Pi_{-}(q_0)\vec{Y}_0 = \vec{Y}_0$. Then, the solution $\vec{Y}_{-}(t)$ of the differential system*

$$(14) \quad \begin{cases} \partial_t \vec{Y}_{-}(t) = B_{-}(\Phi_{-}^{t, t_0}(z_0)) \vec{Y}_{-}(t), & t \in [t_0, t^b) \\ \vec{Y}_{-}(t_0) = \vec{Y}_0 \end{cases}$$

satisfies the following properties:

(1) for all $t \in [t_0, t^b)$, $\vec{Y}_{-}(t)$ is an eigenvector for the minus-mode along the trajectory:

$$\Pi_{-}(q_{-}(t)) \vec{Y}_{-}(t) = \vec{Y}_{-}(t).$$

(2) There exists a normalized real-valued vector \vec{V}_ω such that

$$\lim_{t \rightarrow t^b, t < t^b} \vec{Y}_-(t) = \vec{V}_\omega$$

and

$$(15) \quad \begin{pmatrix} \omega_1 & \omega_2 \\ \omega_2 & -\omega_1 \end{pmatrix} \vec{V}_\omega = \vec{V}_\omega \quad \text{with } \vec{V}_\omega \in \mathbb{R}^2, \quad |\vec{V}_\omega| = 1.$$

(3) There exist $\tau > 0$ and a function $x \mapsto \vec{V}_-(x)$ smooth in a neighborhood of $(\Phi_-^{t,t_0}(z_0))_{t \in [t^b - \tau, t^b]}$ such that $\Pi_- \vec{V}_- = \vec{V}_-$ and $\vec{Y}_-(t) = \vec{V}_-(q_-(t))$.

Note that since \vec{V}_ω is real-valued, the relation (15) fixes \vec{V}_ω up to its sign. Its sign depends on the value of \vec{Y}_0 .

Of course, a similar result holds for the *plus*-mode. More generally, one can construct ingoing and outgoing eigenvectors along the trajectories arising from a non-degenerate conical crossing point z^b .

Proposition 1.5. *Let $t^b \in \mathbb{R}$ and z^b satisfying Assumption 1.1 and $\vec{V}_\omega \in \mathbb{R}^2$ satisfying (15). Let \vec{V}_ω^\perp obtained by the rotation of angle $\frac{\pi}{2}$. There exist two families of eigenvectors $\vec{Y}_\pm(t)$ defined in a neighborhood I of t^b , such that*

$$(16) \quad \partial_t \vec{Y}_\pm(t) = B_\pm(\Phi_\pm^{t,t^b}(z^b)) \vec{Y}_\pm(t), \quad t \in I \setminus \{t^b\}$$

and

$$(17) \quad \lim_{t \rightarrow t^b, t > t^b} \vec{Y}_+(t) = \lim_{t \rightarrow t^b, t < t^b} \vec{Y}_-(t) = \vec{V}_\omega, \quad \lim_{t \rightarrow t^b, t > t^b} \vec{Y}_-(t) = \lim_{t \rightarrow t^b, t < t^b} \vec{Y}_+(t) = \vec{V}_\omega^\perp.$$

As a consequence, starting at time t_0 from a trajectory $\Phi_-^{t,t_0}(z_0)$ for the *minus*-mode that reaches Υ at a non-degenerate conical crossing point z^b , we are left with a family of time-dependent eigenvectors $\vec{Y}_-(t)$ that reaches the crossing and defines a vector \vec{V}_ω . One can then continuously pass through the crossing, while hopping from the *minus*-mode to the *plus*-mode at time t^b . Similarly, with the generalized trajectory arriving at time t^b in z^b for the *plus*-mode, one can associate a family of time-dependent eigenvector for the *plus*-mode that will pass continuously through the crossing with (17), while hopping from the *plus*-mode to the *minus*-mode at time t^b .

1.1.3. *Profile equations.* The profiles of the approximate solutions are linked with the scalar Hamiltonians h_\pm - see (4) - and the associated trajectories. We consider trajectories $\Phi_\pm^{t,t_0}(z_0)$ that do not meet Υ on some time interval I containing t_0 and associate with them the Schrödinger equations with time-dependent harmonic potential

$$(18) \quad i\partial_t u_\pm = -\frac{1}{2}\Delta u_\pm + \frac{1}{2}\text{Hess } \lambda_\pm(\Phi_\pm^{t,t_0}(z_0)) y \cdot y u_\pm^\pm,$$

with initial data in $\mathcal{S}(\mathbb{R}^d)$. In view of [34], these equations have a solution in $\Sigma^k(\mathbb{R}^d)$ on the time interval I for any $k \in \mathbb{N}^*$. Moreover, we have the following proposition.

Proposition 1.6. *Let $(t_0, z_0) \in \mathbb{R}^{2d+1}$ be such that the trajectory Φ_\pm^{t,t_0} reaches Υ at time $t^b > t_0$ and point $z^b = \Phi_\pm^{t^b,t_0}(z_0)$ satisfying Assumption 1.1. Then, there exists a solution $u_\pm(t)$ to (18) on $[t_0, t^b]$ with initial data $u^\pm(t_0) = \varphi_\pm \in \mathcal{S}(\mathbb{R}^d)$. Moreover, for any $t \in [t_0, t^b]$, $u_\pm(t) \in \mathcal{S}(\mathbb{R}^d)$, $\|u_\pm(t)\|_{L^2} = \|\varphi_\pm\|_{L^2}$ and if $k \in \mathbb{N}^*$, there exists a constant $C_k > 0$ such that*

$$(19) \quad \sup_{t \in [t_0, t^b]} \|u_\pm(t)\|_{\Sigma^k} \leq C_k \left(1 + \left|\ln |t - t^b|\right|\right).$$

The result of Proposition 1.6, implies that the time derivatives of the profile functions u_+ and u_- are integrable, up to a phase. With the notations of Assumptions 1.1, we consider the $d \times d$ matrix Γ_0 defined by

$$(20) \quad \Gamma_0 = r^{-1} {}^t dw(q^b) (\text{Id}_{\mathbb{R}^2} - \omega \otimes \omega) dw(q^b)$$

where $\omega \otimes \omega$ is the 2 by 2 matrix $(\omega_i \omega_j)_{i,j}$ and dw is the $2 \times d$ matrix $(\partial_{x_j} w_i)_{i,j}$ (note that $\text{Id}_{\mathbb{R}^2} - \omega \otimes \omega$ is the orthogonal projector on $\mathbb{R} \omega^\perp$).

Corollary 1.7. *Under the assumptions of Proposition 1.6, there exists $u_\pm^{\text{in}} \in \mathcal{S}(\mathbb{R}^d)$ such that for all $k \in \mathbb{N}$, there exists $C_k > 0$ with*

$$(21) \quad \left\| \text{Exp}(\mp \frac{i}{2} \Gamma_0 y \cdot y \ln |t - t^b|) u_\pm(t) - u_\pm^{\text{in}} \right\|_{\Sigma^k} \leq C_k |t - t^b| \left(1 + \left| \ln |t - t^b| \right| \right).$$

Moreover, once given $u_\pm^{\text{out}} \in \mathcal{S}(\mathbb{R}^d)$, there exists a unique pair $u_\pm(t)$ for $t > t^b$ satisfying (18) and such that for all $k \in \mathbb{N}$, there exists $C_k > 0$ with

$$(22) \quad \left\| \text{Exp}(\pm \frac{i}{2} \Gamma_0 y \cdot y \ln |t - t^b|) u_\pm(t) - u_\pm^{\text{out}} \right\|_{\Sigma^k} \leq C_k |t - t^b| \left(1 + \left| \ln |t - t^b| \right| \right).$$

Let us consider an initial data as in (8) and assume that $\Phi_-^{t,t_0}(z_0)$ passes through Υ at time t^b at a point z^b that satisfies Assumption 1.1. Then one can associate a profile $u_-(t)$ with the ingoing trajectory Φ_-^{t,t_0} for $t \in [t_0, t^b]$; this generates an ingoing profile $u_-^{\text{in}} \in \mathcal{S}(\mathbb{R}^d)$. We shall see later how to build an approximate solution to the system (1) thanks to u_-^{in} , and how to associate two outgoing profiles, u_-^{out} and u_+^{out} , with u_-^{in} in an adequate manner; these outgoing profiles then generate two profiles $u_+(t)$ and $u_-(t)$ when $t > t^b$, one for each mode, by solving equation (18) with initial data at time t^b given by u_-^{out} and u_+^{out} respectively.

1.2. Main results. Let us consider an initial data at time t_0 satisfying (8) and assume that the trajectory $\Phi_-^{t,t_0}(z_0)$ does not reach Υ on the interval $[t_0, t_0 + T]$ because $\Phi_-^{t,t_0}(z_0) \in \{|w(x)| \geq \delta\}$ for some $\delta > 0$. Then, there is adiabatic propagation of the wave packet: at leading order, the solution remains in the same eigenspace and can be approximated by a wave packet whose parameters are determined by the classical quantities associated with the related eigenvalue. This type of results are already present in the literature, see [1] for the case of wave packets and [33, 41] for more general results. Our contribution here is intended to emphasize the dependence of the approximation on the parameter δ , encoding the minimum gap along the trajectory, which is a crucial ingredient in the proof of our next result.

Theorem 1.8. *[Propagation with a gap of size δ] Let $k \in \mathbb{N}$. Assume ψ_0^ε is chosen as in Assumption 1.2. Let $\delta > 0$ and assume that $\Phi_-^{t,t_0}(z_0) \in \{|w(x)| \geq \delta\}$ for all $t \in [t_0, t_0 + T]$. Consider the time-dependent eigenvector $\vec{Y}_-(t)$ given by Proposition 1.4 and the profile u_- associated with φ_- by Proposition 1.6. Then, there exists $C_k > 0$ independent of δ such that*

$$\left\| \psi^\varepsilon(t) - \vec{Y}_-(t) e^{\frac{i}{\varepsilon} S_-(t, t^b, z^b)} \text{WP}_{\Phi_-^{t,t^b}(z^b)} u_-(t) \right\|_{\Sigma_\varepsilon^k} \leq C_k (1 + |\ln \delta|) \left(\frac{\varepsilon^{3/2}}{\delta^4} + \frac{\sqrt{\varepsilon}}{\delta} \right).$$

Of course, this result easily extends by linearity to the case of data which have components on both modes with wave packet structures. Theorem 1.8 only gives information when the gap along the trajectory is large enough.

Let us now assume that the trajectory $\Phi_-^{t,t_0}(z_0)$ passes through Υ at time $t^b \in (t_0, t_0 + T)$, $T > 0$ at point z^b where Assumption 1.1 is satisfied. We consider:

- The trajectories $\Phi_-^{t,t_0}(z_0)$ and $\Phi_+^{t,t^b}(z^b)$ built in Proposition 1.3.
- The time-dependent eigenvectors $\vec{Y}_-(t)$ associated with \vec{Y}_0 by Proposition 1.4 for $t \in [t_0, t^b]$, and the pair of time-dependent eigenvectors $(\vec{Y}_+(t), \vec{Y}_-(t))$ of Proposition 1.5 on $[t^b, t_0 + T]$ with (17)
- The profile $u_-(t)$ built for $t \in [t_0, t^b]$, thanks to Proposition 1.6 with data $u_-(t_0) = \varphi_-$. We define u_-^{in} by Corollary 1.7, and associate with u_-^{in} the profiles $u_{\pm}(t)$ defined for $t > t^b$ thanks to the outgoing limiting profiles u_-^{out} and u_+^{out} given by

$$(23) \quad \begin{pmatrix} u_+^{\text{out}} \\ u_-^{\text{out}} \end{pmatrix} = \begin{pmatrix} e^{-i\theta_\varepsilon(\eta)} b(\eta_2) & a(\eta_2) \\ a(\eta_2) & -e^{i\theta_\varepsilon(\eta)} \bar{b}(\eta_2) \end{pmatrix} \begin{pmatrix} 0 \\ e^{\frac{i}{\varepsilon} S_-} u_-^{\text{in}} \end{pmatrix}.$$

where, $S_- = S_-(t^b, t_0, z_0)$ and, with the notations of Assumption 1.1,

$$(24) \quad \eta(y) = \left(\omega \cdot (dw(q^b)y), \omega^\perp \cdot (dw(q^b)y) \right) = (\eta_1(y), \eta_2(y)), \quad \forall y \in \mathbb{R}^d,$$

$$(25) \quad a(\eta_2) = e^{-\frac{\pi\eta_2^2}{2}}, \quad b(\eta_2) = \frac{2i}{\sqrt{\pi\eta_2}} 2^{-i\eta_2^2/2} e^{-\pi\eta_2^2/4} \Gamma\left(1 + i\frac{\eta_2^2}{2}\right) \sinh\left(\frac{\pi\eta_2^2}{2}\right),$$

$$(26) \quad \theta_\varepsilon(\eta) = \frac{\eta_2^2}{2r} \ln\left(\frac{r}{\varepsilon}\right) + \frac{\eta_1^2}{r}$$

We recall the Gamma function and hyperbolic sine function we use:

$$\Gamma(z) = \int_0^1 \left(\ln \frac{1}{t}\right)^{z-1} dt = \int_0^\infty t^{z-1} e^{-t} dt, \quad \sinh(z) = \frac{e^z - e^{-z}}{2}.$$

We then have the following result.

Theorem 1.9. [Propagation of a single wave packet] Let $k \in \mathbb{N}$. Assume ψ_0^ε is chosen as in Assumption 1.2 and that the trajectory $\Phi_-^{t,t_0}(z_0)$ reaches Υ at some time t^b and some point z^b satisfying Assumption 1.1. Consider the above-mentioned classical quantities. Then, as ε tends to 0, the solution to equation (1) with initial data ψ_0^ε satisfies in $\Sigma_\varepsilon^k(\mathbb{R}^d)$: if $t \in [t_0, t^b]$

$$\psi^\varepsilon(t) = e^{\frac{i}{\varepsilon} S_-(t,t_0,z_0)} \vec{Y}_-(t) \text{WP}_{\Phi_-^{t,t_0}(z_0)} u_-(t) + \mathcal{O}\left((1 + |\ln \varepsilon|) \varepsilon^{\frac{1}{14}-}\right)$$

and if $t \in (t^b, t_0 + T]$,

$$(27) \quad \begin{aligned} \psi^\varepsilon(t) &= \vec{Y}_-(t) e^{\frac{i}{\varepsilon} S_-(t,t^b,z^b)} \text{WP}_{\Phi_-^{t,t^b}(z^b)} u_-(t) \\ &\quad + \vec{Y}_+(t) e^{\frac{i}{\varepsilon} S_+(t,t^b,z^b)} \text{WP}_{\Phi_+^{t,t^b}(z^b)} u_+(t) + \mathcal{O}\left((1 + |\ln \varepsilon|) \varepsilon^{\frac{1}{14}-}\right) \end{aligned}$$

By $\varepsilon^{\frac{1}{14}-}$, we mean $\varepsilon^{\frac{1}{14}-\varsigma}$ for some $\varsigma \in (0, \frac{1}{14})$ small enough. Note that the constants involved in the approximation result of Theorem 1.9 depend on the initial data, the potential V and the time length T of the approximation. This is also the case in the next results.

Remark 1.10. The presence of the phase-shift driven by the function $\theta_\varepsilon(\eta)$ in the transfer formula implies that if the L^2 -norms of the outgoing profiles are still uniformly bounded with respect to ε , it will not be the case for their Schwartz semi-norms, that will grow as powers of $\ln(\varepsilon)$. However, setting $f^\varepsilon = \text{WP}_{z_0}(e^{iS(y)\ln(\varepsilon)}\varphi(y))$ with $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and $S \in \mathcal{C}^\infty(\mathbb{R}^d)$ with polynomial growth

together with its derivatives, one can check that the ε -derivatives of f^ε are uniformly bounded. Indeed, one can prove by a recursive argument that for $\alpha \in \mathbb{N}^d$,

$$\varepsilon^{|\alpha|} \partial_x^\alpha f^\varepsilon(y) = \text{WP}_{z_0}(e^{iS(y)\ln(\varepsilon)} \varphi_\alpha^\varepsilon(y))$$

with for $k \in \mathbb{N}$, $\|\varphi_\alpha^\varepsilon\|_{\Sigma^k} \leq c_k(1 + (\sqrt{\varepsilon} \ln(\varepsilon))^{|\alpha|+k})$, $c_k > 0$. The wave packet structure is not excessively deteriorated by this phase shift and the approximate solution in (27) is uniformly bounded in Σ_ε^k with respect to ε for all $k \in \mathbb{N}$.

The result extends, by superposition principles, to the case where two wave packets interact at a crossing point z^b . Assume

$$(28) \quad \psi_0^\varepsilon(x) = \vec{Y}_{0,-} \text{WP}_{z_{0,-}}^\varepsilon \varphi_-(x) + \vec{Y}_{0,+} \text{WP}_{z_{0,+}}^\varepsilon \varphi_+(x),$$

where $\varphi_\pm \in \mathcal{S}(\mathbb{R}^d)$, $z_{0,\pm} = (q_{0,\pm}, p_{0,\pm}) \in \mathbb{R}^{2d} \setminus \Upsilon$ with $\Phi_\pm^{t^b, t_0}(z_{0,\pm}) = z^b$, and $\vec{Y}_{0,\pm} \in \mathbb{R}^2$ are normalized real-valued eigenvectors of the matrix V :

$$V(q_{0,\pm}) \vec{Y}_{0,\pm} = \lambda_\pm(q_{0,\pm}) \vec{Y}_{0,\pm}.$$

We associate with each mode classical quantities:

- One first computes the time-dependent eigenvectors along the trajectories $\vec{Y}_\pm(t)$, carefully handling the fact that if \vec{V}_ω is the vector associated with $\vec{Y}_{0,-}$, the vector associated with $\vec{Y}_{0,+}$ by (2) of Proposition 1.4 adapted to the *plus*-mode is \vec{V}_ω^\perp or $-\vec{V}_\omega^\perp$. If one gets $-\vec{V}_\omega^\perp$, one has to turn the pair $(\vec{Y}_{0,+}, \varphi_+)$ into $(-\vec{Y}_{0,+}, -\varphi_+)$.
- Once this issue is fixed, one computes the profiles $u_\pm(t)$ for $t < t^b$ associated with the trajectories and the initial data φ_\pm . Note that the change of initial data $(\vec{Y}_{0,+}, \varphi_+)$ into $(-\vec{Y}_{0,+}, -\varphi_+)$ corresponds to changing the ingoing profiles u_+^{in} into $-u_+^{\text{in}}$.
- This generates incoming profiles u_-^{in} and u_+^{in} on the *minus*-mode and *plus*-mode, and incoming actions $S_\pm^b = S_\pm(t^b, t_0, z_{0,\pm})$ respectively. Then, we set

$$(29) \quad \begin{pmatrix} u_+^{\text{out}} \\ u_-^{\text{out}} \end{pmatrix} = \begin{pmatrix} -e^{i\theta_\varepsilon(n)} \bar{b}(\eta_2) & a(\eta_2) \\ a(\eta_2) & e^{-i\theta_\varepsilon(n)} b(\eta_2) \end{pmatrix} \begin{pmatrix} e^{\frac{i}{\varepsilon} S_+^b} u_+^{\text{in}} \\ e^{\frac{i}{\varepsilon} S_-^b} u_-^{\text{in}} \end{pmatrix}$$

and one computes the outgoing profiles $u_\pm(t)$ for $t > t^b$ along the trajectories and with initial data u_\pm^{out} at time $t = t^b$.

Then, the following result is a straightforward consequence of Theorem 1.9 and of the linearity of the equation.

Corollary 1.11. *[Interactions of wave packets at conical intersections] The solution of equation (1) with initial data (28) is given for $t \in (t^b, t_0 + T]$ by*

$$\psi^\varepsilon(t) = \vec{Y}_-(t) e^{\frac{i}{\varepsilon} S_-(t, t^b, z^b)} \text{WP}_{\Phi_-^{t, t^b}(z^b)} u_-(t) + \vec{Y}_+(t) e^{\frac{i}{\varepsilon} S_+(t, t^b, z^b)} \text{WP}_{\Phi_+^{t, t^b}(z^b)} u_+(t) + \mathcal{O}((1 + |\ln \varepsilon|) \varepsilon^{\frac{1}{14}})$$

in $\Sigma_\varepsilon^k(\mathbb{R}^d)$.

Remark 1.12. Several remarks are of interest :

- (1) The adjustment of the-time dependent eigenvectors is a crucial issue. It is connected with the choice of the basis $(\vec{V}_\omega, \vec{V}_\omega^\perp)$ at the level of the transition. This basis plays the role of what is sometimes called a *adiabatic* basis and the process that we describe above gives a way of choosing a *adiabatic* basis close to a non-degenerate conical crossing point.

- (2) The actions accumulated during the transport to the conical intersection play a part in the transition process and the new profiles are affected by a ε -dependent phase.
- (3) The analysis performed above extends to the case of time-dependent symmetric Hamiltonian $H(t, z)$ presenting conical intersections. Appendix D is devoted to the generalization of the process.

It is interesting to compute the Wigner measure of the function $\psi^\varepsilon(t)$ ($t > t^b$) of Corollary 1.11.

Corollary 1.13. *The (matrix-valued) Wigner measure of the solution to equation (1) with initial data (28) is given for $t > t^b$ by*

$$(30) \quad \mu(t, z) = c_+ \delta \left(z - \Phi_+^{t, t^b}(z^b) \right) \vec{Y}_+(t) \otimes \vec{Y}_+(t) + c_- \delta \left(z - \Phi_-^{t, t^b}(z^b) \right) \vec{Y}_-(t) \otimes \vec{Y}_-(t)$$

and (with the notations of (24) and (25))

$$c_\pm = \|a(\eta_2)u_\pm^{\text{in}}\|^2 + \|\sqrt{1 - a(\eta_2)^2}u_\mp^{\text{in}}\|^2.$$

Let us conclude this section with a parallel between our main result and Theorem 6.3 of [23]. The latter deals with the propagation of a Hagedorn's wave packet through the conical intersection; it corresponds to our Theorem 1.9 for φ being a Gaussian multiplied by a polynomial function, which implies that the ingoing profile u^{in} has the same structure. The outgoing profiles are decomposed on the basis of Hagedorn's wave packets in formula (6.53). One sees that the component that switches from one mode to the other one only has a finite number of components. In fact, it still has the structure of a Gaussian multiplied by a polynomial function, while the one that keeps going on the same mode has a full decomposition, which is due to the presence of the function Γ in the coefficient $b(\eta)$. The comparison with our result is easier page 100 (last formula of the page): one can observe the oscillating phase and the exponential transition coefficient in the part of the approximate solution that switches of mode, together with a decomposition on Hermite functions at the top of page 101. The other mode is treated page 102 and 103, where the Gamma function can be spotted. The phase shift itself is more visible in [24] where $\lambda(\varepsilon)$ of Theorem 3.1 is the analogue of our $\theta_\varepsilon(y)$. The phase $\lambda(\varepsilon)$ does not depend on y but does depend on the parameters of the avoided crossing that is the subject of [24]. Note that in both references [23] and [24], the scaling of the equation is not the same, as ε in this present article corresponds to ε^2 in those contributions.

1.3. Ideas of the proof, organization of the paper and notations. An important part of the proof consists in the construction of the approximate solutions and, in particular, in the resolution of equation (18), as well as the analysis of the properties of its solutions. This part is performed in Section 2, together with results on the classical quantities. Then the proof proceeds in two steps. We first show that the approximate solution fits outside Υ , which corresponds to times $t \notin (t^b - \delta, t^b + \delta)$ for some δ that will be chosen small. In this region - that can be qualified as *adiabatic* - the solutions of (1) decouples on each of the modes. Using techniques arising from [1, 41] for example, as spelled out in [18], we carefully analyze the order of the approximation (which involves negative powers of δ combined with powers of ε) in Section 3. Then, in $(t^b - \delta, t^b + \delta)$, we are able to reduce to a local model of Landau-Zener's type and exhibit the transitions relations (29) in Section 4. This allows us to fix the ansatz for times $t > t^b + \delta$. All along the proof, it will be convenient to use the notation

$$(31) \quad A(w) = \begin{pmatrix} w_1 & w_2 \\ w_2 & -w_1 \end{pmatrix}, \quad w \in \mathbb{R}^2.$$

Besides, with a vector $V = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \in \mathbb{R}^2$, we associate the vector $V^\perp = \begin{pmatrix} -v_2 \\ v_1 \end{pmatrix}$. Moreover, if $U = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \in \mathbb{R}^2$, we set $U \wedge V = U^\perp \cdot V = u_1 v_2 - u_2 v_1$. Finally, we will use the notation $D_y = \frac{1}{i} \nabla_y$.

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2. ANALYSIS OF CLASSICAL QUANTITIES AND CONSTRUCTION OF THE APPROXIMATE SOLUTION

In this section, we first focus on the properties of the classical trajectories and actions in the neighborhood of the crossing set. Then, the next subsections are intended to construct the time-dependent eigenvectors along the trajectories and the solutions of the profile equation (18), together with a careful analysis of their properties.

2.1. The classical trajectories and actions. It is interesting to compare a generalized classical trajectory $\Phi_\pm^{t,t_0}(z_0)$ reaching the crossing set Υ at time t^b and point z^b with the trajectory $\Phi_0^{t,t^b}(z^b) = (q_0(t), p_0(t))$ associated with the (smooth) Hamiltonian

$$(32) \quad h_0(z) = \frac{|\xi|^2}{2} + v(x).$$

A simple Taylor expansion close to $t = t^b$ gives the following lemma.

Lemma 2.1. *Under the assumptions stated in Proposition 1.3, we have*

$$\begin{cases} q_\pm(t) &= q_0(t) \mp \frac{1}{2} \operatorname{sgn}(t - t^b) (t - t^b)^2 {}^t dw(q^b) \omega + \mathcal{O}((t - t^b)^3), \\ p_\pm(t) &= p_0(t) \mp |t - t^b|^t dw(q^b) \omega + \mathcal{O}((t - t^b)^2). \end{cases}$$

We recall the notation $S_\pm^{t,t_0}(z_0)$ introduced in Section 1.2. The next lemma provides a comparison between the action $S_\pm(t, t^b, z^b) = S_\pm(t, t_0, z_0) - S_\pm^{t,t_0}(z_0)$ associated with a generalized trajectory $\Phi_\pm^{t,t_0}(z_0)$ and the action

$$(33) \quad S_0(t, t^b, z^b) = \int_{t^b}^t (p_0(s) \cdot \dot{q}_0(s) - h_0(z_0(s))) ds$$

associated with the trajectory $\Phi_0^{t,t^b}(z^b)$.

Lemma 2.2. *Using the notations of Proposition 1.3 we have the following asymptotics*

$$S_\pm(t, t^b, z^b) = S_0(t, t^b, z^b) \mp \operatorname{sgn}(t - t^b) r(t - t^b)^2 + \mathcal{O}((t - t^b)^3),$$

and

$$S_0(t, t^b, z^b) = (t - t^b) \left(\frac{1}{2} |p^b|^2 - v(q^b) \right) - p^b \cdot \nabla v(q^b) (t - t^b)^2 + \mathcal{O}((t - t^b)^3).$$

Proof of Lemma 2.2. We use that $h_\pm(z_\pm(t))$ is conserved along the trajectory and we write

$$\dot{S}_\pm(t, t_0, z_0) = p_\pm(t) \cdot \dot{q}_\pm(t) - h_\pm(z^b) = |p_\pm(t)|^2 - h_\pm(z^b).$$

Lemma 1.3 gives

$$\dot{S}_\pm(t, t_0, z_0) = |p^b|^2 - 2p^b \cdot \nabla v(q^b) (t - t^b) \mp 2 dw(q^b) p^b \cdot \omega |t - t^b| - h_\pm(z^b) + \mathcal{O}((t - t^b)^2).$$

Integrating between t and t^b and using $|p^b|^2 - h_\pm(z^b) = \frac{1}{2}|p^b|^2 - v(q^b)$, we obtain

$$S_\pm(t, t_0, z_0) = S^b + (t - t^b) \left(\frac{1}{2}|p^b|^2 - v(q^b) \right) - p^b \cdot \nabla v(q^b)(t - t^b)^2 \\ \mp \operatorname{sgn}(t - t^b) dw(q^b) p^b \cdot \omega(t - t^b)^2 + \mathcal{O}((t - t^b)^3),$$

and we identify the terms $(t - t^b) \left(\frac{1}{2}|p^b|^2 - v(q^b) \right) - p^b \cdot \nabla v(q^b)(t - t^b)^2$ with the first terms of the Taylor expansion of $S_0(t, t^b, z^b)$ close to t^b . \square

2.2. Parallel transport. In this subsection, we prove Propositions 1.4 and 1.5. We begin with preliminary conditions in order to prepare the elements required for the proof. We use the crucial observation that for all $(x, \xi) \in (\mathbb{R}^d \setminus \Upsilon) \times \mathbb{R}^d$, the matrix $\xi \cdot \nabla \Pi_\pm(x)$ is off-diagonal (see Lemma C.1 for details), that is

$$(34) \quad \Pi_\pm(x) \xi \cdot \nabla \Pi_\pm(x) \Pi_\pm(x) = 0$$

and that for $\alpha \in \mathbb{N}^d$, there exist constants $C_\alpha > 0$, $n_\alpha \in \mathbb{N}$ such that

$$(35) \quad \|\partial_x^\alpha \Pi_\pm(x)\|_{\mathcal{C}^{2,2}} \leq C_\alpha |w(x)|^{-|\alpha|} \langle x \rangle^{n_\alpha},$$

which is obtained by combining the estimate (6) at infinity and the analysis of the singularity close to Υ .

A simple calculus shows that the pair (\vec{V}_+, \vec{V}_-) given by $\vec{V}_\pm(x) = \begin{pmatrix} \varsigma_\pm(x) \\ \eta_\pm(x) \end{pmatrix}$ with

$$\varsigma_\pm(x) = \frac{w_2(x)}{\sqrt{2}\sqrt{|w(x)|(|w(x)| \mp w_1(x))}} \quad ; \quad \eta_\pm(x) = \frac{\pm\sqrt{|w(x)| \mp w_1(x)}}{\sqrt{2}}$$

is a pair of real-valued eigenvectors of the matrix $V(x)$ given in (3). These functions are smooth in $\{w_2 \neq 0\}$ (indeed, one has $|w| \neq \pm w_1$ when $w_2 \neq 0$). Actually, one cannot construct pairs of eigenvectors that are smooth in $\mathbb{R}^{2d} \setminus \Upsilon$. However, it is possible to construct pairs of eigenvectors that are smooth in $\mathbb{R}^{2d} \setminus \{w(x) \cdot \vec{e} \neq 0\}$ for all $\vec{e} \in \mathbb{R}^2$, $|\vec{e}| = 1$. Indeed, we introduce the rotation matrix

$$(36) \quad \mathcal{R}(\theta) = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix}, \quad \theta \in \mathbb{R}$$

which satisfies

$$(37) \quad \mathcal{R}(\theta)^* A(w) \mathcal{R}(\theta) = \begin{pmatrix} \vec{e}_\theta \cdot w & \vec{e}_\theta \wedge w \\ \vec{e}_\theta \wedge w & -\vec{e}_\theta \cdot w \end{pmatrix}$$

where $\vec{e}_\theta = (\cos \theta, \sin \theta)$ (recall $w \wedge w' = w_1 w'_2 - w_2 w'_1$ for $w, w' \in \mathbb{R}^2$).

Then, consider the vectors $\vec{V}_\pm^\theta(x) = \begin{pmatrix} \varsigma_\pm^\theta(x) \\ \eta_\pm^\theta(x) \end{pmatrix}$ with

$$\varsigma_\pm^\theta(x) = \frac{w(x) \wedge \vec{e}_\theta}{\sqrt{2}\sqrt{|w(x)|(|w(x)| \mp w(x) \cdot \vec{e}_\theta)}} \quad ; \quad \eta_\pm^\theta(x) = \frac{\pm\sqrt{|w(x)| \mp w(x) \cdot \vec{e}_\theta}}{\sqrt{2}},$$

the pair $(\mathcal{R}(\theta)^* \vec{V}_+^\theta, \mathcal{R}(\theta)^* \vec{V}_-^\theta)$ with gives a pair of eigenvectors of $V(x)$ that are smooth in the region $\mathbb{R}^d \setminus \{w(x) \cdot \vec{e}_\theta^\perp \neq 0\}$.

Lemma 2.3 (Control of real-valued eigenvectors outside Υ). *Let (\vec{V}_+, \vec{V}_-) be a pair of normalized eigenvectors of the matrix $V(x)$ that are smooth in $\Omega = \mathbb{R}^{2d} \setminus \{w(x) \cdot \omega \neq 0\}$ for $\omega \neq 0$. Then, for all $\alpha \in \mathbb{N}^d$, there exist $C_\alpha > 0$, and $n_\alpha \in \mathbb{N}$ such that for $x \in \Omega$*

$$(38) \quad \left\| \partial_x^\alpha \vec{V}_\pm(x) \right\|_{\mathbb{C}^2} \leq C \langle x \rangle^{n_\alpha} |w(x)|^{-\alpha}.$$

Moreover, with the notation of (13), the following relation holds in Ω

$$(39) \quad \xi \cdot \nabla_x \vec{V}_\pm(x) = B_\pm(x, \xi) \vec{V}_\pm(x).$$

Proof. • **Proof of (38).** We proceed by induction on $|\alpha| \geq 1$, using the relations

$$\Pi_\pm \vec{Y}_\pm = \vec{Y}_\pm \quad \text{and} \quad |\vec{Y}_\pm|^2 = 1.$$

When $|\alpha| = 1$ with $\alpha = \mathbf{1}_j$, we derive the second relation in x_j and using the fact that the vectors are real-valued, we obtain that

$$\partial_{x_j} \vec{V}_\pm \cdot \vec{V}_\pm = 0$$

which implies that $\partial_{x_j} \vec{V}_\pm$ is colinear to \vec{V}_\mp . Deriving the first relation, we have

$$\partial_{x_j} \Pi_\pm \vec{V}_\pm + \Pi_\pm \partial_{x_j} \vec{V}_\pm = \partial_{x_j} \vec{V}_\pm$$

that is

$$(40) \quad \partial_{x_j} \Pi_\pm \vec{V}_\pm = (\text{Id}_{\mathbb{R}^2} - \Pi_\pm) \partial_{x_j} \vec{V}_\pm = \Pi_\mp \partial_{x_j} \vec{V}_\pm = \partial_{x_j} \vec{V}_\pm$$

since $\partial_{x_j} \vec{V}_\pm$ is colinear to \vec{V}_\mp . Using (35), we obtain (38) for all $\alpha \in \mathbb{N}^d$ such that $|\alpha| = 1$.

We now fix $\alpha \in \mathbb{N}^d$ and suppose that for some $C_\beta > 0$, $n_\beta \in \mathbb{N}$, we have

$$\forall \beta \in \mathbb{N}^d, |\beta| \leq |\alpha| - 1, \quad |\partial_x^\beta \vec{V}_\pm(x)| \leq C_\beta |w(x)|^{-|\beta|} \langle x \rangle^{n_\beta}.$$

Let $j \in \{1, \dots, d\}$ such that $\alpha_j \neq 0$. We apply $\partial^{\alpha - \mathbf{1}_j}$ to the relation “ $\partial_{x_j} \Pi_\pm \vec{V}_\pm = \partial_{x_j} \vec{V}_\pm$ ” from (40). The chain rule implies that $\partial_x^\alpha \vec{V}_\pm$ is a linear combination of terms $\partial^\beta \Pi_\pm \partial^\gamma \vec{V}_\pm$ for $\beta + \gamma = \alpha$ with $|\beta| > 1$ so that $|\gamma| < |\alpha|$. Using (35) and the assumption on lower order derivatives of \vec{Y}_\pm , we infer that there exist a constant C_α and an integer n_α (taking the sup on (m, ℓ)) such that (38) holds.

• **Proof of (39).** We write the proof for the *plus*-mode, since the other mode is dealt in the same manner. We first notice that

$$\xi \cdot \nabla_x \vec{V}_+ = (\xi \cdot \nabla_x \Pi_+) \vec{V}_+ + \Pi_+(\xi \cdot \nabla_x \vec{V}_+).$$

Since \vec{V}_+ is normalized and real-valued, $\Pi_+(\xi \cdot \nabla_x \vec{V}_+) = 0$ and we are left with the relation

$$\xi \cdot \nabla_x \vec{V}_+ = (\xi \cdot \nabla_x \Pi_+) \vec{V}_+ = (\xi \cdot \nabla_x \Pi_+) \Pi_+ \vec{V}_+ = \Pi_-(\xi \cdot \nabla_x \Pi_+) \Pi_+ \vec{V}_+ = B_+ \vec{V}_+.$$

□

We can now prove Propositions 1.4 and 1.5.

Proof of Proposition 1.4. 1- Differentiating in time the expression $\Pi_+(q_-(t)) \vec{Y}_-(t)$, we obtain

$$\frac{d}{dt} (\Pi_+(q_-(t)) \vec{Y}_-(t)) = p_-(t) \cdot \nabla \Pi_+(q_-(t)) \vec{Y}_-(t) + \Pi_+(q_-(t)) B_-(q_-(t)) \vec{Y}_-(t) = 0.$$

Indeed,

$$\begin{aligned} p_-(t) \cdot \nabla \Pi_+(q_-(t)) \vec{Y}_-(t) &= \Pi_+(q_-(t)) p_-(t) \cdot \nabla \Pi_+(q_-(t)) \Pi_-(q_-(t)) \vec{Y}_-(t) \\ &= -\Pi_+(q_-(t)) B_-(q_-(t)) \vec{Y}_-(t) \end{aligned}$$

by (13), (34) and $\vec{Y}_- = \Pi_- \vec{Y}_-$. Therefore, $\Pi_+(q_-(t)) \vec{Y}_-(t) = \Pi_+(q_-(t_0)) \vec{Y}_-(t_0) = 0$

2- We start by analyzing $\Pi_-(\Phi_-^{t,t_0}(z_0))$ and $(\xi \cdot \nabla \Pi_{\pm})(\Phi_{\pm}^{t,t_0}(z_0))$ when t goes to t^b with $t < t^b$. We recall

$$\Pi_-(x) = \frac{1}{2} (\text{Id} - |w(x)|^{-1} A(w(x))).$$

By equation (11) setting $\omega = (\omega_1, \omega_2)^t$, We obtain

$$(41) \quad \Pi_-(\Phi_-^{t,t_0}(z_0)) = \frac{1}{2} (\text{Id} + A(\omega)) + O(t - t^b).$$

We now consider the limit of $B_-(\Phi_-^{t,t_0}(z_0))$. Using Lemma C.1, we obtain

$$(42) \quad \begin{aligned} B_-(x, \xi) &= -\frac{\xi \cdot \nabla w(x) \wedge w(x)}{2|w(x)|^3} \Pi_+(x) \begin{pmatrix} w_2(x) & -w_1(x) \\ -w_1(x) & -w_2(x) \end{pmatrix} \Pi_-(x) \\ &= -\frac{1}{2} \Pi_+(x) \left[\frac{1}{|w(x)|} \begin{pmatrix} \xi \cdot \nabla_x w_1 & \xi \cdot \nabla_x w_2 \\ \xi \cdot \nabla_x w_2 & -\xi \cdot \nabla_x w_1 \end{pmatrix} \right. \\ &\quad \left. - \frac{(\xi \cdot \nabla_x w_1)w_1 + (\xi \cdot \nabla_x w_2)w_2}{|w(x)|^3} \begin{pmatrix} w_1 & w_2 \\ w_2 & -w_1 \end{pmatrix} \right] \Pi_-(x) \end{aligned}$$

We now specify this relation to $(x, \xi) = \Phi_-^{t,t_0}(z_0)$. By definition

$$p_-(t) \cdot \nabla_x w(q_-(t)) = r\omega + O(|t - t^b|),$$

and, using (11), we obtain

$$\frac{1}{|w(x)|} \begin{pmatrix} \xi \cdot \nabla_x w_1 & \xi \cdot \nabla_x w_2 \\ \xi \cdot \nabla_x w_2 & -\xi \cdot \nabla_x w_1 \end{pmatrix} \Big|_{(x,\xi)=\Phi_-^{t,t_0}(z_0)} = \frac{1}{|t - t^b|} \begin{pmatrix} \omega_1 & \omega_2 \\ \omega_2 & -\omega_1 \end{pmatrix} + O(1)$$

and

$$\frac{(\xi \cdot \nabla_x w_1)w_1 + (\xi \cdot \nabla_x w_2)w_2}{|w(x)|^3} \begin{pmatrix} w_1 & w_2 \\ w_2 & -w_1 \end{pmatrix} \Big|_{(x,\xi)=\Phi_-^{t,t_0}(z_0)} = \frac{1}{|t - t^b|} \begin{pmatrix} \omega_1 & \omega_2 \\ \omega_2 & -\omega_1 \end{pmatrix} + O(1),$$

that is

$$\frac{\xi \cdot \nabla w(x) \wedge w(x)}{2|w(x)|^2} \Big|_{(x,\xi)=\Phi_-^{t,t_0}(z_0)} = O(1)$$

and the singularity in $|t - t^b|^{-1}$ disappears in the expression of $B_-(\Phi_-^{t,t_0}(z_0))$. We obtain that $B_-(\Phi_-^{t,t_0}(z_0))$ is uniformly bounded in a neighborhood of t^b .

As a consequence of the last observation, we deduce the boundedness of $\partial_t \vec{Y}_-(t)$ for $t \in [t_0, t^b)$, which - in turn - implies that $\vec{Y}_-(t)$ has a limit \vec{V}_ω when t goes to $(t^b)^-$ which is normalized and real-valued. Besides, by (41), \vec{V}_ω is in the range of $\frac{1}{2}(\text{Id}_{\mathbb{C}^2} + A(\omega))$, thus an eigenvector of $A(\omega)$.

3- One checks that the function $w(x) \cdot \omega$ is non zero along the curves $\Phi_-^{t,t_0}(z_0)$ for t close to t^b . Therefore, we choose the function $\vec{V}_-(x)$ that is a smooth real-valued eigenvector of $V(x)$ for the *minus*-mode in the region $\{w(x) \cdot \omega \neq 0\}$ and so that $\vec{V}_-(q_-(t))$ has the same limit \vec{V}_ω than $\vec{Y}_-(t)$

as t goes to t^b with $t < t^b$ by turning \vec{V}_- into $-\vec{V}_-$ if necessary. Then, the result comes from the observation

$$\begin{aligned} \frac{d}{dt} \vec{V}_-(q_-(t)) &= p_-(t) \cdot \nabla \vec{V}_-(q_-(t)) = \Pi_+(q_-(t)) p_-(t) \cdot \nabla \vec{V}_-(q_-(t)) \\ &= \Pi_+(q_-(t)) p_-(t) \cdot \nabla \Pi_-(q_-(t)) \vec{V}_-(q_-(t)) = B_-(\Phi_-^{t,t^b}(z_0)) \vec{Y}_-(t), \end{aligned}$$

where we have used $(\xi \cdot \nabla \Pi_-) \vec{Y}_- = \Pi_+ \xi \cdot \nabla \vec{V}_- = \xi \cdot \nabla \vec{V}_-$. \square

Proof of Proposition 1.5. The proposition follows the same ideas than in the preceding one and is based on the following observations

$$(43) \quad \Pi_-(\Phi_-^{t,t^b}(z^b)) \xrightarrow{t \rightarrow (t^b)^-} V_\omega \otimes \bar{V}_\omega, \quad \Pi_+(\Phi_+^{t,t^b}(z^b)) \xrightarrow{t \rightarrow (t^b)^-} V_\omega^\perp \otimes \bar{V}_\omega^\perp,$$

$$(44) \quad \Pi_+(\Phi_+^{t,t^b}(z^b)) \xrightarrow{t \rightarrow (t^b)^+} V_\omega \otimes \bar{V}_\omega, \quad \Pi_-(\Phi_-^{t,t^b}(z^b)) \xrightarrow{t \rightarrow (t^b)^+} V_\omega^\perp \otimes \bar{V}_\omega^\perp,$$

$$(45) \quad (\xi \cdot \nabla \Pi_\pm)(\Phi_\pm^{t,t^b}(z^b)) = O(1) \quad \text{when } t \sim t^b.$$

\square

2.3. Resolution of the profile equations. In this section, properties of the solutions of equation (18) are discussed and Proposition 1.6 and Corollary 1.7 are proved. A crucial element of the proof is a good understanding of the singularity of the Hessian of the function λ_\pm along the trajectories. We start by a technical Lemma that we shall use later.

Lemma 2.4. *There exist smooth matrices $M_\pm(t)$ defined on $[t_0, t^b]$ (resp. $[t^b, t^b + \tau]$) such that when t tends to t^b with $t < t^b$ (resp. $t > t^b$),*

$$(46) \quad \text{Hess } \lambda_\pm(q_\pm(t)) = M_\pm(t) \pm |t - t^b|^{-1} \Gamma_0$$

with Γ_0 given by (20).

Proof. We have $\text{Hess } \lambda_\pm = \text{Hess } v \pm \text{Hess}(|w|)$ and

$$\partial_{x_i x_j}^2(|w|) = \partial_{x_i x_j}^2 w \cdot \frac{w}{|w|} + \frac{\partial_{x_i} w \cdot \partial_{x_j} w}{|w|} - \frac{(\partial_{x_i} w \cdot w)(\partial_{x_j} w \cdot w)}{|w|^3}.$$

We deduce from (11) that

$$\text{Hess } \lambda_\pm(q_\pm(t)) = \pm \frac{1}{|t - t^b|} \Gamma_0 \pm \text{sgn}(t - t^b) d^2 w(z^b) \omega + \text{Hess } v(q^b) + \mathcal{O}(t - t^b)$$

with

$$\Gamma_0 = r^{-1} (\partial_{x_i} w \cdot \partial_{x_j} w - (\partial_{x_j} w \cdot \omega)(\partial_{x_i} w \cdot \omega))_{1 \leq i, j \leq d},$$

whence (20) \square

We now prove Proposition 1.6.

Proof of Proposition 1.6. Let us consider the operator

$$(47) \quad Q_\pm(t) = -\frac{1}{2} \Delta_y + \frac{1}{2} \text{Hess } \lambda_\pm(q_\pm(t)) y \cdot y.$$

This operator has a classical symbol $(y, \xi) \mapsto \frac{1}{2} |\xi|^2 + \frac{1}{2} \text{Hess}(\lambda_\pm(\Phi_\pm^{t,t^b}(z_0))) y \cdot y$ that enjoys subquadratic estimates in the interval $[t_0, t^b[$, which guarantees the existence of the solution (see [34]):

the solution $u_{\pm}(t)$ exists for all $t \in [t_0, t^b[$ and is in all spaces Σ^k for $k \in \mathbb{N}$. Since we know that the L^2 -norm is conserved, we focus on $\|u_{\pm}(t)\|_{\Sigma^k}$ for $k \geq 1$.

For convenience, we fix a mode, the *plus*-mode, and choose $t < t^b$. So we drop any mention of the mode as it will cause no confusion in this part of the paper:

$$Q(t) = Q_+(t), \quad \lambda(q(t)) = \lambda_+(q_+(t)), \quad u = u_+.$$

The proofs for the *minus*-mode or for $t > t^b$ are similar. We set the following notation,

$$U = {}^t(yu, D_y u),$$

and our aim is to prove that the norms $\|U\|_{\Sigma^k}$ are bounded for all $k \in \mathbb{N}$. Using

$$(48) \quad [Q(t), D_y] = -i \text{Hess } \lambda(q(t))y \quad \text{and} \quad [Q(t), y] = -\nabla_y = -iD_y,$$

we obtain

$$[Q(t), {}^t(y, D_y)]u_{\pm} = {}^t(-iD_y u, i \text{Hess } \lambda(q(t))y u) = -i \begin{pmatrix} 0 & \text{Id}_{\mathbb{R}^d} \\ \text{Hess } \lambda(q(t)) & 0 \end{pmatrix} {}^t(yu, D_y u)U.$$

We deduce the equation

$$i\partial_t U - Q(t)U = \left[Q(t), \begin{pmatrix} y \\ D_y \end{pmatrix} \right] u = -i \begin{pmatrix} 0 & \text{Id}_{\mathbb{R}^d} \\ \text{Hess } \lambda(q(t)) & 0 \end{pmatrix} U$$

This system is closed and by Lemma 2.4 it is a system of the form

$$i\partial_t U - Q(t)U = (M(t) + i(t - t^b)^{-1}\Gamma)U,$$

where $t \mapsto M(t)$ smoothly depends on t for $t \in [t_0, t^b[$ (meaning that it has - as its derivatives - limits when t goes to t^b from below) and

$$\Gamma = \begin{pmatrix} 0 & 0 \\ -\Gamma_0 & 0 \end{pmatrix},$$

for Γ_0 defined in (20). Our aim is to prove the following claim :

Claim: *For all $k \in \mathbb{N}$, there exists $C_k > 0$ such that for all $t \in [t_0, t^b[$*

$$\|U(t)\|_{\Sigma^k(\mathbb{R}^d, \mathbb{C}^{2d})} \leq C_k \left(1 + \left| \ln |t - t^b| \right| \right).$$

For that purpose, we introduce the following projector of rank d

$$\mathbb{P} = \begin{pmatrix} 0 & 0 \\ 0 & \text{Id}_{\mathbb{R}^d} \end{pmatrix} \quad ; \quad \text{satisfying} \quad (1 - \mathbb{P})\Gamma = 0 \quad \text{and} \quad \mathbb{P}\Gamma = \mathbb{P}\Gamma(1 - \mathbb{P}).$$

Step one: $k = 0$. We set $V = (1 - \mathbb{P})U$ and $W = \mathbb{P}U$. Then, because $(1 - \mathbb{P})\Gamma = 0$,

$$i\partial_t V - Q(t)V = (1 - \mathbb{P})M(t)(V + W)$$

and

$$i\partial_t W - Q(t)W = i(t - t^b)^{-1}\mathbb{P}\Gamma V + \mathbb{P}M(t)(V + W).$$

We then introduce the variable

$$\tilde{V} = W - \ln |t - t^b| \mathbb{P}\Gamma V$$

so that \tilde{V} satisfies

$$\begin{aligned} i\partial_t \tilde{V} - Q(t)\tilde{V} &= \mathbb{P}M(t)(V + W) - \ln|t - t^b| \mathbb{P}\Gamma(i\partial_t V - Q(t)V) \\ &= \mathbb{P}M(t)(V + W) - \ln|t - t^b| \mathbb{P}\Gamma(1 - \mathbb{P})M(t)(V + W) \\ &= (\mathbb{P} - \ln|t - t^b| \mathbb{P}\Gamma)M(t)(V + \tilde{V} + \ln|t - t^b| \mathbb{P}\Gamma V). \end{aligned}$$

To conclude, V and \tilde{V} satisfy the system

$$(49) \quad \begin{cases} i\partial_t V - Q(t)V &= A(t)V + B(t)\tilde{V} \\ i\partial_t \tilde{V} - Q(t)\tilde{V} &= \tilde{A}(t)V + \tilde{B}(t)\tilde{V}, \end{cases}$$

with $t \mapsto A(t), B(t), \tilde{A}(t), \tilde{B}(t)$ are smooth on $[t_0, t^b)$ and integrable on $[t_0, t^b]$. The change of unknown has contributed to improve the integrability of the functions of the right-hand side of the system. It allows us to conclude thanks to an energy estimate and Grönwall lemma. As a consequence, there exists a constant $C > 0$ such that

$$\forall t \in [t_0, t^b), \quad \|V(t)\|_{L^2} + \|\tilde{V}(t)\|_{L^2} \leq C.$$

Since we can write

$$U = V + W = V + \tilde{V} + \ln|t - t^b| \mathbb{P}\Gamma V,$$

this implies the existence of $C_1 > 0$ such that for all $t \in [t_0, t^b)$

$$\begin{aligned} \|U(t)\|_{L^2} &\leq \|V(t)\|_{L^2} + \|\tilde{V}(t)\|_{L^2} + \|\ln|t - t^b| \mathbb{P}\Gamma V(t)\|_{L^2} \\ &\leq C_1 \left(1 + \left|\ln|t - t^b|\right|\right). \end{aligned}$$

Step two: $k = 1$. In view of (48), the quantities

$$y_j V, \quad y_j \tilde{V}, \quad D_{y_j} V, \quad D_{y_j} \tilde{V}, \quad 1 \leq j \leq d$$

satisfy a closed system of equations of the form

$$\begin{aligned} i\partial_t(y_j V) - Q(t)(y_j V) &= A(t)(y_j V) + B(t)(y_j \tilde{V}) + iD_{y_j} V, \\ i\partial_t(y_j \tilde{V}) - Q(t)(y_j \tilde{V}) &= \tilde{A}(t)(y_j V) + \tilde{B}(t)(y_j \tilde{V}) + iD_{y_j} \tilde{V}, \\ i\partial_t(D_{y_j} V) - Q(t)(D_{y_j} V) &= A(t)(D_{y_j} V) + B(t)(D_{y_j} \tilde{V}) + C(t) \cdot y V \\ &\quad + i|t - t^b|^{-1}(e_j \cdot \Gamma_0 y) V, \\ i\partial_t(D_{y_j} \tilde{V}) - Q(t)(D_{y_j} \tilde{V}) &= \tilde{A}(t)D_{y_j} V + \tilde{B}(t)(D_{y_j} \tilde{V}) + \tilde{C}(t) \cdot y \tilde{V} \\ &\quad + i|t - t^b|^{-1}(e_j \cdot \Gamma_0 y) \tilde{V}, \end{aligned}$$

where $A(t), \tilde{A}(t), B(t), \tilde{B}(t), C(t)$ and $\tilde{C}(t)$ are smooth maps. Again, this system presents the non-integrable singularity $|t - t^b|^{-1}$ in the right-hand side that calls for a change of unknown, as we previously did. We write $V_1 = V \in \mathbb{C}^d$, $\tilde{V}_1 = \tilde{V} \in \mathbb{C}^d$ and consider the derivatives and momenta of V_1 and \tilde{V}_1 . We set

$$V_2 = (y_1 V, \dots, y_d V, y_1 \tilde{V}, \dots, y_d \tilde{V})$$

and

$$\tilde{V}_2 = ((D_{y_j} V + \ln|t - t^b|(e_j \cdot \Gamma_0 y)V)_{1 \leq j \leq d}, (D_{y_j} \tilde{V} + \ln|t - t^b|(e_j \cdot \Gamma_0 y)\tilde{V})_{1 \leq j \leq d}),$$

where $(e_j)_j$ is the canonical basis of \mathbb{R}^d . We have: $V_2, \tilde{V}_2 \in \mathbb{C}^{(2d)^2}$ and the functions $t \mapsto V_2(t), \tilde{V}_2(t)$ satisfy a system of the form

$$\begin{cases} i\partial_t V_2 - Q(t)V_2 &= A_2(t)V_2 + B_2(t)\tilde{V}_2 \\ i\partial_t \tilde{V}_2 - Q(t)\tilde{V}_2 &= \tilde{A}_2(t)V_2 + \tilde{B}_2(t)\tilde{V}_2 \end{cases}$$

with $A_2(t), B_2(t), \tilde{A}_2(t), \tilde{B}_2(t)$ are integrable.

Arguing as above by using an energy estimate and Grönwall lemma, together with the control established for V_1, \tilde{V}_1 , we obtain a control of the L^2 -norm of $(V_2(t), \tilde{V}_2(t))$ of the form

$$\|V_2(t)\|_{L^2(\mathbb{R}^d, \mathbb{C}^{(2d)^2})} + \|\tilde{V}_2(t)\|_{L^2(\mathbb{R}^d, \mathbb{C}^{(2d)^2})} \leq C'_2.$$

We then write

$$\begin{aligned} \|U(t)\|_{\Sigma^1} &\leq \|U(t)\|_{L^2} + \|V_2(t)\|_{L^2} + \|\tilde{V}_2(t)\|_{L^2} + \|\ln|t - t^b|(e_j \cdot \Gamma_0 y)V_1(t)\|_{L^2} \\ &\quad + \|\ln|t - t^b|(e_j \cdot \Gamma_0 y)\tilde{V}_1(t)\|_{L^2} \\ &\leq C_2 \left(1 + \left| \ln|t - t^b| \right| \right), \end{aligned}$$

where we have noticed that $\|(e_j \cdot \Gamma_0 y)V_1(t)\|_{L^2}$ is controlled by $\|V_2(t)\|_{L^2}$, and the same holds with the *tilda*-term.

Step three: from k to $k+1$. At the $(k-1)$ -th step, we are left with a vector

$$(V_k(t), \tilde{V}_k(t)) \in \mathbb{C}^{(2d)^k}$$

satisfying a system of the form

$$\begin{cases} i\partial_t V_k - Q(t)V_k &= A_k(t)V_k + B_k(t)\tilde{V}_k \\ i\partial_t \tilde{V}_k - Q(t)\tilde{V}_k &= \tilde{A}_k(t)V_k + \tilde{B}_k(t)\tilde{V}_k \end{cases}$$

with $A_k(t), B_k(t), \tilde{A}_k(t), \tilde{B}_k(t)$ are integrable. This leads to the construction of a vectors of $(2d)^k = d(2d)^{k-1} + d(2d)^{k-1}$ variables. Re-organizing the equation in order to cancel the singularity generated by the commutator $[D_y, Q(t)]$: we set

$$V_{k+1} = (y_1 V_k, \dots, y_d V_k, y_1 \tilde{V}_k, \dots, y_d \tilde{V}_k)$$

$$\text{and } \tilde{V}_{k+1} = ((D_{y_j} V_k + \ln|t - t^b|(e_j \cdot \Gamma_0 y)V_k)_{1 \leq j \leq d}, (D_{y_j} \tilde{V}_k + \ln|t - t^b|(e_j \cdot \Gamma_0 y)\tilde{V}_k)_{1 \leq j \leq d}).$$

One can proceed as before and one obtains the boundedness of $(V_{\ell+1}, \tilde{V}_{\ell+1})$ in L^2 , whence the existence of $C_{k+1}, C'_{k+1} > 0$ such that

$$\|(V_k, \tilde{V}_k)\|_{\Sigma^1} \leq c_k \|(V_{k+1}, \tilde{V}_{k+1})\|_{L^2} \leq C'_{k+1},$$

which implies $\|U\|_{\Sigma^k} \leq C_{k+1} \left(1 + \left| \ln|t - t^b| \right| \right)$. □

With Proposition 1.6, we have a precise information on the behavior of the Σ^k -norms of the solutions to the system (18). This allows to characterize their behaviors on the crossing set and to solve the equation (18) after the crossing time. This is the subject of Corollary 1.7 that we now prove.

Proof of Corollary 1.7. Let us assume $t < t^b$ and set

$$v_{\pm}(t) = \text{Exp} \left[\mp \frac{i}{2} \Gamma_0 y \cdot y \ln |t - t^b| \right] u_{\pm}(t).$$

We have

$$\begin{aligned} i\partial_t v_{\pm}(t) &= \text{Exp} \left[\mp \frac{i}{2} \Gamma_0 y \cdot y \ln |t - t^b| \right] \times \left(i\partial_t u_{\pm} \mp \frac{1}{2|t - t^b|} \Gamma_0 y \cdot y u_{\pm} \right), \\ &= \text{Exp} \left[\mp \frac{i}{2} \Gamma_0 y \cdot y \ln |t - t^b| \right] \times \\ &\quad \left(-\frac{1}{2} \Delta_y u_{\pm}(t) + \frac{1}{2} (\text{Hess} \lambda_{\pm}(q_{\pm}(t)) y \cdot y) u_{\pm}(t) \mp \frac{1}{2|t - t^b|} \Gamma_0 y \cdot y u_{\pm} \right) \\ &= \text{Exp} \left[\mp \frac{i}{2} \Gamma_0 y \cdot y \ln |t - t^b| \right] \times \left(-\frac{1}{2} \Delta_y u_{\pm}(t) + \frac{1}{2} M_{\pm}(t) y \cdot y u_{\pm} \right) \end{aligned}$$

where the matrix $M_{\pm}(t)$ is defined in Lemma 2.4 and is smooth on $[t_0, t^b]$ (the term $\pm(t - t^b)^{-1} \Gamma_0 y \cdot y$ compensates for the singularity of the potential of the operator $Q(t)$ (see (47)). We now use Proposition 1.6. Therefore, for all $t \in [t_0, t^b]$, $\partial_t v_{\pm}(t) \in \Sigma^k$ for all $k \in \mathbb{N}$. Besides, for each $k \in \mathbb{N}$, in view of the control (19), there exist constants $C_k, \tilde{C}_k > 0$ and $N_k, \tilde{N}_k \in \mathbb{N}$ such that

$$\|\partial_t v_{\pm}(t)\|_{\Sigma^k} \leq C_k \left(1 + |\ln |t - t^b|| \right)^{N_k} \|u_{\pm}(t)\|_{\Sigma^{k+2}} \leq \tilde{C}_k \left(1 + |\ln |t - t^b|| \right)^{\tilde{N}_k}$$

We deduce that $\int_{t_0}^{t^b} \partial_t v_{\pm}(s) ds$ is well-defined as a function of Σ^k and we denote by u_{\pm}^{in} this function that satisfies (21).

We now want to use u_{\pm}^{in} as an initial data at time t^b . We observe that the function $v_{\pm}(t)$ solves an equation of the form

$$(50) \quad i\partial_t v_{\pm} = H(t)v_{\pm}$$

with

$$\begin{aligned} H(t) &= -\frac{1}{2} \Delta \pm a(t)y \cdot D_y \pm c(t) + b(t)y \cdot y, \\ a(t) &= \Gamma_0 \ln |t - t^b|, \quad c(t) = -\frac{i}{2} \text{tr}(\Gamma_0) \ln |t - t^b| \\ b(t)y \cdot y &= \frac{1}{2} M_{\pm}(t)y \cdot y + \frac{1}{2} (\ln |t - t^b|)^2 |\Gamma_0 y|^2. \end{aligned}$$

Note that

$$a(t)y \cdot D_y + c(t) = \frac{1}{2} (a(t)y \cdot D_y) + \frac{1}{2} (a(t)y \cdot D_y)^*.$$

The operator $H(t)$ is a self-adjoint quadratic operator with time-integrable coefficients to which we can associate a two-parameters propagator $\tilde{\mathcal{U}}(t, s)$ defined for $t, s \in [t_0, t^b]$ (see [34]). our aim is to construct $\mathcal{U}(s, t^b)$. We use the following facts:

- (1) It is equivalent to say that $u_{\pm}(t)$ solves (18) and to say that $v_{\pm}(t)$ solves (50).
- (2) There is conservation of the L^2 -norm and

$$\|v_{\pm}(t)\|_{L^2} = \|v_{\pm}(t_0)\|_{L^2} = \|u_{\pm}(t_0)\|_{L^2}.$$

- (3) When t tends to t^b , $\tilde{\mathcal{U}}(t, s)u_{\pm}(t_0)$ has a limit u_{\pm}^{in} with $\|u_{\pm}(t_0)\|_{L^2} = \|u_{\pm}^{\text{in}}\|_{L^2}$. Let us denote by $\tilde{\mathcal{U}}(t^b, s)$ the operator mapping $u_{\pm}(t_0)$ to u_{\pm}^{in} .

(4) For all $f \in \mathcal{S}(\mathbb{R}^d)$, $k \in \mathbb{N}$ there exists $C_k > 0$ such that

$$\forall f \in \mathcal{S}(\mathbb{R}^d), \quad \|\tilde{\mathcal{U}}(t^b, s)f\|_{\Sigma^k} \leq C_k \|f\|_{\Sigma^{k+3}}.$$

We claim that for $t, s \in [t_0, t^b)$ we have $\tilde{\mathcal{U}}(s, t) = \tilde{\mathcal{U}}(t, s)^*$, which allows to define the operator $\tilde{\mathcal{U}}(s, t^b)$ by

$$\tilde{\mathcal{U}}(s, t^b) := \tilde{\mathcal{U}}(t^b, s)^*.$$

Indeed, from the definition of $\tilde{\mathcal{U}}(t, s)$ as solving

$$(51) \quad i\partial_t \tilde{\mathcal{U}}(t, s) = H(t)\tilde{\mathcal{U}}(t, s), \quad \tilde{\mathcal{U}}(s, s) = \text{Id}_{\mathbb{R}^2},$$

we deduce on one hand, that

$$i\partial_t \tilde{\mathcal{U}}(t, s)^* = -\tilde{\mathcal{U}}(t, s)^* H(t), \quad \tilde{\mathcal{U}}(s, s) = \text{Id}_{\mathbb{R}^2},$$

and on the other hand, differentiating in s the relation (51), we obtain that $V(t, s) = \partial_s \tilde{\mathcal{U}}(t, s)$ satisfies

$$i\partial_t V(t, s) = H(t)V(t, s), \quad V(s, s) = -\partial_t \tilde{\mathcal{U}}(s, s) = iH(s).$$

Therefore, $V(t, s) = \tilde{\mathcal{U}}(t, s)iH(s)$, which gives $i\partial_s \tilde{\mathcal{U}}(t, s) = -\tilde{\mathcal{U}}(t, s)H(s)$. Exchanging the roles of t and s we obtain that $\tilde{\mathcal{U}}(s, t)$ solves the same equation as $\tilde{\mathcal{U}}(t, s)^*$ with the same initial data and thus, they are equal.

Therefore, we have proved that we can build a function $u^\pm(t)$ solving (18) for $t \leq t^b$, starting from a profile u_\pm^{in} on t^b with enough regularity, in particular for $u_\pm^{\text{in}} \in \mathcal{S}(\mathbb{R}^d)$. Arguing in a similar way in the zone $t > t^b$, we deduce that there exists a unique solution to (18) satisfying (22) for some given $u_\pm^{\text{out}} \in \mathcal{S}(\mathbb{R}^d)$. \square

3. ADIABATIC TRANSPORT OUTSIDE THE GAP REGION

This section is inspired by [18] and discussions with Caroline Lasser and Didier Robert. We focus here on zones that are far enough from the gap region in the sense that $|w(x)| > \delta$, along the trajectories concerned by the process. In this adiabatic region, we prove the following result showing that one can approximate the solution of the system (1) by solutions of scalar type equations.

Proposition 3.1. *Let $k \in \mathbb{N}$ and $\delta \in (0, 1)$ such that $\sqrt{\varepsilon}\delta^{-1} \ll 1$. Consider $s_1, s_2 \in \mathbb{R}$, $s_1 < s_2$ and two classical trajectories $z_\pm(t)_{t \in [s_1, s_2]}$ that reach the crossing set Υ at time t^b at a point where Assumptions 1.1 are satisfied. We assume $[s_1, s_2] \subset \{|t - t^b| > \delta\}$ and that at initial time s_1 ,*

$$\left\| \psi^\varepsilon(s_1) - \vec{Y}_+(s_1)v_+^\varepsilon(s_1) - \vec{Y}_-(s_1)v_-^\varepsilon(s_1) \right\|_{\Sigma_\varepsilon^k} \leq C\sqrt{\varepsilon},$$

$$v_\pm^\varepsilon(s_1) = \text{WP}_{z_\pm(s_1)}^\varepsilon(u_\pm(s_1)), \quad u_\pm(s_1) \in \mathcal{S}(\mathbb{R}^d), \quad z_\pm(s_1) = (q_\pm(s_1), p_\pm(s_1)) \in \mathbb{R}^{2d},$$

and with $\Pi_\pm(q_\pm(s_1))\vec{Y}_\pm(s_1) = \vec{Y}_\pm(s_1)$. Then, for all $k \in \mathbb{N}$, one has

$$\sup_{t \in [s_1, s_2]} \left\| \Pi_\pm \psi^\varepsilon(t) - \vec{Y}_\pm(t)v_\pm^\varepsilon(t) \right\|_{\Sigma_\varepsilon^k} \leq C_k(1 + |\ln \delta|) \left(\frac{\varepsilon^{3/2}}{\delta^4} + \frac{\sqrt{\varepsilon}}{\delta} \right),$$

where the constant C_k is uniform in δ and ε , and for $t \in [s_1, s_2]$

- the functions $v_\pm^\varepsilon(t)$ are wave packets:

$$(52) \quad v_\pm^\varepsilon(t) = e^{\frac{i}{\varepsilon}S_\pm(t)} \text{WP}_{z_\pm(t)}^\varepsilon(u_\pm(t)),$$

- the trajectory $z_{\pm}(t)$ is the classical trajectory $z_{\pm}(t) = \Phi_{\pm}^{t,s_1}(z_{\pm}(s_1))$ and $S_{\pm}(t)$ is the related action $S_{\pm}(t) = S_{\pm}(t, s_1, z_{\pm}(s_1))$ (see (12)),
- the functions $u_{\pm}(t)$ satisfy (18) with data $u_{\pm}(s_1)$ at time s_1 and their norms in spaces Σ^k satisfy (19),
- the vectors $\vec{Y}_{\pm}(t)$ are defined in Section 1.1.2 and satisfy $\Pi_{\pm}(z_{\pm}(t))\vec{Y}_{\pm}(t) = \vec{Y}_{\pm}(t)$, together with $\partial_t \vec{Y}_{\pm}(t) = B_{\pm}(z_{\pm}(t))\vec{Y}_{\pm}(t)$.

Note first that, by the results of Section 2, all the quantities involved in Proposition 3.1 are well defined for $t \in [s_1, s_2]$. Besides, the solution at time $t \in [s_1, s_2]$ on each mode only depends on the data on the same mode at time s_1 . This is the reason why one may say that the approximation is of “scalar type” as mentioned before.

Note also that the assumptions of Proposition 3.1 imply that there exists $c > 0$ such that

$$\forall t \in [s_1, s_2], \quad |w(z_{\pm}(t))| > c\delta.$$

In the proof of Theorem 1.9, we will use Proposition 3.1 twice: first between $s_1 = t_0$ and $s_2 = t^b - \delta$ with $u_+(t_0) = 0$ and $u_-(t_0) = a$, then, between $s_1 = t^b + \delta$ and s_2 equal to some final time t with the profiles $u_{\pm}(t^b + \delta)$ arising from the process of passing through the crossing.

For proving Proposition 3.1, we use the semi-classical formalism of Appendix A and the pseudo-differential operators introduced therein: with $a \in \mathcal{C}^{\infty}(\mathbb{R}^{2d}, \mathbb{C}^N)$ ($N = 1$ or 2), we associate the operator $\text{op}_{\varepsilon}(a)$ defined by (79). We shall use the matrices \mathbb{P} , $\mathbb{P}_{\pm}^{(2)}$, Ω and $\Omega_{\pm}^{(2)}$ of Section C.2. We work close enough to the crossing time t^b so that the curves $z_{\pm}(t)$ are included in $\{w(x) \cdot \omega \neq 0\}$ for all $t \in [s_1, s_2]$. Indeed, far from t^b , the proof is easier since one does not see the singularities of the involved quantities. The proof is divided into two steps: we first identify an approximate solution satisfied by an auxiliary ansatz that is close to the function $\vec{Y}_{\pm}(t)v_{\pm}^{\varepsilon}(t)$ (Lemma 3.4 in Section 3.1), then we prove that $\Pi_{\pm}\psi^{\varepsilon}(t)$ (up to some remainder) satisfies the same equation (Section 3.2).

3.1. The adiabatic ansatz. For proving Proposition 3.1, we first introduce cut-off functions that allow us to restrict the analysis close to the trajectories, where the functions λ_{\pm} and related quantities are smooth. Let I be an interval containing $[s_1, s_2]$. We construct $\chi_{\pm}^{\delta} \in \mathcal{C}(I, \mathcal{C}_0^{\infty}(\mathbb{R}^{2d}))$, compactly supported in $\{|w(x)| > \delta\}$, equal to 1 close to the curve $(z_{\pm}(t))_{t \in [s_1, s_2]}$ and satisfying

$$(53) \quad \partial_t \chi_{\pm}^{\delta} + \left\{ \frac{|\xi|^2}{2} + \lambda_{\pm}, \chi_{\pm}^{\delta} \right\} = 0.$$

Remark 3.2. Let s_1, s_2 as in Proposition 3.1. The functions χ_{\pm}^{δ} can be taken for $t \in [s_1, s_2]$ as

$$\chi_{\pm}^{\delta}(t, x, \xi) = \chi \left(\frac{\Phi_{\pm}^{t, s_2}(x, \xi) - z_{\pm}(s_2)}{\delta} \right)$$

where $0 \leq \chi \leq 1$ with $\chi = 1$ close to 0 and $\chi = 0$ far from 0.

We also introduce $\tilde{\chi}_{\pm}^{\delta} \in \mathcal{C}(I, \mathcal{C}_0^{\infty}(\mathbb{R}^{2d}))$ compactly supported, such that for all $t \in [s_1, s_2]$, we have $\tilde{\chi}_{\pm}^{\delta}(t) = 1$ on $\text{supp } \chi_{\pm}^{\delta}(t)$. We have

$$(54) \quad \text{for } \alpha \in \mathbb{N}^{2d}, \quad \partial^{\alpha} \chi_{\pm}^{\delta} = \mathcal{O}(\delta^{-|\alpha|}) ; \quad \partial^{\alpha} \tilde{\chi}_{\pm}^{\delta} = \mathcal{O}(\delta^{-|\alpha|})$$

Step one: reduction to an auxiliary ansatz. Let \vec{V}_{\pm} be the smooth functions defined in (3) of Proposition 1.4, that is a smooth eigenvector of the matrix $V(x)$ satisfying $\vec{Y}_{\pm}(t) = \vec{V}_{\pm}(q_{\pm}(t))$.

Lemma 3.3. *Let $\delta \in (0, 1]$ be such that $\sqrt{\varepsilon}\delta^{-1} \ll 1$. Then, we have for $t \in [s_1, s_2]$,*

$$\vec{Y}_{\pm}(q_{\pm}(t))v_{\pm}^{\varepsilon}(t) = \text{op}_{\varepsilon} \left(\chi_{\pm}^{\delta}(t, x, \xi) \vec{V}_{\pm}(x) \right) v_{\pm}^{\varepsilon}(t) + \mathcal{O}(\sqrt{\varepsilon}\delta^{-1}(1 + |\ln \delta|)).$$

Proof. The proof relies on the application of Lemma B.2 with $n_0 = 0$ to the symbol $a(t, x, \xi) = \chi_{\pm}^{\delta}(t, x, \xi) \vec{V}_{\pm}(x)$, which requires the computation of the semi-norms

$$N_{d+k+1}^{\varepsilon}(\partial_{z_j} a) = \sum_{\alpha \in \mathbb{N}^{2d}, |\alpha| \leq n_{d+k+1}} \varepsilon^{\frac{|\alpha|}{2}} \sup_{\mathbb{R}^{2d}} |\partial_z^{\alpha} \partial_{z_j} a|, \quad 1 \leq j \leq 2d,$$

where for $\ell \in \mathbb{N}$, $n_{\ell} = M\ell$, $M \geq 1$. With $a = \chi_{\pm}^{\delta} \vec{V}_{\pm}$ and in view of Lemma 2.3 and equation (54), we obtain

$$\begin{aligned} \sqrt{\varepsilon} N_{d+k+1}^{\varepsilon}(\partial_{z_j} a) &\leq C\sqrt{\varepsilon} \left(\sum_{|\alpha| \leq n_{d+k+1}} \varepsilon^{|\alpha|/2} \sup_{\mathbb{R}^{2d}} \left| \partial_z^{\alpha} ((\partial_{z_j} \chi_{\pm}^{\delta}) \vec{V}_{\pm}) \right| + \sum_{|\alpha| \leq n_{d+k+1}} \varepsilon^{|\alpha|/2} \sup_{\mathbb{R}^{2d}} \left| \partial_z^{\alpha} (\chi_{\pm}^{\delta} \partial_{z_j} \vec{V}_{\pm}) \right| \right) \\ &\leq C'\sqrt{\varepsilon} \sum_{|\alpha| \leq n_{d+k+1}} \varepsilon^{|\alpha|/2} \delta^{-|\alpha|-1} = C' \sum_{|\alpha| \leq n_{d+k+1}} (\sqrt{\varepsilon}\delta^{-1})^{|\alpha|+1} = O(\sqrt{\varepsilon}\delta^{-1}) \end{aligned}$$

since $\sqrt{\varepsilon}\delta^{-1} \ll 1$.

We can now see, thanks to Lemma B.2 and the previous computation, that we have in Σ_{ε}^k , for some integer N'

$$\begin{aligned} \text{op}_{\varepsilon} \left(\chi_{\pm}^{\delta}(t, x, \xi) \vec{V}_{\pm}(x) \right) v_{\pm}^{\varepsilon}(t) &= e^{\frac{i}{\varepsilon} S_{\pm}(t)} \text{op}_{\varepsilon} \left(\chi_{\pm}^{\delta}(t, x, \xi) \vec{V}_{\pm}(x) \right) \text{WP}_{z_{\pm}(t)}^{\varepsilon}(u_{\pm}(t)) \\ &= e^{\frac{i}{\varepsilon} S_{\pm}(t)} \text{WP}_{z_{\pm}(t)}^{\varepsilon} \left(\chi_{\pm}^{\delta}(t, z_{\pm}(t)) \vec{V}_{\pm}(q_{\pm}(t)) \right) u_{\pm}(t) + \mathcal{O}(\sqrt{\varepsilon}\delta^{-1} \|u_{\pm}(t)\|_{\Sigma^{N'}}) \\ &= \vec{Y}_{\pm}(t) e^{\frac{i}{\varepsilon} S_{\pm}(t)} \text{WP}_{z_{\pm}(t)}^{\varepsilon} u_{\pm}(t) + \mathcal{O}(\sqrt{\varepsilon}\delta^{-1}(1 + |\ln \delta|)) \\ &= \vec{Y}_{\pm}(t) v_{\pm}^{\varepsilon}(t) + \mathcal{O}(\sqrt{\varepsilon}\delta^{-1}(1 + |\ln \delta|)) \end{aligned}$$

where we have used to definition of χ_{\pm}^{δ} , the estimation on the profiles (19), $\chi_{\pm}^{\delta}(t, z_{\pm}(t)) = 1$ and Lemma B.1. \square

Step two: Analysis of the ansatz. We now study the properties of the ansatz

$$(55) \quad \psi_{\pm, \text{app}}^{\varepsilon}(t) = \text{op}_{\varepsilon} \left(\chi_{\pm}^{\delta}(t, x, \xi) \vec{V}_{\pm}(x) \right) v_{\pm}^{\varepsilon}(t).$$

We analyze the equations satisfied by $\psi_{\pm, \text{app}}^{\varepsilon}$ and use the notations of Section C.2.

Lemma 3.4. *Let $k \in \mathbb{N}$ and $\delta \in (0, 1]$ be such that $\sqrt{\varepsilon}\delta^{-1} \ll 1$. With the notations of Proposition 3.1 and Equation (55), for $t \in [s_1, s_2]$, we have*

$$\begin{aligned} i\varepsilon \partial_t \psi_{\pm, \text{app}}^{\varepsilon} &= -\frac{\varepsilon^2}{2} \Delta \psi_{\pm, \text{app}}^{\varepsilon} + \lambda_{\pm}(x) \psi_{\pm, \text{app}}^{\varepsilon} + \varepsilon \text{op}_{\varepsilon}(\Omega \tilde{\chi}_{\pm}^{\delta}) \psi_{\pm, \text{app}}^{\varepsilon} + \varepsilon^2 \text{op}_{\varepsilon}(\Omega_{\pm}^{(2)} \tilde{\chi}_{\pm}^{\delta}) \psi_{\pm, \text{app}}^{\varepsilon} \\ &\quad + \mathcal{O}\left((\varepsilon^{3/2} + \varepsilon^2 \delta^{-2} + \varepsilon^{5/2} \delta^{-4})(1 + |\ln \delta|)\right) \end{aligned}$$

in Σ_{ε}^k , where $\Omega_{\pm}^{(2)}$ is given in (90) and Ω is the self-adjoint matrix

$$(56) \quad \begin{aligned} \Omega &= i(B_+ + B_-) = i(\Pi_- \xi \cdot \nabla \Pi_+ \Pi_+ - \Pi_+ \xi \cdot \nabla \Pi_+ \Pi_-) \\ &= -\frac{i}{2|w(x)|} \xi \cdot \nabla w(x) \wedge \frac{w(x)}{|w(x)|} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \end{aligned}$$

We recall that the matrices B_{\pm} are defined in (13) and we point out that Ω is self-adjoint because

$$\Omega^* = -i(B_+^* + B_-^*) = i(B_+ + B_-) = \Omega.$$

Moreover, by (13) and (6), the operator $\text{op}_{\varepsilon}(\Omega)$ is a differential operator of order 1 with matrix-valued coefficients that are growing polynomially at infinity and are singular on Υ . The various expressions of the matrix Ω are proved in Lemma C.1.

Remark 3.5. We shall use $\delta = \varepsilon^{\alpha}$ with $3/2 - 4\alpha > 0$, that is $\alpha \leq 3/8$. We shall see in the next section that the analysis requires $\delta^3 \varepsilon^1 \ll 1$ (see Remark 4.7), which is possible since one has $1/3 < 3/8$. Besides, $\varepsilon^2 \delta^{-2} \ll \varepsilon^{5/2} \delta^{-4}$ as soon as $\alpha > 1/4$, which is satisfied when $\alpha \in (1/3, 3/8)$. An optimal choice of δ will then consist in choosing $\delta = \varepsilon^{\frac{5}{14}}$, leading to $\varepsilon^{3/2} \delta^{-4} = \delta^3 \varepsilon^{-1} = \varepsilon^{\frac{1}{14}}$ (and of course $\sqrt{\varepsilon} \ll \varepsilon^{5/14}$).

Proof. We begin by considering for $t \in [s_1, s_2]$ the family $(v_{\pm}^{\varepsilon}(t))$ defined in (52). It comes from a computation (see [7] for example) that $v_{\pm}^{\varepsilon}(t)$ solves in Σ^k ,

$$(57) \quad i\varepsilon \partial_t v_{\pm}^{\varepsilon}(t) = -\frac{\varepsilon^2}{2} \Delta v_{\pm}^{\varepsilon}(t) + \lambda_{\pm}(x) v_{\pm}^{\varepsilon}(t) + \mathcal{O}(\varepsilon^{3/2} \|u_{\pm}(t)\|_{\Sigma^{k+3}}).$$

Since the profiles satisfy (19), we have

$$\mathcal{O}(\varepsilon^{3/2} \|u_{\pm}\|_{\Sigma^{k+3}}) = \mathcal{O}(\varepsilon^{3/2}(1 + |\ln \delta|)).$$

Considering $\psi_{\pm, \text{app}}^{\varepsilon}$, we write in Σ_{ε}^k ,

$$(58) \quad i\varepsilon \partial_t \psi_{\pm, \text{app}}^{\varepsilon} = \text{op}_{\varepsilon}(i\varepsilon \partial_t \chi_{\pm}^{\delta}(t) \vec{V}_{\pm}) v_{\pm}^{\varepsilon} + \text{op}_{\varepsilon}(\chi_{\pm}^{\delta}(t) \vec{V}_{\pm}) i\varepsilon \partial_t v_{\pm}^{\varepsilon}.$$

Using (53) in the first term of (58), we get

$$\text{op}_{\varepsilon}(i\varepsilon \partial_t \chi_{\pm}^{\delta}(t) \vec{V}_{\pm}) v_{\pm}^{\varepsilon} = -i\varepsilon \text{op}_{\varepsilon} \left(\left\{ \frac{|\xi|^2}{2} + \lambda_{\pm}, \chi_{\pm}^{\delta}(t) \right\} \vec{V}_{\pm} \right) v_{\pm}^{\varepsilon}.$$

Writing $\left\{ \frac{|\xi|^2}{2} + \lambda_{\pm}(x), \chi_{\pm}^{\delta}(t, z) \right\} \vec{V}_{\pm}(x) = \left\{ \frac{|\xi|^2}{2} + \lambda_{\pm}(x), \chi_{\pm}^{\delta}(t, z) \vec{V}_{\pm}(x) \right\} + \xi \cdot \nabla_x \vec{V}_{\pm}(x) \chi_{\pm}^{\delta}(t, z)$, and using (39) together with $\Pi_{\mp} \vec{V}_{\pm} = 0$, we deduce

$$\text{op}_{\varepsilon}(i\varepsilon \partial_t \chi_{\pm}^{\delta}(t) \vec{V}_{\pm}) v_{\pm}^{\varepsilon} = -i\varepsilon \text{op}_{\varepsilon} \left(\left\{ \frac{|\xi|^2}{2} + \lambda_{\pm}, \chi_{\pm}^{\delta}(t) \vec{V}_{\pm} \right\} \right) v_{\pm}^{\varepsilon} + \varepsilon \text{op}_{\varepsilon} \left(\Omega \vec{V}_{\pm} \chi_{\pm}^{\delta}(t) \right) v_{\pm}^{\varepsilon}.$$

On the other hand, using (57), the second term of (58) can be handled as

$$\begin{aligned} \text{op}_{\varepsilon}(\chi_{\pm}^{\delta}(t) \vec{V}_{\pm}) i\varepsilon \partial_t v_{\pm}^{\varepsilon} &= \text{op}_{\varepsilon} \left(\frac{|\xi|^2}{2} + \lambda_{\pm} \right) \text{op}_{\varepsilon}(\chi_{\pm}^{\delta}(t) \vec{V}_{\pm}) v_{\pm}^{\varepsilon} \\ &\quad - \left[\text{op}_{\varepsilon} \left(\frac{|\xi|^2}{2} + \lambda_{\pm} \right), \text{op}_{\varepsilon}(\chi_{\pm}^{\delta}(t) \vec{V}_{\pm}) \right] v_{\pm}^{\varepsilon} + \mathcal{O}(\varepsilon^{3/2}(1 + |\ln \delta|)) \\ &= \text{op}_{\varepsilon} \left(\frac{|\xi|^2}{2} + \lambda_{\pm} \right) \text{op}_{\varepsilon}(\chi_{\pm}^{\delta}(t) \vec{V}_{\pm}) v_{\pm}^{\varepsilon} - \frac{\varepsilon}{i} \text{op}_{\varepsilon} \left(\left\{ \frac{|\xi|^2}{2} + \lambda_{\pm}, \chi_{\pm}^{\delta}(t) \vec{V}_{\pm} \right\} \right) v_{\pm}^{\varepsilon} \\ &\quad + \mathcal{O}(\varepsilon^{3/2}(1 + |\ln \delta|)) + \mathcal{O}(\varepsilon^2 \delta^{-2}) \end{aligned}$$

thanks to Proposition A.1.

As a consequence of these two computations, we obtain

$$i\varepsilon \partial_t \psi_{\pm, \text{app}}^{\varepsilon} = \left(-\frac{\varepsilon^2}{2} \Delta + \lambda_{\pm} \right) \psi_{\pm, \text{app}}^{\varepsilon} + \varepsilon \text{op}_{\varepsilon} \left(\Omega \vec{V}_{\pm} \chi_{\pm}^{\delta}(t) \right) v_{\pm}^{\varepsilon} + \mathcal{O}(\varepsilon^{3/2}(1 + |\ln \delta|)) + \mathcal{O}(\varepsilon^2 \delta^{-2}(1 + |\ln \delta|))$$

We then use

$$\text{op}_\varepsilon \left(\Omega \vec{V}_\pm \chi_\pm^\delta(t) \right) = \text{op}_\varepsilon \left(\Omega \tilde{\chi}_\pm^\delta(t) \right) \text{op}_\varepsilon \left(\chi_\pm^\delta(t) \vec{V}_\pm \right) - \frac{i\varepsilon}{2} \text{op}_\varepsilon \left(\left\{ \Omega \tilde{\chi}_\pm^\delta(t), \vec{V}_\pm \chi_\pm^\delta(t) \right\} \right) + \mathcal{O}(\varepsilon^3 \delta^{-5}).$$

Therefore,

$$\begin{aligned} i\varepsilon \partial_t \psi_{\pm, \text{app}}^\varepsilon &= \left(-\frac{\varepsilon^2}{2} \Delta + \lambda_\pm + \varepsilon \text{op}_\varepsilon \left(\Omega \tilde{\chi}_\pm^\delta(t) \right) + \varepsilon^2 \text{op}_\varepsilon \left(\Omega_\pm^{(2)} \tilde{\chi}_\pm^\delta(t) \right) \right) \psi_{\pm, \text{app}}^\varepsilon \\ &\quad - \varepsilon^2 \text{op}_\varepsilon \left(\Omega_\pm^{(2)} \tilde{\chi}_\pm^\delta(t) \right) \text{op}_\varepsilon \left(\vec{V}_\pm \chi_\pm^\delta(t) \right) v_\pm^\varepsilon - \frac{i\varepsilon^2}{2} \text{op}_\varepsilon \left(\left\{ \Omega \tilde{\chi}_\pm^\delta(t), \vec{V}_\pm \chi_\pm^\delta(t) \right\} \right) v_\pm^\varepsilon \\ &\quad + \mathcal{O}(\varepsilon^{3/2} (1 + |\ln \delta|)) + \mathcal{O}(\varepsilon^2 \delta^{-2} (1 + |\ln \delta|)) + \mathcal{O}(\varepsilon^4 \delta^{-5} (1 + |\ln \delta|)) \end{aligned}$$

To handle the last terms, we rely on Proposition A.1, Remark C.3 and estimates (54), (38), together with (19). We write in Σ_ε^k

$$\text{op}_\varepsilon \left(\Omega_\pm^{(2)} \tilde{\chi}_\pm^\delta(t) \right) \text{op}_\varepsilon \left(\chi_\pm^\delta(t) \vec{V}_\pm \right) v_\pm^\varepsilon = \text{op}_\varepsilon \left(\Omega_\pm^{(2)} \chi_\pm^\delta(t) \vec{V}_\pm \right) v_\pm^\varepsilon + \mathcal{O}(\varepsilon \delta^{-5} (1 + |\ln \delta|)).$$

We finally use Lemma B.2, noticing that $\chi_\pm^\delta, \tilde{\chi}_\pm^\delta$ are equal to one close to the curve $z_\pm(t)$ and write in Σ_ε^k

$$\begin{aligned} \text{op}_\varepsilon \left(\Omega_\pm^{(2)} \chi_\pm^\delta(t) \vec{V}_\pm \right) v_\pm^\varepsilon &= \Omega_\pm^{(2)}(z_\pm(t)) \vec{V}_\pm(q_\pm(t)) v_\pm^\varepsilon + \mathcal{O}(\varepsilon^{5/2} \delta^{-4} \|v^\varepsilon\|_{\Sigma_\varepsilon^{k+1}}) \\ &= \mathcal{O}(\delta^{-2} (1 + |\ln \delta|)) + \mathcal{O}(\varepsilon^{1/2} \delta^{-4} (1 + |\ln \delta|)) \end{aligned}$$

thanks to Lemma C.4. We treat the term $\text{op}_\varepsilon \left(\left\{ \Omega \tilde{\chi}_\pm^\delta(t), \vec{V}_\pm \chi_\pm^\delta(t) \right\} \right) v_\pm^\varepsilon$ in a similar way. One notices

$$\left\{ \Omega \tilde{\chi}_\pm^\delta(t), \vec{V}_\pm \chi_\pm^\delta(t) \right\} (z_\pm(t)) = \{ \Omega, V_\pm \} (z_\pm(t)) = \nabla_\xi \Omega \cdot \nabla V_\pm(z_\pm(t)) = \mathcal{O}(\delta^{-2})$$

because $\partial_{z_j} \chi_\pm^\delta(z_\pm(t)) = \partial_{z_j} \tilde{\chi}_\pm^\delta(z_\pm(t)) = 0$. Then Lemma B.2 gives

$$\begin{aligned} \text{op}_\varepsilon \left(\left\{ \Omega \tilde{\chi}_\pm^\delta(t), \vec{V}_\pm \chi_\pm^\delta(t) \right\} \right) v_\pm^\varepsilon &= \left\{ \Omega \tilde{\chi}_\pm^\delta(t), \vec{V}_\pm \chi_\pm^\delta(t) \right\} (z_\pm(t)) v_\pm^\varepsilon \\ &\quad + \mathcal{O} \left(\sqrt{\varepsilon} (1 + |\ln \delta|) N_{d+k+1}^\varepsilon (d(\{ \Omega \tilde{\chi}_\pm^\delta(t), \vec{V}_\pm \chi_\pm^\delta(t) \})) \right). \end{aligned}$$

One has $\left\{ \Omega \tilde{\chi}_\pm^\delta(t), \vec{V}_\pm \chi_\pm^\delta(t) \right\} (z_\pm(t)) = \mathcal{O}(\delta^{-4})$, which gives

$$\text{op}_\varepsilon \left(\left\{ \Omega \tilde{\chi}_\pm^\delta(t), \vec{V}_\pm \chi_\pm^\delta(t) \right\} \right) v_\pm^\varepsilon = \mathcal{O} \left((\varepsilon^{1/2} \delta^{-4} + \delta^{-2}) (1 + |\ln \delta|) \right).$$

One then concludes by observing that $\varepsilon^4 \delta^{-5} \ll \varepsilon^{5/2} \delta^{-4}$ since $\sqrt{\varepsilon} \delta^{-1} \ll 1$. □

3.2. Superadiabatic correctors of the projectors. In this section, we proceed with the study of the equation satisfied by the projections of $\psi^\varepsilon(t)$ on the modes, the functions $\Pi_\pm \psi^\varepsilon(t)$. We use ideas issued from [41, 1, 36, 37, 33], aiming at improving the projectors $\Pi_\pm(x)$ into operators called superadiabatic projectors that are pseudodifferential operators with symbols that are series in ε . For our purpose, we only need the first two terms of these series. We set

$$H(x, \xi) = \frac{|\xi|^2}{2} + V(x), \quad h_\pm(x, \xi) = \frac{|\xi|^2}{2} + \lambda_\pm(x),$$

and consider for $x \notin \Upsilon$, the matrices $\Omega(x, \xi)$ defined by (56), $\mathbb{P}(x, \xi)$ given by

$$(59) \quad \begin{aligned} \mathbb{P}(x, \xi) &= \frac{i}{2|w(x)|} (\Pi_-(x)\xi \cdot \nabla \Pi_+(x) - \Pi_+(x)\xi \cdot \nabla \Pi_-(x)) \\ &= \frac{-i}{4|w(x)|^2} \xi \cdot \nabla w \wedge \frac{w}{|w|} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \end{aligned}$$

and $\mathbb{P}_\pm^{(2)}, \Omega_\pm^{(2)}$ written in details in Section C.2. The superadiabatic projectors at order 2 are the functions

$$\Pi_\pm^\varepsilon(x, \xi) = \Pi_\pm(x) \pm \varepsilon \mathbb{P}(x, \xi) + \varepsilon^2 \mathbb{P}_\pm^{(2)}(x, \xi).$$

These matrices are smooth outside Υ . From Lemma C.2, outside Υ , we have equation (85), i.e.

$$\Pi_\pm^\varepsilon \#_\varepsilon H = (h_\pm + \varepsilon \Omega_\pm^{(1)} + \varepsilon^2 \Omega_\pm^{(2)}) \#_\varepsilon \Pi_\pm^\varepsilon + \varepsilon^3 R^\varepsilon$$

where R^ε satisfies the estimate (86). Besides, Estimate (35) and Remark C.3 give precise information about these matrices at infinity and close to Υ . Because these corrected projectors may grow in the variables x and ξ , we shall localize them by use of the cut-off functions of Section 3.1. It will also allow to restrict the analysis to the zone where they are smooth. By construction, we have the following Lemma.

Lemma 3.6. *Let $k \in \mathbb{N}$, $\delta \in (0, 1)$ such that $\sqrt{\varepsilon} \delta^{-1} \ll 1$. Then, in $\mathcal{L}(\Sigma_\varepsilon^k)$, we have for all function $\tilde{\chi}_\pm^\delta(t) \in C^\infty(\mathbb{R}^{2d})$ satisfying (54) and supported on $\{\chi^\delta(t) = 1\}$ for $t \in [t_0, t^b]$,*

$$\text{op}_\varepsilon(\tilde{\chi}_\pm^\delta(t)) \text{op}_\varepsilon(\Pi_\pm^\varepsilon \chi_\pm^\delta(t)) \left(-\frac{\varepsilon^2}{2} \Delta + V(x) \right) = \text{op}_\varepsilon(\tilde{\chi}_\pm^\delta(t)) \text{op}_\varepsilon(H_{\text{adiab}, \pm}^\varepsilon) \text{op}_\varepsilon(\Pi_\pm^\varepsilon \chi_\pm^\delta(t)) + \mathcal{O}(\varepsilon^3 \delta^{-5}).$$

with

$$H_{\text{adiab}, \pm}^\varepsilon(t) := h_\pm + \varepsilon \Omega \tilde{\chi}_\pm^\delta(t) + \varepsilon^2 \Omega_\pm^{(2)} \tilde{\chi}_\pm^\delta(t)$$

Remark 3.7. Note that if $\delta = \varepsilon^\alpha$ with $\alpha \in (\frac{1}{3}, \frac{3}{8})$, as suggested in Remark 3.5, then $\varepsilon^2 \delta^{-5} \ll \varepsilon^{3/2} \delta^{-4}$.

This lemma emphasizes the purpose of these superadiabatic projectors: they allow to diagonalize the operator $\text{op}_\varepsilon(H)$ up to the correction $\varepsilon \text{op}_\varepsilon(\Omega) + \varepsilon^2 \text{op}_\varepsilon(\Omega^{(2)})$ which is of lower order in ε (recall that $\Omega = i(B_+ + B_-)$ is self-adjoint).

Proof. The proof comes from the symbolic calculus of Proposition A.1 and Remark A.3, keeping in mind that we have $|w(x)| > \delta$ on the support of the cut-off functions. We observe

$$\text{op}_\varepsilon(\Pi_\pm^\varepsilon \chi_\pm^\delta(t)) \text{op}_\varepsilon(H) = \text{op}_\varepsilon((\Pi_\pm^\varepsilon \chi_\pm^\delta(t)) \#_\varepsilon H) = \text{op}_\varepsilon(\chi_\pm^\delta(t) (\Pi_\pm^\varepsilon \#_\varepsilon H)) + \text{op}_\varepsilon(b_\pm^\varepsilon)$$

with $b_\pm^\varepsilon = (\Pi_\pm^\varepsilon \chi_\pm^\delta(t)) \#_\varepsilon H - \chi_\pm^\delta(t) (\Pi_\pm^\varepsilon \#_\varepsilon H)$ depending linearly on derivatives of χ_\pm^δ of order larger or equal to 1. Using (85), we obtain

$$\begin{aligned} \text{op}_\varepsilon(\Pi_\pm^\varepsilon \chi_\pm^\delta(t)) \text{op}_\varepsilon(H) &= \text{op}_\varepsilon\left(\chi_\pm^\delta(t) ((h_\pm + \varepsilon \Omega + \varepsilon^2 \Omega_\pm^{(2)}) \#_\varepsilon \Pi_\pm^\varepsilon)\right) + \text{op}_\varepsilon(b_\pm^\varepsilon) + \varepsilon^3 \text{op}_\varepsilon(\chi_\pm^\delta(t) R_\varepsilon) \\ &= \text{op}_\varepsilon\left((\chi_\pm^\delta(t) h_\pm + \tilde{\chi}_\pm^\delta(t) \chi_\pm^\delta(t) (\varepsilon \Omega + \varepsilon^2 \Omega_\pm^{(2)}) \#_\varepsilon \Pi_\pm^\varepsilon)\right) + \text{op}_\varepsilon(b_\pm^\varepsilon) + \varepsilon^3 \text{op}_\varepsilon(\chi_\pm^\delta(t) R_\varepsilon) \\ &= \text{op}_\varepsilon((\chi_\pm^\delta(t) H_{\text{adiab}, \pm}^\varepsilon(t)) \#_\varepsilon \Pi_\pm^\varepsilon) + \text{op}_\varepsilon(b_\pm^\varepsilon) + \varepsilon^3 \text{op}_\varepsilon(\chi_\pm^\delta(t) R_\varepsilon) \end{aligned}$$

where we have used in the last equation that $\tilde{\chi}_\pm^\delta(t)$ is identically equal to 1 on the support of $\chi_\pm^\delta(t)$. Then, we can write

$$\text{op}_\varepsilon(\Pi_\pm^\varepsilon \chi_\pm^\delta(t)) \text{op}_\varepsilon(H) = \text{op}_\varepsilon(H_{\text{adiab}, \pm}^\varepsilon(t)) \text{op}_\varepsilon(\chi_\pm^\delta(t) \Pi_\pm^\varepsilon) + \text{op}_\varepsilon(\tilde{b}_\pm^\varepsilon) + \varepsilon^3 \text{op}_\varepsilon(\chi_\pm^\delta(t) R_\varepsilon)$$

where $\tilde{b}_\pm^\varepsilon = b_\pm^\varepsilon + (\chi_\pm^\delta H_{\text{adiab},\pm}^\varepsilon(t))\#_\varepsilon \Pi_\pm^\varepsilon - H_{\text{adiab},\pm}^\varepsilon(t)\#_\varepsilon (\Pi_\pm^\varepsilon \chi_\pm^\delta)$ satisfies the same properties as b_\pm^ε . Using (86), we have

$$\text{op}_\varepsilon(\chi_\pm^\delta(t)R_\varepsilon) = \mathcal{O}(\delta^{-5}).$$

Besides, on the support of $\tilde{\chi}_+^\delta(t)$, the functions $\partial_z^\alpha \tilde{\chi}_+^\delta(t)$, $\partial_z^\alpha \chi_+^\delta(t)$, and thus \tilde{b}_+^ε and its derivatives, are all identically equal to 0 for any $\alpha \in \mathbb{N}^{2d}$, and similarly for the *minus*-mode. Therefore, using Remark A.2, we obtain

$$\text{op}_\varepsilon(\tilde{\chi}_\pm^\delta(t))\text{op}_\varepsilon(\tilde{b}_\pm^\varepsilon) = \mathcal{O}(\varepsilon^{N+1}\delta^{-3-N})$$

because for $\gamma \in \mathbb{N}^{2d}$, using Remark C.3 (the worst term being Π_\pm^ε), we have

$$N_d^\varepsilon(\tilde{b}_\pm^\varepsilon) = \mathcal{O}(\varepsilon\delta^{-|\gamma|-3}) \quad \text{and} \quad N_d^\varepsilon(\partial_z^\gamma \tilde{\chi}_\pm^\delta) = \mathcal{O}(\delta^{-|\gamma|}).$$

One then concludes by choosing $N = 2$. □

We can now perform the proof of Proposition 3.1.

Proof of Proposition 3.1. Without loss of generality, we can reduce to only one mode and we can assume $v_+^\varepsilon(s_1) = 0$, what we do from now on. Indeed, the same scheme of proof then extends to the other mode and one gets the general case because of the linearity of the equation. It is also enough to prove

$$\|\Pi_\pm \psi^\varepsilon(s_2) - \psi_{\pm,\text{app}}^\varepsilon(s_2)\|_{\Sigma_k^\varepsilon} \leq C_k(1 + |\ln \delta|) \left(\frac{\varepsilon^{3/2}}{\delta^4} + \frac{\sqrt{\varepsilon}}{\delta} \right),$$

where $\psi_{\pm,\text{app}}^\varepsilon$ has been defined in (55). Indeed, the same argument will be valid for any $s^* \in [s_1, s_2]$, with the same constant C_k because that constant will only depend on the sup-norm of quantities that are continuous functions in $\{|w(x)| > \delta\}$.

We choose δ such that $\sqrt{\varepsilon}\delta^{-1} \leq 1$ and consider $\chi_\pm^\delta(t)$, $\tilde{\chi}_\pm^\delta(t)$ and $\check{\chi}_\pm^\delta(t)$ as in the preceding section (see Remark 3.2 and Lemma 3.6); they enjoy the following relations:

$$0 \leq \check{\chi}_\pm^\delta(t) \leq \chi_\pm^\delta(t) \leq \tilde{\chi}_\pm^\delta(t) \leq 1$$

$$\tilde{\chi}_\pm^\delta(t) = 1 \text{ on } \text{supp } \chi_\pm^\delta(t) \quad \text{and} \quad \chi_\pm^\delta(t) = 1 \text{ on } \text{supp } \check{\chi}_\pm^\delta(t).$$

We additionally require

$$\partial_t \tilde{\chi}_\pm^\delta(t) = \{h_\pm, \tilde{\chi}_\pm^\delta(t)\}.$$

and $\check{\chi}_+^\delta(s_2) = \check{\chi}_-^\delta(s_2) =: \check{\chi}^\delta(s_2)$. Then, the functions $\chi_\pm^\delta(s_2)$ localize close to the point $z_-(s_2)$ while for $t \in [s_1, s_2]$, $\chi_\pm^\delta(t)$ localize on separated points, $\Phi_\pm^{t,s_2}(z_-(s_2))$, and similarly for $\check{\chi}_\pm^\delta$ and $\tilde{\chi}_\pm^\delta$. We set for $t \in [s_1, s_2]$

$$w_-^\varepsilon(t) = \text{op}_\varepsilon(\check{\chi}_-^\delta(t)) \left(\text{op}_\varepsilon(\chi_-^\delta(t)\Pi_-^\varepsilon)\psi^\varepsilon(t) - \text{op}_\varepsilon(\chi_-^\delta(t))\psi_{-,\text{app}}^\varepsilon(t) \right)$$

and

$$w_+^\varepsilon(t) = \text{op}_\varepsilon(\tilde{\chi}_+^\delta(t)) \text{op}_\varepsilon(\chi_+^\delta(t)\Pi_+^\varepsilon)\psi^\varepsilon(t).$$

The crucial point of the proof is to establish the equation satisfied by $w_\pm^\varepsilon(t)$.

Lemma 3.8. *Let $k \in \mathbb{N}$, $\delta \in (0, 1)$ with $\sqrt{\varepsilon}\delta^{-1} \ll 1$. For $t \in [s_1, s_2]$, we have in Σ_ε^k ,*

$$i\varepsilon\partial_t w_+^\varepsilon = -\frac{\varepsilon^2}{2}\Delta w_+^\varepsilon + \lambda_+ w_+^\varepsilon + \varepsilon \text{op}_\varepsilon \left(\tilde{\chi}_\pm^\delta(t)(\Omega + \varepsilon\Omega_+^{(2)}) \right) w_+^\varepsilon + \mathcal{O}(\varepsilon^3\delta^{-5})$$

$$i\varepsilon\partial_t w_-^\varepsilon = -\frac{\varepsilon^2}{2}\Delta w_-^\varepsilon + \lambda_- w_-^\varepsilon + \varepsilon \text{op}_\varepsilon \left(\tilde{\chi}_\pm^\delta(t)(\Omega + \varepsilon\Omega_-^{(2)}) \right) w_-^\varepsilon + \mathcal{O}((\varepsilon^{5/2}\delta^{-4} + \varepsilon^{3/2}\delta^{-1})(1 + |\ln \delta|))$$

with initial data $w_\pm^\varepsilon(s_1) = \mathcal{O}(\sqrt{\varepsilon})$.

Proof of Lemma 3.8. Let us begin with $w_+^\varepsilon(t)$. We have

$$\begin{aligned} i\varepsilon\partial_t w_+^\varepsilon(t) &= \text{op}_\varepsilon(\tilde{\chi}_+^\delta(t))\text{op}_\varepsilon(\chi_+^\delta(t)\Pi_+^\varepsilon)\text{op}_\varepsilon(H)\psi^\varepsilon(t) \\ &\quad + i\varepsilon\text{op}_\varepsilon(\partial_t\tilde{\chi}_+^\delta(t))\text{op}_\varepsilon(\chi_+^\delta(t)\Pi_+^\varepsilon)\psi^\varepsilon(t) + i\varepsilon\text{op}_\varepsilon(\tilde{\chi}_+^\delta(t))\text{op}_\varepsilon(\partial_t\chi_+^\delta(t)\Pi_+^\varepsilon)\psi^\varepsilon(t). \end{aligned}$$

Using $\partial_t\tilde{\chi}_+^\delta(t) = \{h_+, \tilde{\chi}_+^\delta(t)\}$ and the fact that $\partial_z\chi_+^\delta(t) = 0$ on the support of $\tilde{\chi}_+^\delta(t)$, we obtain by Remark A.2 as in the proof of Lemma 3.6,

$$\varepsilon\text{op}_\varepsilon(\tilde{\chi}_+^\delta(t))\text{op}_\varepsilon(\partial_t\chi_+^\delta(t)\Pi_+^\varepsilon)\psi^\varepsilon(t) = \mathcal{O}(\varepsilon^{N+1}\delta^{-3-N})$$

and we choose as before $N = 2$. By Lemma 3.6, we are left with

$$(60) \quad \begin{aligned} i\varepsilon\partial_t w_+^\varepsilon(t) &= \text{op}_\varepsilon(\tilde{\chi}_+^\delta(t))\text{op}_\varepsilon(H_{\text{adiab},+}^\varepsilon)\text{op}_\varepsilon(\chi_+^\delta(t)\Pi_+^\varepsilon)\psi^\varepsilon(t) \\ &\quad + i\varepsilon\text{op}_\varepsilon(\partial_t\tilde{\chi}_+^\delta(t))\text{op}_\varepsilon(\chi_+^\delta(t)\Pi_+^\varepsilon)\psi^\varepsilon(t) + \mathcal{O}(\varepsilon^3\delta^{-5}). \end{aligned}$$

We now take advantage of Remark A.3 for writing

$$[\text{op}_\varepsilon(\tilde{\chi}_+^\delta(t)), \text{op}_\varepsilon(H_{\text{adiab},+}^\varepsilon)] = -i\varepsilon\text{op}_\varepsilon(\{\tilde{\chi}_+^\delta(t), H_{\text{adiab},\pm}^\varepsilon\}) + \mathcal{O}(\varepsilon^3\delta^{-5}),$$

where we have used the analysis of the singularities of Ω and $\Omega_+^{(2)}$ (see Lemma C.2). We deduce

$$\begin{aligned} \text{op}_\varepsilon(\tilde{\chi}_+^\delta(t))\text{op}_\varepsilon(H_{\text{adiab},+}^\varepsilon)\text{op}_\varepsilon(\chi_+^\delta(t)\Pi_+^\varepsilon)\psi^\varepsilon(t) &= \text{op}_\varepsilon(H_{\text{adiab},+}^\varepsilon)w_+^\varepsilon \\ &\quad - i\varepsilon\text{op}_\varepsilon(\{h_+, \tilde{\chi}_+^\delta(t)\})\text{op}_\varepsilon(\chi_+^\delta(t)\Pi_+^\varepsilon)\psi^\varepsilon(t) + \mathcal{O}(\varepsilon^3\delta^{-5}). \end{aligned}$$

Combining the latter with (60) and the relation $\partial_t\tilde{\chi}_+^\delta(t) = \{h_+, \tilde{\chi}_+^\delta(t)\}$, we obtain

$$i\varepsilon\partial_t w_+^\varepsilon(t) = \text{op}_\varepsilon(H_{\text{adiab},+}^\varepsilon)w_+^\varepsilon(t) + \mathcal{O}(\varepsilon^3\delta^{-5}).$$

For $w_-^\varepsilon(t)$, the computation follows the same steps with the difference that there is an additional term due to the presence of $\psi_{-, \text{app}}^\varepsilon$. Using Lemma 3.4, an additional remainder in

$$\mathcal{O}((\varepsilon^{5/2}\delta^{-4} + \varepsilon^{3/2}\delta^{-1})(1 + |\ln \delta|)),$$

is generated, which is much larger than $\mathcal{O}(\varepsilon^3\delta^{-5})$ (again because of $\sqrt{\varepsilon}\delta^{-1} \leq 1$). \square

We can now conclude the proof of Proposition 3.1. Using Lemma 3.8, and by the properties of the unitary propagator associated with the operators

$$\text{op}_\varepsilon(H_{\text{adiab},\pm}^\varepsilon) = -\frac{\varepsilon^2}{2}\Delta + \lambda_\pm + \varepsilon\text{op}_\varepsilon(\Omega\tilde{\chi}_\pm^\delta(t)) + \varepsilon^2\text{op}_\varepsilon(\Omega_\pm^2\tilde{\chi}_\pm^\delta(t)),$$

(see [34]), we obtain the existence of a constant C_k such that

$$(61) \quad \|w_+^\varepsilon(s_2)\|_{\Sigma_\varepsilon^k} + \|w_-^\varepsilon(s_2)\|_{\Sigma_\varepsilon^k} \leq C_k((\varepsilon^{3/2}\delta^{-4} + \sqrt{\varepsilon}\delta^{-1})(1 + |\ln \delta|)).$$

Equivalently, using $\tilde{\chi}^\delta(s_2) = \tilde{\chi}^\delta(s_2)\chi_\pm^\delta(s_2)$,

$$\text{op}_\varepsilon(\Pi_+^\varepsilon + \Pi_-^\varepsilon) = \text{Id} + \mathcal{O}(\varepsilon^2\delta^{-4})$$

(see Remark C.3), and the localization properties of $\psi_{-, \text{app}}^\varepsilon$ (see Lemma B.2 (2)), the latter relation writes

$$\text{op}_\varepsilon(\tilde{\chi}^\delta(s_2))\psi^\varepsilon(s_2) = \psi_{-, \text{app}}^\varepsilon(s_2) + \mathcal{O}((\varepsilon^{3/2}\delta^{-4} + \sqrt{\varepsilon}\delta^{-1})(1 + |\ln \delta|))$$

in Σ_ε^k . The argument could have been worked out between s_1 and any $s \in [s_1, s_2]$. Therefore, at this stage of the proof, varying the function $\tilde{\chi}_\delta$, we have obtained that for any $t \in [s_1, s_2]$ and any cut-off function χ_δ supported in $\{|w(x)| > \delta\}$, we have in Σ_ε^k ,

$$(62) \quad \text{op}_\varepsilon(\chi_\delta(t))\psi^\varepsilon(t) = \psi_{-, \text{app}}^\varepsilon(t) + \mathcal{O}((\varepsilon^{3/2}\delta^{-4} + \sqrt{\varepsilon}\delta^{-1})(1 + |\ln \delta|)).$$

We now want to extend this approximation to $\psi^\varepsilon(t)$ itself. We define θ_-^δ localizing close to the trajectory $z_-(t)$ and in $\{|w(x)| > \delta\}$ (we denote it θ_-^δ to emphasize that it is independent of the functions χ_-^δ used before). The analysis performed above applies to the special case of θ_-^δ and we have in Σ_ε^k and for $t \in [s_1, s_2]$

$$\text{op}_\varepsilon(\theta_-^\delta(t))\psi^\varepsilon(t) = \psi_{-, \text{app}}^\varepsilon(t) + \mathcal{O}((\varepsilon^{3/2}\delta^{-4} + \sqrt{\varepsilon}\delta^{-1})(1 + |\ln \delta|)).$$

We study

$$w^\varepsilon(t) = \text{op}_\varepsilon(1 - \theta_-^\delta(t))\psi^\varepsilon(t)$$

and aim at proving that $w^\varepsilon(s_2)$ is negligible, which is the case for $w^\varepsilon(s_1)$. Moreover, for $t \in [s_1, s_2]$,

$$(63) \quad i\varepsilon\partial_t w^\varepsilon = -\frac{\varepsilon^2}{2}\Delta w^\varepsilon + Vw^\varepsilon + \frac{1}{2}[\varepsilon^2\Delta, \text{op}_\varepsilon(\theta_-^\delta(t))]\psi^\varepsilon.$$

Let us study the source term. By symbolic calculus (see Remark A.3), we have

$$\left[-\frac{\varepsilon^2}{2}\Delta, \text{op}_\varepsilon(\theta_-^\delta(t))\right] = \varepsilon \text{op}_\varepsilon(\chi^\delta(t)) + \mathcal{O}(\varepsilon^3\delta^{-3})$$

where $\chi^\delta = \xi \cdot \nabla_x \theta_-^\delta \in \mathcal{C}^\infty(\mathbb{R}^{2d+1})$ is supported in $\{|w(x)| > c\delta\}$ for some $c > 0$, with $\chi^\delta(t)$ identically equal to 0 in a neighborhood of $\Phi^{t, s_2}(z_-(s_2))$ and $|\partial^\alpha \chi^\delta(t, x, \xi)| \leq C\delta^{-1-|\alpha|}$ for all $\alpha \in \mathbb{N}^{2d}$.

We deduce from (63) and from (2) of Lemma B.2 that for $N \in \mathbb{N}^*$, $t \in [s_1, s_2]$ and in Σ_ε^k

$$\text{op}_\varepsilon(\chi^\delta(t))\psi^\varepsilon(t) = \mathcal{O}(\delta^{-1}(\sqrt{\varepsilon}\delta^{-1})^N(1 + |\ln \delta|)) + \mathcal{O}((\varepsilon^{3/2}\delta^{-4} + \sqrt{\varepsilon}\delta^{-1})(1 + |\ln \delta|)).$$

Therefore, equation (63) gives in Σ_ε^k

$$w^\varepsilon(s_2) = w^\varepsilon(s_1) + \mathcal{O}(\delta^{-1}(\sqrt{\varepsilon}\delta^{-1})^N(1 + |\ln \delta|)) + \mathcal{O}((\varepsilon^{3/2}\delta^{-4} + \sqrt{\varepsilon}\delta^{-1})(1 + |\ln \delta|)) + \mathcal{O}(\varepsilon^2\delta^{-3}).$$

By choosing $N = 3$ and using $\varepsilon^2\delta^{-3} \ll \varepsilon^{3/2}\delta^{-4}$, we deduce

$$\psi^\varepsilon(s_2) = \psi_{-, \text{app}}^\varepsilon(s_2) + \mathcal{O}((\varepsilon^{3/2}\delta^{-4} + \sqrt{\varepsilon}\delta^{-1})(1 + |\ln \delta|)),$$

whence Proposition 3.1. □

4. PASSING THROUGH THE GAP REGION

At this stage of the proof, we have obtained an approximation of the solution as long as the trajectories do not enter in the region $\{|w(q)| \leq c\delta\}$, for some $c > 0$ fixed, i.e. in a neighborhood of the crossing set Υ . We now focus on trajectories that reach their minimal gap inside this region and enter in the region at time $t^b - \delta$ and leaves it at time $t^b + \delta$.

The strategy is the following.

- (1) We first perform a change of time and unknown in order to reduce the system (1) into a Landau-Zener model in the region $\{|w(q)| \leq c\delta\}$.
- (2) We identify the ingoing wave packet in the new coordinates, i.e. the function $\psi^\varepsilon(t^b - \delta)$ that satisfy in $L^2(\mathbb{R}^d)$,

$$\psi^\varepsilon(t^b - \delta) = \psi_{\text{app}}^\varepsilon(t^b - \delta) + \mathcal{O}((\sqrt{\varepsilon}\delta^{-1} + \varepsilon^{3/2}\delta^{-4})(1 + |\ln \delta|)).$$

- (3) We prove that we can use the resolution of the Landau-Zener model to obtain an approximation of the solution at time $t^b + \delta$.

4.1. Reduction to a Landau-Zener model. To pass through the region Υ , following ideas from [23], we use a Taylor approximation along the trajectory $\Phi_0^{t,t^b}(z^b) = (q_0(t), p_0(t))$ introduced in Section 2.1. We make the time-scaling $t = t^b + s\sqrt{\varepsilon}$ and consider the new unknown function $u^\varepsilon(s) \in L^2(\mathbb{R}^d, \mathbb{C}^2)$ defined by

$$(64) \quad \psi^\varepsilon(t) = e^{\frac{i}{\varepsilon} S_0(t, t^b, z^b)} \text{WP}_{\Phi_0^{t,t^b}(z^b)}^\varepsilon(u^\varepsilon(s)), \quad t = t^b + s\sqrt{\varepsilon}$$

where the action $S_0(t, t^b, z^b)$ is associated with h_0 , defined in (32), and $\Phi_0^{t,t^b}(z^b)$ as introduced in Lemma 2.2.

Remark 4.1. (1) Note that when $t = t^b - \delta$, then $s = -s_0 := -\delta/\sqrt{\varepsilon}$ and when $t = t^b + \delta$, then $s = s_0 = \delta/\sqrt{\varepsilon}$. Since we have assumed $\sqrt{\varepsilon}\delta^{-1} \ll 1$ in the preceding section, we will have $s_0 \gg 1$. Through the change of variable (64), for $k \in \mathbb{N}$ and $s \in [-s_0, s_0]$, there exist constants c, C such that

$$c\|u^\varepsilon(s)\|_{\widetilde{\Sigma}_\varepsilon^k} \leq \|\psi^\varepsilon(t)\|_{\Sigma_\varepsilon^k} \leq C\|u^\varepsilon(s)\|_{\widetilde{\Sigma}_\varepsilon^k}$$

with

$$(65) \quad \|f\|_{\widetilde{\Sigma}_\varepsilon^k} = \sup_{|\alpha|+|\beta| \leq k} \varepsilon^{\frac{|\alpha|+|\beta|}{2}} \|f\|_{\Sigma^{|\alpha|+|\beta|}}.$$

Therefore, it is natural to use these sets $\widetilde{\Sigma}_\varepsilon^k$ for estimations.

Lemma 4.2. *Let $k \in \mathbb{N}$. The family $(u^\varepsilon(s))_{\varepsilon>0}$ satisfies for all $(s, y) \in \mathbb{R}^{2d+1}$*

$$(66) \quad i\partial_s u^\varepsilon = A \left(s r \omega + dw(q^b)y \right) u^\varepsilon + \sqrt{\varepsilon} \left(-\frac{1}{2} \Delta u^\varepsilon + B^\varepsilon(s, y) u^\varepsilon \right)$$

where B^ε is a smooth hermitian matrix valued potential with the following properties: there exist constants $C_0, C_1 > 0$ such that for all $s \in [-s_0, s_0]$ and $y \in \mathbb{R}^d$,

$$|B^\varepsilon(s, y)| \leq C_0 (s^2 \langle \sqrt{\varepsilon}|y| \rangle + |y|^2), \quad |\nabla B^\varepsilon(s, y)| \leq C_1 (\sqrt{\varepsilon}|y|^2 + |y| + \sqrt{\varepsilon}s^2)$$

and for all $|\beta| \geq 2$, there exists $C_\beta > 0$ such that for all $s \in [-s_0, s_0]$ and $y \in \mathbb{R}^d$,

$$|\partial_y^\beta B^\varepsilon(s, y)| \leq C_\beta \varepsilon^{\frac{|\beta|-2}{2}} \langle \sqrt{\varepsilon}y \rangle^2.$$

Remark 4.3. When (t^b, z^b) is the point of the trajectory $\Phi_-^{t,t^b}(z_0)$ where the quantity $|w(\Phi_-^{t,t^b}(z_0))|$ (called the gap) is minimal, a similar analysis yields to the system

$$i\partial_s u^\varepsilon = A \left(\frac{w(q^b)}{\sqrt{\varepsilon}} + s r \omega + dw(q^b)y \right) u^\varepsilon + \sqrt{\varepsilon} \left(-\frac{1}{2} \Delta u^\varepsilon + B^\varepsilon(s, y) u^\varepsilon \right).$$

This observation gives a starting point for the analysis of the propagation of a wave packet passing close to a crossing point, while not exactly through it. The size of the gap comparatively to $\sqrt{\varepsilon}$ then is a crucial point of the description.

Recall that $r\omega = dw(q^b)p^b$ and that $w(q^b) = 0$. We shall set in the following $\eta(y) := dw(q^b)y$ and compare u^ε with the solution u of the equation

$$i\partial_s u = A(s r \omega + \eta(y)) u.$$

The important point to note here is that the leading part $A(s r \omega + \eta(y))$ of the system has the same structure as the well-known Landau-Zener system (see references [29, 43] and equation (67)

below). The latter is well understood as it will be detailed in the next sections. We shall use the initial data at time $s = -s_0$ with

$$s_0 = \delta/\sqrt{\varepsilon}.$$

The time $-s_0$ corresponds to $t = t^b - \delta$, i.e. to the ingoing solution, and we shall deduce the value of the outgoing solution at time $t = t^b + \delta$ or equivalently $s = +s_0$. This will be done assuming $\delta \gg \sqrt{\varepsilon}$, thanks to the scattering result of the next section.

Proof. We use the formalism of Section 2.3, together with the observation of Appendix B. The first step consists in observing that

$$\begin{aligned} \left(i\varepsilon\partial_t + \frac{\varepsilon^2}{2}\Delta - v(x) \right) \psi^\varepsilon(t, x) &= e^{\frac{i}{\varepsilon}S_0(t, t^b, z^b)} e^{\frac{i}{\varepsilon}p_0(t) \cdot (\sqrt{\varepsilon}y)} \left(i\sqrt{\varepsilon}\partial_s u^\varepsilon(s, y) + \frac{\varepsilon}{2}\Delta_y u^\varepsilon(s, y) \right. \\ &\quad \left. - (v(q_0(t) + \sqrt{\varepsilon}y) - v(q_0(t)) - y\sqrt{\varepsilon}dv(q_0(t))) u^\varepsilon(s, y) \right) \Big|_{y=\frac{x-q_0(t)}{\sqrt{\varepsilon}}} \\ &= e^{\frac{i}{\varepsilon}S_0(t, t^b, z^b)} e^{\frac{i}{\varepsilon}p_0(t) \cdot (\sqrt{\varepsilon}y)} \left(i\sqrt{\varepsilon}\partial_s u^\varepsilon(s, y) + \frac{\varepsilon}{2}\Delta_y u^\varepsilon(s, y) + \varepsilon\mathcal{W}^\varepsilon(t, y)u^\varepsilon(s, y) \right) \Big|_{y=\frac{x-q_0(t)}{\sqrt{\varepsilon}}} \end{aligned}$$

where we have used Lemma B.2 (1) and the definition of the action. Besides,

$$\mathcal{W}^\varepsilon(s, y) = R_0(t, y\sqrt{\varepsilon})y \cdot y, \quad R_0(t, y\sqrt{\varepsilon}) = \int_0^1 \text{Hess } v(q_0(t) + \sqrt{\varepsilon}\theta y)(1 - \theta)d\theta,$$

and R_0 is bounded with bounded derivatives according to (2). Similarly, we have

$$A(w(x))\psi^\varepsilon(t, x) = e^{\frac{i}{\varepsilon}S_0(t, t^b, z^b)} \left(e^{\frac{i}{\varepsilon}p_0(t) \cdot (\sqrt{\varepsilon}y)} A(w(q_0(t) + \sqrt{\varepsilon}y))u^\varepsilon(s, y) \right) \Big|_{y=\frac{x-q_0(t)}{\sqrt{\varepsilon}}}.$$

Therefore, Equation (1) becomes

$$i\sqrt{\varepsilon}\partial_s u^\varepsilon + \frac{\varepsilon}{2}\Delta u^\varepsilon + \varepsilon\mathcal{W}^\varepsilon(s, y)u^\varepsilon(s, y) = A(w(q_0(t) + \sqrt{\varepsilon}y))u^\varepsilon(s, y).$$

Writing $w(q_0(t) + \sqrt{\varepsilon}y) = w(q_0(t)) + \sqrt{\varepsilon}dw(q_0(t))y + \varepsilon R_1(t, y\sqrt{\varepsilon})y \cdot y$

$$i\sqrt{\varepsilon}\partial_s u^\varepsilon = A \left(w(q_0(t^b + s\sqrt{\varepsilon})) + \sqrt{\varepsilon}dw(q_0(t^b + s\sqrt{\varepsilon}))y \right) u^\varepsilon + \varepsilon R_2(s\sqrt{\varepsilon}, y\sqrt{\varepsilon})y \cdot y u^\varepsilon(s, y),$$

for some bounded smooth matrix R_1 and tensor R_2 , with bounded derivatives coming from (2). We conclude by performing a Taylor expansion in s , writing

$$\begin{aligned} q_0(t^b + s\sqrt{\varepsilon}) &= q^b + \sqrt{\varepsilon}sp^b + \varepsilon s^2 R_3(s\sqrt{\varepsilon}) \\ \text{and} \quad w(q_0(t^b + s\sqrt{\varepsilon})) + \sqrt{\varepsilon}dw(q_0(t^b + s\sqrt{\varepsilon}))y &= \sqrt{\varepsilon}sdw(q^b)p^b + \sqrt{\varepsilon}dw(q^b)y + \varepsilon R_4(s\sqrt{\varepsilon})s^2 + \varepsilon^{3/2}s^2 R_5(s\sqrt{\varepsilon})y \end{aligned}$$

for some smooth bounded vector-valued R_3 and R_4 , and matrix-valued R_5 , with bounded derivatives because of the assumption (2).

The properties of $B^\varepsilon(s, y)$ come from its expression in terms of the R_j , $j \in \{1, \dots, 5\}$

$$B^\varepsilon(s, y) = \mathcal{W}(t^b + s\sqrt{\varepsilon}, y) + s^2 A \left(R_4(s\sqrt{\varepsilon}) + \sqrt{\varepsilon}R_5(s\sqrt{\varepsilon})y \right) + R_2(s\sqrt{\varepsilon}, y\sqrt{\varepsilon})y \cdot y$$

and the assumption (2) made on the potential. \square

4.2. The Landau-Zener model and the structure of the solutions. The structure of the system (66) suggests that we consider the model problem

$$(67) \quad \begin{cases} i\partial_s u = A(sr\omega + \eta)u, \\ u(0, \eta) = u_0(\eta) \in \mathbb{C}^2 \end{cases}$$

where $\eta \in \mathbb{C}^2$ is a parameter. As we shall see below, this problem can be turned into the following Landau-Zener problem by elementary computations

$$(68) \quad \frac{1}{i}\partial_s u_{LZ}(s, z) = \begin{pmatrix} s + z_1 & z_2 \\ z_2 & -s - z_1 \end{pmatrix} u_{LZ}(s, z).$$

Therefore, one can deduce the behavior of the solutions to (67) from the asymptotics, as $s \rightarrow \pm\infty$, of the solutions to the Landau-Zener problem (68). Besides the historical references [29, 43], the reader can refer to [12] where an analysis of the behavior of the solutions of the Landau-Zener model is given with a stationary phase approach; or to [23] where the proof is given in terms of parabolic-cylinder functions. We follow the results of the Appendix of [12] which are obtained for η taken in a fixed compact, while the analysis in terms of the size R of this compact is performed in [Appendix, [14]]: as $s \rightarrow \pm\infty$

$$(69) \quad u_{LZ}(s) = e^{i\frac{(s+z_1)^2}{2} + i\frac{z_2^2}{2} \ln|s+z_1|} \begin{pmatrix} u_1^\pm(z_2) \\ 0 \end{pmatrix} + e^{-i\frac{(s+z_1)^2}{2} - i\frac{z_2^2}{2} \ln|s+z_1|} \begin{pmatrix} 0 \\ u_2^\pm(z_2) \end{pmatrix} + \mathcal{O}(R^2|s|^{-1}),$$

with

$$u_1^\pm = a(z_2)u_1^- - \bar{b}(z_2)u_2^-, \quad u_2^\pm = b(z_2)u_1^- + a(z_2)u_2^-$$

where the coefficients a and b are given by (25). It is then possible to derive the next proposition about solutions to (67) in which $(\vec{V}_\omega, \vec{V}_\omega^\perp)$ is a direct orthogonal basis of \mathbb{R}^2 as in (15) consisting of normalized real-valued eigenvectors of $A(\omega)$ satisfying

$$A(\omega)\vec{V}_\omega = \vec{V}_\omega \quad \text{and} \quad A(\omega)\vec{V}_\omega^\perp = -\vec{V}_\omega^\perp.$$

Note that they are uniquely defined up to a sign. The next lemma gives the form of the asymptotics of $u(s, \eta)$ when $s \rightarrow \pm\infty$ in such a basis, together with scattering relations.

Lemma 4.4. *There exists $\alpha_1^{\text{in}}, \alpha_2^{\text{in}}, \alpha_1^{\text{out}}, \alpha_2^{\text{out}} \in \mathcal{S}(\mathbb{R}^d)$ such that as s goes to $-\infty$ and for $|\eta| \leq R$,*

$$u(s, \eta) = e^{i\Lambda(s, \eta)} \alpha_1^{\text{in}}(\eta) \vec{V}_\omega^\perp + e^{-i\Lambda(s, \eta)} \alpha_2^{\text{in}}(\eta) \vec{V}_\omega + \mathcal{O}(R^3|s|^{-1}),$$

¹ and as s goes to $+\infty$ and $|\eta| \leq R$

$$u(s, \eta) = e^{i\Lambda(s, \eta)} \alpha_1^{\text{out}}(\eta) \vec{V}_\omega^\perp + e^{-i\Lambda(s, \eta)} \alpha_2^{\text{out}}(\eta) \vec{V}_\omega + \mathcal{O}(R^3|s|^{-1}),$$

where

$$(70) \quad \Lambda(s, \eta) = \frac{1}{2r} |\omega \cdot \eta + rs|^2 + \frac{1}{2r} |\omega^\perp \cdot \eta|^2 \ln(\sqrt{r}|s|).$$

Besides

$$\begin{pmatrix} \alpha_1^{\text{out}} \\ \alpha_2^{\text{out}} \end{pmatrix} = S(r^{-1/2}\omega^\perp \cdot \eta) \begin{pmatrix} \alpha_1^{\text{in}} \\ \alpha_2^{\text{in}} \end{pmatrix}$$

with

$$S(\eta) = \begin{pmatrix} a(\eta) & -\bar{b}(\eta) \\ b(\eta) & a(\eta) \end{pmatrix},$$

where the coefficients a and b are given by (25).

¹check R^3

Proof. For proving Lemma 4.4, we relate the solution u of the system (67) to u_{LZ} thanks to a change of variables via the rotation matrix $\mathcal{R}(\theta)$ defined in (36) and its property (37). Therefore, choosing $\theta \in \mathbb{R}$ such that $\omega_\theta = -\omega$, we have

$$\mathcal{R}(\theta)^{-1}A(\eta + sr\omega)\mathcal{R}(\theta) = - \begin{pmatrix} \eta \cdot \omega + sr & \eta \cdot \omega^\perp \\ \eta \cdot \omega^\perp & -\eta \cdot \omega - sr \end{pmatrix}.$$

We then write

$$\begin{aligned} \frac{1}{i}\partial_s(\mathcal{R}(\theta)^{-1}u) &= \mathcal{R}(\theta)^{-1}A(-\eta - sr\omega)\mathcal{R}(\theta)(\mathcal{R}(\theta)^{-1}u) \\ &= \begin{pmatrix} \eta \cdot \omega + sr & \eta \cdot \omega^\perp \\ \eta \cdot \omega^\perp & -\eta \cdot \omega - sr \end{pmatrix}(\mathcal{R}(\theta)^{-1}u). \end{aligned}$$

and we deduce that

$$v(s, \eta) = \mathcal{R}(\theta)^{-1}u(sr^{-1/2}, r^{1/2}\eta)$$

solves

$$\frac{1}{i}\partial_s v(s, \eta) = \begin{pmatrix} \eta \cdot \omega + s & \eta \cdot \omega^\perp \\ \eta \cdot \omega^\perp & -\eta \cdot \omega - s \end{pmatrix} v(s, \eta),$$

i.e. the equation (68) for $z = (\eta \cdot \omega, \eta \cdot \omega^\perp)$ and we can write

$$u(s, \eta) = \mathcal{R}(\theta)u_{LZ}(sr^{1/2}, r^{-1/2}z).$$

Then, Equation (69) motivates the following:

$$\begin{aligned} \Lambda(s, \eta) &:= \frac{1}{2}|sr^{1/2} + r^{-1/2}\eta \cdot \omega|^2 + \frac{1}{2}|r^{-1/2}\eta \cdot \omega^\perp|^2 \ln |sr^{1/2} + r^{-1/2}\eta \cdot \omega| \\ &= \frac{1}{2r}|sr + \eta \cdot \omega|^2 + \frac{1}{2r}|\eta \cdot \omega^\perp|^2 \ln |sr^{1/2}| + O(R^3|s|^{-1}) \end{aligned}$$

where we have performed a Taylor expansion of $\ln \left| 1 + \frac{\eta \cdot \omega}{sr} \right|$ and used $|\eta| \leq R$. As $s \rightarrow \pm\infty$, we deduce that Equation (69) yields to

$$u(s, \eta) = e^{i\Lambda(s, \eta)}u_1^\pm \mathcal{R}(\theta) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + e^{-i\Lambda(s, \eta)}u_2^\pm \mathcal{R}(\theta) \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \mathcal{O}(R^3|s|^{-1}).$$

In view of

$$\mathcal{R}(\theta)^{-1}A(\omega)\mathcal{R}(\theta) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

we deduce that there exists $\varsigma \in \{-1, +1\}$ such that

$$\vec{V}_\omega = \varsigma \mathcal{R}(\theta) \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \vec{V}_\omega^\perp = \varsigma \mathcal{R}(\theta) \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

up to a sign. The result of Lemma 4.4 then follows with $\alpha_j^{\text{in}} = \varsigma u_j^-$ and $\alpha_j^{\text{out}} = \varsigma u_j^+$, $j \in \{1, 2\}$. \square

In the following, we wish to compare u^ε with u from (67) with $\eta = \eta(y)$ and use Lemma 4.4 to deduce the leading behavior of u^ε at $s_0 = \delta/\sqrt{\varepsilon}$ from information available at time $-s_0 = -\delta/\sqrt{\varepsilon}$. For that purpose, it is required to identify the ingoing profiles α_1^{in} and α_2^{in} related with the data $u(-s_0) := u^\varepsilon(-s_0)$, that is known from Section 3. We will do that in the next section and will make use of the following property of $u^\varepsilon(s, y)$.

Lemma 4.5. *Assume $u(-s_0) \in \Sigma^k(\mathbb{R}^d)$, $\alpha, \beta \in \mathbb{N}^2$. Then, there exists a constant $C_{\alpha, \beta} > 0$ such that the solution of (67) satisfies for $s \in (-s_0, s_0)$ we have*

$$\|\eta^\alpha \partial_\eta^\beta u(s)\|_{L^2} \leq C_{\alpha, \beta} \langle s \rangle^{|\beta|}.$$

Proof. When $\beta = 0$, one easily checks that the result holds (because η^α commutes with the equation). One then fixes α , uses a recursive argument on the length of β , starting from the conservation of the L^2 -norm ($\beta = 0$) and based on the observation

$$i\partial_s(\eta^\alpha \partial^\beta u) = A(sr\omega + \eta)(\eta^\alpha \partial^\beta u) + \sum_{j=1,2} \mathbf{1}_{\beta_j > 0} c_j A(e_j) \eta^\alpha \partial^{\beta-1_j} u$$

where c_j are universal constants and (e_1, e_2) the canonical basis of \mathbb{R}^2 . An energy inequality generates the growth in s . \square

4.3. The ingoing wave packet. Here we prove the following proposition.

Proposition 4.6. *With the assumptions of Theorem 1.9, the solution of (1) satisfies (64) at time $t = t^\flat - \delta$, i.e. $s = -s_0 = -\delta/\sqrt{\varepsilon}$ with*

$$u^\varepsilon(-s_0, y) = e^{-i\Lambda(-s_0, \eta)} \alpha_2^{\text{in}}(\eta(y)) \vec{V}_\omega + \mathcal{O}\left((\sqrt{\varepsilon}\delta^{-1} + \varepsilon^{3/2}\delta^{-4} + \delta^3\varepsilon^{-1})(1 + |\ln \delta|)\right) \text{ in } \widetilde{\Sigma}_\varepsilon^k$$

where $\Lambda(s, \eta)$ is defined in (70), η is given by $\eta = dw(q^\flat)y$ and we have

$$(71) \quad \alpha_2^{\text{in}}(\eta) = \text{Exp}\left(\frac{i}{\varepsilon} S_-^\flat + \frac{i}{4r}(\eta \cdot \omega^\perp)^2 \ln\left(\frac{r}{\varepsilon}\right) + \frac{i}{2r}|\omega \cdot \eta|^2\right) u_-^{\text{in}}(y),$$

with $S_-^\flat = S_-(t^\flat, t_0, z_0)$.

Remark 4.7. This result suggests that δ has to be chosen so that $\delta^3 \ll \varepsilon$, accordingly with the constraints mentioned in Remark 3.5 and fits with the choice of $\delta = \varepsilon^{\frac{5}{14}}$.

Proof. We start from the estimate obtained for $t \leq t^\flat - \delta$, namely

$$\begin{aligned} \psi^\varepsilon(t, x) &= \varepsilon^{-d/4} e^{\frac{i}{\varepsilon} S_-(t, t_0, z_0) + \frac{i}{\varepsilon} p_-(t)(x - q_-(t))} \vec{V}_-(t, \Phi_-^{t, t_0}(z_0)) \\ &\quad \times u_- \left(t, \frac{x - q_-(t)}{\sqrt{\varepsilon}}\right) + \mathcal{O}\left((\sqrt{\varepsilon}\delta^{-1} + \varepsilon^{3/2}\delta^{-4})(1 + |\ln \delta|)\right) \end{aligned}$$

in Σ_ε^k . We fix $k \in \mathbb{N}$ and prove the estimates in this set.

We begin by considering the phase. The asymptotics of Lemma 2.1 and Lemma 2.2 imply that when $t = t^\flat + \sqrt{\varepsilon}s$ with $s < 0$ and $x = q_0(t) + \sqrt{\varepsilon}y$, we have the pointwise estimates

$$\frac{i}{\varepsilon} S_-(t, t^\flat, z^\flat) = \frac{i}{\varepsilon} S_0(t, t^\flat, z^\flat) - irs^2 + \mathcal{O}(\sqrt{\varepsilon}s^3)$$

and

$$\begin{aligned} \frac{i}{\varepsilon} p_-(t) \cdot (x - q_-(t)) &= \frac{i}{\varepsilon} \left(p_0(t) - \sqrt{\varepsilon}s^t dw(q^\flat)\omega + \mathcal{O}(\varepsilon s^2)\right) \cdot \left(x - q_0(t) + \frac{\varepsilon}{2}s^2{}^t dw(q^\flat)\omega + \mathcal{O}(\varepsilon^{3/2}s^3)\right) \\ &= \frac{i}{\sqrt{\varepsilon}} p_0(t) \cdot y - is\omega \cdot dw(q^\flat)y + \frac{i}{2}s^2\omega \cdot dw(q^\flat)p_0(t) + \mathcal{O}(\sqrt{\varepsilon}s^2|y|) + \mathcal{O}(\sqrt{\varepsilon}s^3). \end{aligned}$$

We observe that

$$\omega \cdot dw(q^\flat)p_0(t) = \omega \cdot dw(q^\flat)p^\flat + \mathcal{O}(s\sqrt{\varepsilon}) = r + \mathcal{O}(s\sqrt{\varepsilon}).$$

Therefore

$$\begin{aligned} \frac{i}{\varepsilon} S_-(t, t^b, z^b) + \frac{i}{\varepsilon} p_-(t) \cdot (x - q_-(t)) &= \frac{i}{\varepsilon} S_0(t, t^b, z^b) + \frac{i}{\sqrt{\varepsilon}} y \cdot p_0(t) \\ &\quad - \frac{i}{2} r s^2 - i s \omega \cdot dw(q^b) y + \mathcal{O}(\sqrt{\varepsilon} s^2 |y|) + \mathcal{O}(\sqrt{\varepsilon} s^3) \end{aligned}$$

We now consider the profile and takes into account Corollary 1.7. We obtain the estimate in Σ_ε^k

$$\begin{aligned} \psi^\varepsilon(t, x) &= \varepsilon^{-d/4} \text{Exp} \left(\frac{i}{\varepsilon} S_0(t^b + \sqrt{\varepsilon} s, t^b, z^b) + \frac{i}{\sqrt{\varepsilon}} p_0(t) \cdot y \right) \\ &\quad \times \vec{V}_\omega \text{Exp} \left(-\frac{i}{2} \Gamma_0 y \cdot y \ln |s \sqrt{\varepsilon}| - \frac{i}{2} r s^2 - i s \omega \cdot dw(q^b) y + \mathcal{O}(s^3 \sqrt{\varepsilon}) \right) \\ &\quad \times e^{\frac{i}{\varepsilon} S_-^b} u_-^{\text{in}}(y + y^\varepsilon(s)) + \mathcal{O} \left((\sqrt{\varepsilon} \delta^{-1} + \varepsilon^{3/2} \delta^{-4} + \delta)(1 + |\ln \delta|) \right) \end{aligned}$$

where we have approximated $u_-(t)$ by u_-^{in} and $\vec{Y}_-(t)$ by $\vec{V}_\omega(t)$ for t close to t^b ($|t - t^b| \sim \delta$) and $y^\varepsilon(s)$ satisfies the pointwise estimate $y^\varepsilon(s) = \mathcal{O}(s^2 \sqrt{\varepsilon} \langle y \rangle)$. We deduce from the fact that $u_-^{\text{in}} \in \mathcal{S}(\mathbb{R}^d)$

$$\begin{aligned} u^\varepsilon(-s_0, y) &= \vec{V}_\omega e^{\frac{i}{\varepsilon} S_-^b} \text{Exp} \left(-\frac{i}{2} \Gamma_0 y \cdot y \ln |s \sqrt{\varepsilon}| - \frac{i}{2} r s^2 - i s \omega \cdot dw(q^b) y \right) u_-^{\text{in}}(y) \\ &\quad + \mathcal{O} \left((\sqrt{\varepsilon} \delta^{-1} + \varepsilon^{3/2} \delta^{-4} + \delta + \delta^3 \varepsilon^{-1})(1 + |\ln \delta|) \right) \end{aligned}$$

where we have used that $\frac{\delta^2}{\sqrt{\varepsilon}} \ll \frac{\delta^3}{\varepsilon}$ since $\sqrt{\varepsilon} \ll \delta$. Given the definition of $\Lambda(s, \eta)$ in (70) with $\eta = dw(q^b) y$, we obtain

$$\Lambda(s, \eta) = \frac{r}{2} s^2 + s \omega \cdot dw(q^b) y + \frac{1}{2r} |\omega \cdot \eta|^2 + \frac{1}{2r} |\omega^\perp \cdot \eta|^2 \ln(\sqrt{r} |s|).$$

Moreover

$$\Gamma_0 y \cdot y = r^{-1} \left((\text{Id}_{\mathbb{R}^2} - \omega \otimes \omega) dw(q^b) y \right) \cdot \left(dw(q^b) y \right) = r^{-1} (dw(q^b) y \cdot \omega^\perp)^2.$$

Therefore, in $\tilde{\Sigma}_\varepsilon^k$

$$\begin{aligned} u^\varepsilon(-s_0, y) &= \vec{V}_\omega \text{Exp}(-i\Lambda(s, y)) \text{Exp} \left(\frac{i}{\varepsilon} S_-^b + \frac{i}{4r} (\eta \cdot \omega^\perp)^2 \ln\left(\frac{r}{\varepsilon}\right) + \frac{i}{2r} |\omega \cdot \eta|^2 \right) u_-^{\text{in}}(y) \\ &\quad + \mathcal{O} \left((\sqrt{\varepsilon} \delta^{-1} + \varepsilon^{3/2} \delta^{-4} + \delta + \delta^3 \varepsilon^{-1})(1 + |\ln \delta|) \right), \end{aligned}$$

which concludes the proof in view of (71). \square

4.4. The outgoing solution. We now compare $u^\varepsilon(s)$ with a solution to the Landau-Zener model problem. Let u be the solution of (67) for $\eta = \eta(y)$ and the initial data

$$u(-s_0) = e^{i\Lambda(-s_0, \eta)} \alpha_2^{\text{in}}(\eta) \vec{V}_\omega$$

where $\alpha_2^{\text{in}}(\eta)$ is given by (71), $R > 0$, $\eta = \eta(y)$. We consider $\chi_0 \in \mathcal{C}_0^\infty(\mathbb{R}^d, [0, 1])$ such that $|\eta(y)| \leq cR$ when $y/R \in \text{supp} \chi_0$. We consider the function $u_R(s) = \chi_0(y/R) u(s)$. Then, u_R is the solution to (67) for $\eta = \eta(y)$ and the initial data

$$(72) \quad u_R(-s_0) = e^{i\Lambda(-s_0, \eta)} \alpha_2^{\text{in}}(\eta) \chi_0(y/R) \vec{V}_\omega$$

This cut-off allows us to use the scattering results of Lemma 4.4 for u_R . As noticed in Remark 4.1, we shall use the norms $\tilde{\Sigma}_\varepsilon^k$ introduced in (65).

Lemma 4.8. *Let $u_R(s)$ be the solution of the Landau-Zener model problem (67) for $\eta = \eta(y)$ and the initial data $u_R(-s_0)$ given by (72), and $u^\varepsilon(s)$ be the solution of (66). Let $k \in \mathbb{N}$, then for all $N_0 \in \mathbb{N}$ and for all $s \in [-s_0, s_0]$, for all $R \geq 1$ with $R^2\sqrt{\varepsilon} \ll 1$, $R\delta \ll 1$ and $R\varepsilon^2\delta^{-4} \ll 1$, in $\widetilde{\Sigma}_\varepsilon^k(\mathbb{R}^d)$,*

$$u^\varepsilon(s) - u_R(s) = \mathcal{O}\left((\sqrt{\varepsilon}\delta^{-1} + \varepsilon^{3/2}\delta^{-4} + \delta + R\delta^3\varepsilon^{-1} + R^{-N_0})(1 + |\ln \delta|)\right).$$

Remark 4.9. We are going to take $\alpha = \frac{5}{14}$ as in Remark 3.5, which implies $\delta^3\varepsilon^{-1} = \varepsilon^{\frac{1}{14}}$. We choose $R = \varepsilon^{-\beta}$ with $\beta \in (0, \frac{1}{14})$ small enough so that $R^2\sqrt{\varepsilon} \ll 1$, $R\delta \ll 1$ and $R\varepsilon^2\delta^{-4} \ll 1$. Since R produces an error of size $R^3\sqrt{\varepsilon}\delta^{-1} \ll 1$ by Lemma 4.4, we additionally ask $R^3\sqrt{\varepsilon}\delta^{-1} \leq \varepsilon^{\frac{1}{14}}$. We choose N_0 as large as necessary to ensure $R^{-N_0} \leq \varepsilon^{\frac{1}{14}}$. We are then left with an approximation of order $\mathcal{O}(\varepsilon^{\frac{1}{14}-\beta}) = \mathcal{O}\left(\varepsilon^{\frac{1}{14}-}\right)$.

Proof. We set $r^\varepsilon(s) = u^\varepsilon(s) - u_R(s)$. We observe that using that $u_-^{\text{in}} \in \mathcal{S}(\mathbb{R}^d)$ (see Proposition 4.6), we deduce that we have in $\widetilde{\Sigma}_\varepsilon^k$ and for any $N_0 \in \mathbb{N}$,

$$r^\varepsilon(-s_0) = \mathcal{O}\left((\sqrt{\varepsilon}\delta^{-1} + \varepsilon^{3/2}\delta^{-4} + \delta + \delta^3\varepsilon^{-1} + R^{-N_0})(1 + |\ln \delta|)\right) = \mathcal{O}(\varsigma_\varepsilon).$$

where we set for short $\mathcal{O}(\varsigma_\varepsilon) = \mathcal{O}\left((\sqrt{\varepsilon}\delta^{-1} + \varepsilon^{3/2}\delta^{-4} + \delta + R\delta^3\varepsilon^{-1} + R^{-N_0})(1 + |\ln \delta|)\right)$. Besides, we have (with the notations of Lemma 4.2)

$$i\partial_s r^\varepsilon(s) - P^\varepsilon(s)r^\varepsilon(s) = \sqrt{\varepsilon}f^\varepsilon(s, y)$$

where

$$\begin{aligned} P^\varepsilon(s) &= A(sE + dw(q^b)y) + \frac{\sqrt{\varepsilon}}{2}\Delta + \sqrt{\varepsilon}B^\varepsilon(s, y) \\ f^\varepsilon(s) &= \frac{1}{2}\Delta u_R(s) + B^\varepsilon(s, y)u_R(s). \end{aligned}$$

We shall use the two following properties:

- (i) By Lemma 4.2, there exist constants C_0, C_1, C_β , $|\beta| \geq 2$, such that on the support of u_R (where $|y| \leq c'R$, $c' > 0$), and for $s \in [-s_0, s_0]$, we have

$$|B^\varepsilon(s, y)| \leq C_0(Rs^2 + |y|^2), \quad |\nabla B^\varepsilon(s, y)| \leq C_1(R|y| + \delta s), \quad |\partial_y^\beta B^\varepsilon(s, y)| \leq C_\beta R^2 \varepsilon^{\frac{|\beta|-2}{2}}.$$

- (ii) By Lemma 4.5, f^ε satisfies the following: for all $\alpha, \beta \in \mathbb{N}^d$, there exists $C_{\alpha, \beta}$ such that

$$(73) \quad \|y^\alpha \partial_y^\beta f^\varepsilon(s, y)\|_{L^2} \leq C_{\alpha, \beta} (R s_0^{|\beta|+2} + R^2 s_0^{(|\beta|-2)}) \leq C_{\alpha, \beta} R s_0^{|\beta|+2}$$

where we used $R s_0^{-4} \leq 1$. We prove by a recursive argument that

$$(74) \quad \sup_{s \in [-s_0, s_0]} \|y^\alpha \partial_y^\beta r^\varepsilon(s, y)\|_{L^2} = \mathcal{O}(\sqrt{\varepsilon} R s_0^{|\alpha|+|\beta|+3}) + \mathcal{O}(\varsigma_\varepsilon)$$

which implies the Lemma since

$$\varepsilon^{\frac{|\alpha|+|\beta|}{2}} R \sqrt{\varepsilon} s_0^{|\alpha|+|\beta|+3} = R \sqrt{\varepsilon} s_0^3 = R \frac{\delta^3}{\varepsilon}.$$

- $k = 0$. An energy estimate gives

$$(75) \quad \|r^\varepsilon(s)\|_{L^2} \leq C\sqrt{\varepsilon} \int_{-s_0}^s \|f^\varepsilon(s')\|_{L^2} ds' + \mathcal{O}(\varsigma_\varepsilon) \leq CR\sqrt{\varepsilon} s_0^3 + \mathcal{O}(\varsigma_\varepsilon),$$

whence (74) for $k = 0$.

- $k = 1$. Using the equation satisfied by r^ε , we write for $j \in \{1, \dots, d\}$

$$\begin{aligned} (i\partial_s - P^\varepsilon(s))(y_j r^\varepsilon) &= \sqrt{\varepsilon}(y_j f^\varepsilon) + \sqrt{\varepsilon}(\partial_{y_j} r^\varepsilon), \\ (i\partial_s - P^\varepsilon(s))(\partial_{y_j} r^\varepsilon) &= \sqrt{\varepsilon}(\partial_{y_j} f^\varepsilon) + \sqrt{\varepsilon}(\partial_{y_j} B^\varepsilon r^\varepsilon) + A(\partial_{x_j} w(q^b))r^\varepsilon. \end{aligned}$$

Note that $|\partial_{y_j} B^\varepsilon r^\varepsilon| \leq C(R|y| + \delta s)|r^\varepsilon|$ and $R \geq 1$. Using Point (i) above, an energy argument gives for some constant c_1

$$\begin{aligned} \|y r^\varepsilon(s)\|_{L^2} + \|\nabla_y r^\varepsilon(s)\|_{L^2} &\leq \mathcal{O}(\varsigma_\varepsilon) + c_1(R\sqrt{\varepsilon}) \int_{-s_0}^s (\|y r^\varepsilon(s')\|_{L^2} + \|\nabla_y r^\varepsilon(s')\|_{L^2}) ds' \\ &+ \sqrt{\varepsilon} \int_{-s_0}^s (\|y f^\varepsilon(s')\|_{L^2} + \|\nabla_y f^\varepsilon(s')\|_{L^2}) ds' + c_1 \delta \sqrt{\varepsilon} \int_{-s_0}^s \langle s' \rangle \|r^\varepsilon(s')\|_{L^2} ds' + c_1 \int_0^s \|r^\varepsilon(s')\|_{L^2} ds' \\ &\leq 2c_1 R \sqrt{\varepsilon} s_0 \sup_{s \in [-s_0, s_0]} (\|y r^\varepsilon(s)\|_{L^2} + \|\nabla_y r^\varepsilon(s)\|_{L^2}) + c_1 \int_0^s \|r^\varepsilon(s')\|_{L^2} ds' \\ &+ \sqrt{\varepsilon} \int_{-s_0}^s (\|y f^\varepsilon(s')\|_{L^2} + \|\nabla_y f^\varepsilon(s')\|_{L^2}) ds' + c_1 \delta \sqrt{\varepsilon} s_0 \int_{-s_0}^s \|r^\varepsilon(s')\|_{L^2} ds' + \mathcal{O}(\varsigma_\varepsilon) \end{aligned}$$

where we have used $\sqrt{\varepsilon} s_0 \leq \delta$. Using $R\sqrt{\varepsilon} s_0 \leq R\delta \ll 1$, (73) and (75), we deduce (changing the constant c_1 as necessary)

$$\sup_{s \in [-s_0, s_0]} (\|y r^\varepsilon(s)\|_{L^2} + \|\nabla_y r^\varepsilon(s)\|_{L^2}) \leq c_1(R\sqrt{\varepsilon} s_0^4 + \delta \varepsilon R s_0^5) + \mathcal{O}(\varsigma_\varepsilon) \leq c_1 R \sqrt{\varepsilon} s_0^4 + \mathcal{O}(\varsigma_\varepsilon),$$

where we have used $s_0 \sqrt{\varepsilon} \leq \delta$, whence (74) for $k = 1$.

- $k \rightarrow k + 1$. We assume that there exists some $k \in \mathbb{N}$ such that for all $\ell \in \{0, \dots, k\}$

$$\sup_{|\alpha|+|\beta|=\ell} \sup_{s \in [-s_0, s_0]} \|y^\alpha \partial_y^\beta r^\varepsilon(s)\|_{L^2} \leq c_k R \sqrt{\varepsilon} s_0^{\ell+3}$$

and that for any term of the form $y^\alpha \partial_y^\beta r^\varepsilon$ with $|\alpha| + |\beta| = k$, we have

$$(i\partial_s - P^\varepsilon(s))(y^\alpha \partial_y^\beta r^\varepsilon) = \sqrt{\varepsilon} y^\alpha \partial_y^\beta f^\varepsilon + \sum_{\ell=0}^k \sum_{|\alpha'|+|\beta'|=\ell} c_{\alpha',\beta}^\varepsilon(s, y) y^{\alpha'} \partial_y^{\beta'} r^\varepsilon$$

for some smooth functions $c_{\alpha',\beta}^\varepsilon$ bounded together with their derivatives uniformly in ε with

$$\begin{aligned} |c_{\alpha',\beta'}^\varepsilon(s, y)| + |\nabla_y c_{\alpha',\beta'}^\varepsilon(s, y)| &= \mathcal{O}(\sqrt{\varepsilon}(\langle s \rangle + |y|) + 1) \text{ for } |\alpha'| + |\beta'| < k \\ |c_{\alpha',\beta'}^\varepsilon(s, y)| + |\nabla_y c_{\alpha',\beta'}^\varepsilon(s, y)| &= \mathcal{O}(R\sqrt{\varepsilon}) \text{ for } |\alpha'| + |\beta'| = k. \end{aligned}$$

Multiplying the equation by y_j and applying ∂_{y_j} for all $j \in \{1, \dots, d\}$, one obtains that the form of the equation passes to the $(k + 1)$ -th step, which gives the norm estimate by an energy argument. This concludes the proof. \square

5. PROOF OF THE MAIN RESULTS

5.1. Proof of Theorem 1.8. When the trajectory $\Phi_-^{t,t_0}(z_0)$ remains in the domain $\{|w(q)| > \delta\}$, the results of Proposition 3.1 apply and imply Theorem 1.8.

5.2. Proof of Theorem 1.9. Inside the gap region, for $t \in [t^b - \delta, t^b + \delta]$, we apply Lemma 4.3 to pass through it. Then over the time $[t^b + \delta, t_0 + T]$ we use Proposition 3.1 again to propagate further, with initial data found from the resulting solution $\psi^\varepsilon(t^b + \delta)$ from Lemma 4.3 in the gap region. Then, we optimize δ and R to get the best approximation in terms of ε according to Remarks 3.5 and 4.9.

5.2.1. Away from the gap region. Given the initial assumptions of the theorem, we start at time t_0 far from the crossing point with initial data ψ_0^ε satisfying (8). We consider the trajectory $\Phi_-^{t, t_0}(z_0)$ and the classical quantities that are associated with it. Applying Proposition 3.1 on $[t_0, t^b - \delta]$ with $u_+(t_0) = 0$ and $u_-(t_0) = a$, we propagate the solution up to the gap region: at $t = t^b - s_0\sqrt{\varepsilon} = t^b - \delta$, we have in $L^2(\mathbb{R}^d)$

$$\begin{aligned} \psi^\varepsilon(t, x) = & \varepsilon^{-d/4} e^{\frac{i}{\varepsilon} S_-(t, t_0, z_0) + \frac{i}{\varepsilon} p_-(t)(x - q_-(t))} \vec{V}_-(t, \Phi_-^{t, t_0}(z_0)) \\ & \times u_- \left(t, \frac{x - q_-(t)}{\sqrt{\varepsilon}} \right) + \mathcal{O} \left((\sqrt{\varepsilon} \delta^{-1} + \varepsilon^{3/2} \delta^{-4})(1 + |\ln \delta|) \right). \end{aligned}$$

Using the minimal gap of the avoided crossing, $\delta_c \gg \sqrt{\varepsilon}$, we are left with error terms $o(1)$.

5.2.2. Passing through the gap region. In this section, we compute an approximation of $\psi^\varepsilon(t^b + \delta)$, thanks to the representation of ψ^ε as (64) which reduces the analysis to one of function $u^\varepsilon(s)$ satisfying (66). Then, by Lemma 4.8, it is possible to use Lemma 4.4 to link $u^\varepsilon(+s_0)$ and $u^\varepsilon(-s_0)$. Proposition 4.6 allow to identify the entering data at time $s = -s_0$ that we use in Lemma 4.4 : $\alpha_1 = 0$ and α_2 satisfying (71). We define $(\alpha_1^{\text{out}}, \alpha_2^{\text{out}})$ as

$$(76) \quad \begin{aligned} \alpha_1^{\text{out}}(\eta) &= -\bar{b}(r^{-1/2} \eta \cdot \omega^\perp) \alpha_2^{\text{in}}(\eta) \\ \alpha_2^{\text{out}}(\eta) &= a(r^{-1/2} \eta \cdot \omega^\perp) \alpha_2^{\text{in}}(\eta). \end{aligned}$$

This follows from the formula giving $\begin{pmatrix} \alpha_1^{\text{out}} \\ \alpha_2^{\text{out}} \end{pmatrix}$ in Lemma 4.4. Besides, we know that when $t = t^b + \delta = t^b + s_0\sqrt{\varepsilon}$, $\psi^\varepsilon(t)$ satisfies (64) with

$$\begin{aligned} u^\varepsilon(s_0, y) = & e^{i\Lambda(s, \eta)} \alpha_1^{\text{out}}(\eta) \vec{V}_\omega^\perp + e^{-i\Lambda(s, \eta)} \alpha_2^{\text{out}}(\eta) \vec{V}_\omega \\ & + \mathcal{O} \left((\sqrt{\varepsilon} \delta^{-1} + \varepsilon^{3/2} \delta^{-4} + \delta + R\delta^3 \varepsilon^{-1})(1 + |\ln \delta|) \right). \end{aligned}$$

This implies that for $t = t^b + \delta = t^b + \sqrt{\varepsilon} s_0$,

$$\psi^\varepsilon(t, x) = \psi_+^\varepsilon(t, x) + \psi_-^\varepsilon(t, x) + \mathcal{O} \left((\sqrt{\varepsilon} \delta^{-1} + \varepsilon^{3/2} \delta^{-4} + \delta + R\delta^3 \varepsilon^{-1})(1 + |\ln \delta|) \right)$$

with

$$(77) \quad \psi_+^\varepsilon(t, x) = e^{\frac{i}{\varepsilon} S_0(t, t^b, z^b) + \frac{i}{\varepsilon} (x - q_0(t)) \cdot p_0(t)} \left(e^{-i\Lambda(s_0, \eta(y))} \alpha_2^{\text{out}}(\eta) \right) \Big|_{y = \frac{x - q_0(t)}{\sqrt{\varepsilon}}} \vec{V}_\omega,$$

$$(78) \quad \psi_-^\varepsilon(t, x) = e^{\frac{i}{\varepsilon} S_0(t, t^b, z^b) + \frac{i}{\varepsilon} (x - q_0(t)) \cdot p_0(t)} \left(e^{+i\Lambda(s_0, \eta(y))} \alpha_1^{\text{out}}(\eta) \right) \Big|_{y = \frac{x - q_0(t)}{\sqrt{\varepsilon}}} \vec{V}_\omega^\perp$$

in $L^2(\mathbb{R}^d)$. It remains to see why the functions $\psi_\pm^\varepsilon(t, x)$ can be approximated by wave packets associated with the curves $\Phi_\pm^{t, t^b}(z^b)$ respectively. For this, we study the asymptotics of the phase and of the profiles for $t > t^b$, as we did in Section 4.3 for times $t < t^b$.

Let us begin with the phases. We observe that the asymptotics of Lemma 2.1 and Lemma 2.2 imply that when $t = t^b + \sqrt{\varepsilon}s$ with $s > 0$ and $x = q_0(t) + \sqrt{\varepsilon}y$, we have the pointwise estimates

$$\frac{i}{\varepsilon}S_{\pm}(t, t^b, z^b) = \frac{i}{\varepsilon}S_0(t, t^b, z^b) \mp irs^2 + \mathcal{O}(\sqrt{\varepsilon}s^3)$$

and

$$\begin{aligned} \frac{i}{\varepsilon}p_{\pm}(t) \cdot (x - q_{\pm}(t)) &= \frac{i}{\varepsilon} \left(p_0(t) \mp \sqrt{\varepsilon}s^t dw(q^b)\omega + \mathcal{O}(\varepsilon s^2) \right) \cdot \left(x - q_0(t) \pm \frac{\varepsilon}{2}s^2 dw(q^b)\omega + \mathcal{O}(\varepsilon^{3/2}s^3) \right) \\ &= \frac{i}{\sqrt{\varepsilon}}p_0(t) \cdot y \mp is\omega \cdot dw(q^b)y + \mathcal{O}(\sqrt{\varepsilon}s^2|y|) \pm \frac{i}{2}s^2\omega \cdot dw(q^b)p_0(t) + \mathcal{O}(\sqrt{\varepsilon}s^3) + \mathcal{O}(\varepsilon s^3) \end{aligned}$$

We observe that

$$\omega \cdot dw(q^b)p_0(t) = \omega \cdot dw(q^b)p^b + \mathcal{O}(s\sqrt{\varepsilon}) = r + \mathcal{O}(s\sqrt{\varepsilon}).$$

Therefore

$$\frac{i}{\varepsilon}p_{\pm}(t) \cdot (x - q_{\pm}(t)) = \frac{i}{\sqrt{\varepsilon}}y \cdot p_0(t) \mp is\omega \cdot dw(q^b)y \pm \frac{i}{2}rs^2 + \mathcal{O}(\sqrt{\varepsilon}s^2|y|) + \mathcal{O}(\sqrt{\varepsilon}s^3).$$

Then,

$$\begin{aligned} \frac{i}{\varepsilon}S_{\pm}(t, t^b, z^b) + \frac{i}{\varepsilon}p_{\pm}(t) \cdot (x - q_{\pm}(t)) &= \frac{i}{\varepsilon}S_0(t, t^b, z^b) + \frac{i}{\sqrt{\varepsilon}}y \cdot p_0(t) \\ &\mp \frac{i}{2}rs^2 \mp is\omega \cdot dw(q^b)y + \mathcal{O}(\sqrt{\varepsilon}s^2|y|) + \mathcal{O}(\sqrt{\varepsilon}s^3) \end{aligned}$$

Given the definition of $\Lambda(s, \eta)$, (70),

$$i\Lambda(s, \eta) = \frac{i}{2r}|\omega \cdot \eta + rs|^2 + \frac{i}{4r}|\omega^{\perp} \cdot \eta|^2 \ln(rs^2),$$

we obtain

$$\begin{aligned} i\Lambda(s, \eta) &= \frac{i}{2r} \left(|\omega \cdot \eta|^2 + 2rs\omega \cdot dw(q^b)y + r^2s^2 \right) + \frac{i}{4r}|\omega^{\perp} \cdot \eta|^2 \ln(rs^2) \\ &= \frac{i}{2r}|\omega \cdot \eta|^2 + is\omega \cdot dw(q^b)y + \frac{i}{2}rs^2 + \frac{i}{4r}|\omega^{\perp} \cdot \eta|^2 \ln(rs^2) \end{aligned}$$

Using all of these ingredients together, we have the pointwise estimate

$$\begin{aligned} \frac{i}{\varepsilon}S_{\pm}(t, t^b, z^b) + \frac{i}{\varepsilon}p_{\pm}(t) \cdot (x - q_{\pm}(t)) &= \frac{i}{\varepsilon}S_0(t, t^b, z^b) \\ &+ \frac{i}{\sqrt{\varepsilon}}y \cdot p_0(t) \mp i\Lambda(s, \eta) \pm \frac{i}{2r}|\omega \cdot \eta|^2 \pm \frac{i}{2r}|\omega^{\perp} \cdot \eta|^2 (\ln(\sqrt{r}s)) \\ &+ \mathcal{O}(\sqrt{\varepsilon}s^2|y|) + \mathcal{O}(\sqrt{\varepsilon}s^3) \end{aligned}$$

At this stage of the proof, we are able to see the wave packet structure of the functions $\psi_{\pm}^{\varepsilon}(t^b + \delta)$ defined in (77) and (78). Let us study more precisely $\psi_{-}^{\varepsilon}(t, x)$, the computation for the other mode being similar. In view of the relations stated above, we have in $L^2(\mathbb{R}^d)$

$$\begin{aligned} \psi_{-}^{\varepsilon}(t, x) &= e^{\frac{i}{\varepsilon}S_{-}(t, t^b, z^b) + \frac{i}{\varepsilon}(x - q_{-}(t)) \cdot p_{-}(t) + \frac{i}{2r}|\omega \cdot \eta|^2 + \frac{i}{2r}|\omega^{\perp} \cdot \eta|^2 \ln(\sqrt{r}s)} \alpha_1^{\text{out}}(\eta) \vec{V}_{\omega}^{\perp} \\ &+ \mathcal{O}((\sqrt{\varepsilon}s^2|y| + \sqrt{\varepsilon}s^3)(1 + |\ln(s\sqrt{r})|)). \end{aligned}$$

Here again

$$\frac{1}{r}(\omega^{\perp} \cdot \eta(y))^2 \ln(s\sqrt{r}) = \Gamma_0 y \cdot y \ln(s\sqrt{r}) = \Gamma_0 y \cdot y \ln(s\sqrt{\varepsilon}) + \frac{1}{2r}(\omega^{\perp} \cdot \eta(y))^2 \ln\left(\frac{r}{\varepsilon}\right).$$

and we obtain for $t = t^b + \delta = t^b + s_0\sqrt{\varepsilon}$

$$\begin{aligned} \psi_-^\varepsilon(t, x) &= V_\omega^\perp \text{Exp} \left(\frac{i}{\varepsilon} S_-(t, t^b, z^b) + \frac{i}{\varepsilon} (x - q_-(t)) \cdot p_-(t) \right) \\ &\times \left(\text{Exp} \left(\frac{i}{2} \Gamma_0 y \cdot y \ln(s\sqrt{\varepsilon}) \right) \text{Exp} \left(\frac{i}{4r} (\omega^\perp \cdot \eta(y))^2 \ln(r/\varepsilon) + \frac{i}{2r} (\omega \cdot \eta)^2 \right) \alpha_1^{\text{out}}(\eta) \right) \Big|_{y=\frac{x-q_0(t)}{\sqrt{\varepsilon}}} \\ &+ \mathcal{O}((\sqrt{\varepsilon}s^2|y| + \sqrt{\varepsilon}s^3)(1 + |\ln(s\sqrt{r})|)) \end{aligned}$$

in $L^2(\mathbb{R}^d)$. Using the regularity of α_1^{out} , we deduce $\alpha_1^{\text{out}} \left(\frac{x-q_0(t)}{\sqrt{\varepsilon}} \right) = \alpha_1^{\text{out}} \left(\frac{x-q_-(t)}{\sqrt{\varepsilon}} \right) + \mathcal{O}(\sqrt{\varepsilon}s^2)$ with $\mathcal{O}(\sqrt{\varepsilon}s^2) = \mathcal{O}(\delta^2\varepsilon^{-1/2})$, we identify a wave packet approximation in $L^2(\mathbb{R}^d)$

$$\begin{aligned} \psi_-^\varepsilon(t, x) &= e^{\frac{i}{\varepsilon} S_-(t, t^b, z^b)} \text{WP}_{\Phi_-^{t, t^b}(z^b)}^\varepsilon \left(e^{\frac{i}{2} \Gamma_0 y \cdot y \ln(s\sqrt{\varepsilon})} e^{\frac{i}{4r} (\omega^\perp \cdot \eta(y))^2 \ln(r/\varepsilon) + \frac{i}{2r} (\omega \cdot \eta)^2} \alpha_1^{\text{out}}(\eta) \right) V_\omega^\perp \\ &+ \mathcal{O}(\sqrt{\varepsilon}s^2(1 + |y|)) + \mathcal{O}(\sqrt{\varepsilon}s^3). \end{aligned}$$

For $t \in [t^b - \delta, t^b + \delta]$, $\mathcal{O}(\sqrt{\varepsilon}s^2(1 + |y|)) + \mathcal{O}(\sqrt{\varepsilon}s^3) = \mathcal{O}(\varepsilon^{-1/2}\delta^2(1 + |y|)) + \mathcal{O}(\varepsilon^{-1}\delta^3)$. Using $y = \frac{x-q(t)}{\sqrt{\varepsilon}}$ for this region, we are left with the error terms $\mathcal{O}(\delta^3\varepsilon^{-1})$. In view of (22), this suggests that we set

$$\begin{aligned} u_-^{\text{out}}(y) &= \text{Exp} \left(\frac{i}{4r} (\omega^\perp \cdot \eta(y))^2 \ln(r/\varepsilon) + \frac{i}{2r} |\omega \cdot \eta|^2 \right) \alpha_1^{\text{out}}(\eta) \\ &= -\text{Exp} \left(\frac{i}{4r} (\omega^\perp \cdot \eta(y))^2 \ln(r/\varepsilon) + \frac{i}{2r} |\omega \cdot \eta|^2 \right) \bar{b}(r^{-1/2}\eta \cdot \omega^\perp) \alpha_2^{\text{in}}(\eta) \end{aligned}$$

A similar computation for the *plus*-mode gives

$$\begin{aligned} u_+^{\text{out}}(y) &= \text{Exp} \left(-\frac{i}{4r} (\omega^\perp \cdot \eta(y))^2 \ln(r/\varepsilon) - \frac{i}{2r} |\omega \cdot \eta|^2 \right) \alpha_2^{\text{out}}(\eta), \\ &= \text{Exp} \left(-\frac{i}{4r} (\omega^\perp \cdot \eta(y))^2 \ln(r/\varepsilon) - \frac{i}{2r} |\omega \cdot \eta|^2 \right) a(r^{-1/2}\eta \cdot \omega^\perp) \alpha_2^{\text{in}}(\eta). \end{aligned}$$

In view of (71), we deduce

$$\begin{aligned} u_+^{\text{out}}(y) &= e^{\frac{i}{\varepsilon} S^b} a(r^{-1/2}\eta \cdot \omega^\perp) u_-^{\text{in}}(y), \\ u_-^{\text{out}}(y) &= -e^{\frac{i}{\varepsilon} S^b} \text{Exp} \left(\frac{i}{2r} (\omega^\perp \cdot \eta(y))^2 \ln(r/\varepsilon) + \frac{i}{r} |\omega \cdot \eta|^2 \right) \bar{b}(r^{-1/2}\eta \cdot \omega^\perp) u_-^{\text{in}}(y). \end{aligned}$$

which is equivalent to (23).

5.2.3. Leaving the gap region. We define $u_\pm(t, y)$ for $t \geq t^b + \delta$ as the solution of (18) satisfying (22). Then, we have (27) when $t = t^b + \delta$ and the result for $[t \in t^b + \delta, T]$ comes by applying Proposition 3.1.

5.3. Proof of Corollary 1.13. Since for $t \in (t^b, t^b + T)$, we have $\Phi_+^{t, t^b}(z^b) \neq \Phi_-^{t, t^b}(z^b)$, any Wigner measure of $(\psi^\varepsilon(t))_{\varepsilon > 0}$ is of the form (30). Besides the coefficients c_+ and c_- are limits in ε of $\|u_+(t)\|_{L^2}^2$ and $\|u_-(t)\|_{L^2}^2$ respectively. We focus on c_+ (the proof for c_- is similar). We have

$$\|u_+(t)\|_{L^2}^2 = \|u_+^{\text{out}}\|_{L^2}^2 = \|a(\eta_2)u_+^{\text{in}}\|_{L^2}^2 + \|b(\eta_2)u_-^{\text{in}}\|_{L^2}^2 - 2\text{Re} \left(e^{\frac{i}{\varepsilon}(S_+^b - S_-^b)} \gamma_\varepsilon \right)$$

with

$$\gamma_\varepsilon = \int_{\mathbb{R}^d} a(\eta_2(y)) b(\eta_2(y)) u_+^{\text{in}}(y) \overline{u_-^{\text{in}}(y)} e^{i\theta_\varepsilon(\eta(y))} dy.$$

In view of $|b(\eta_2)|^2 = 1 - a(\eta_2)^2$, we have $\|b(\eta_2)u_{-}^{\text{in}}\|^2 = \|\sqrt{1 - a(\eta_2)}u_{-}^{\text{in}}\|^2$. Moreover, by (26) and using $b(0) = 0$, the term γ_ε writes

$$\gamma_\varepsilon = \int \eta_2(y) f(y) e^{-\frac{i}{2r} \eta_2(y)^2 \ln \varepsilon} dy$$

for some smooth function f . Together with $\eta_2(y) = \omega^\perp \cdot dw(q^b)y$ where $dw(q^b)$ of rank 2, one writes

$$\int_{\mathbb{R}^d} \eta_2(y) f(y) e^{-\frac{i}{2r} \eta_2(y)^2 \ln \varepsilon} dy = \frac{r}{i \ln \varepsilon} \int_{\mathbb{R}^d} |{}^t dw(q^b) \omega^\perp|^{-2} {}^t dw(q^b) \omega^\perp \cdot \nabla_y f(y) e^{-\frac{i}{2r} \eta_2(y)^2 \ln \varepsilon} dy,$$

which implies $c_+ = \|a(\eta_2)u_{+}^{\text{in}}\|^2 + \|\sqrt{1 - a(\eta_2)}u_{-}^{\text{in}}\|^2$.

APPENDIX A. SEMI-CLASSICAL PSEUDO-DIFFERENTIAL CALCULUS

This section contains results about semi-classical pseudo-differential operators. We consider matrix-valued functions $a \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^{2,2})$ which are bounded, as well as their derivatives. Then, one defines the Weyl semi-classical pseudo-differential operator of symbol a as

$$(79) \quad \text{op}_\varepsilon(a)f(x) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} e^{\frac{i}{\varepsilon} \xi \cdot (x-y)} a\left(\frac{x+y}{2}, \xi\right) f(y) dy d\xi, \quad \forall f \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^2).$$

The reader may find proofs of the results presented here in [8, 44, 11], for instance. In the following, we denote by $z = (x, \xi) \in \mathbb{R}^{2d}$ the variable of the functions $a \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^{2,2})$.

The Calderón-Vaillancourt Theorem [2] ensures the existence of constants $C_d, n_d > 0$ such that for every $a \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C}^{2,2})$, bounded with bounded derivatives, one has

$$(80) \quad \|\text{op}_\varepsilon(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d, \mathbb{C}^2))} \leq C_d N_d^\varepsilon(a),$$

where

$$N_d^\varepsilon(a) := \sum_{\alpha \in \mathbb{N}^{2d}, |\alpha| \leq n_d} \varepsilon^{\frac{|\alpha|}{2}} \sup_{\mathbb{R}^{2d}} |\partial_z^\alpha a|$$

with $n_d = Md$ for some constant $M \geq 1$ (see [44] for example). It is then easy to check that, since $\varepsilon \in (0, 1]$,

$$(81) \quad \sqrt{\varepsilon} N_d^\varepsilon(\partial_{z_j} a) \leq N_{d+1}^\varepsilon(a) \quad \text{for all } j \in \{1, \dots, 2d\}.$$

Matrix-valued pseudodifferential operators enjoy a symbolic calculus:

Proposition A.1. *Let $a, b \in \mathcal{C}_0^\infty(\mathbb{R}^d, \mathbb{C}^{2,2})$, then*

$$\text{op}_\varepsilon(a)\text{op}_\varepsilon(b) = \text{op}_\varepsilon(ab) + \varepsilon R_\varepsilon^{(1)}(a, b) = \text{op}_\varepsilon(ab) + \frac{\varepsilon}{2i} \text{op}_\varepsilon(\{a, b\}) + \varepsilon^2 R_\varepsilon^{(2)}(a, b),$$

with $\{a, b\} = \sum_{j=1}^d \partial_{\xi_j} a \partial_{x_j} b - \partial_{x_j} a \partial_{\xi_j} b$ and

$$\|R_\varepsilon^{(j)}(a, b)\|_{\mathcal{L}(L^2(\mathbb{R}^d, \mathbb{C}^2))} \leq C \sup_{|\alpha|+|\beta|=j} N_d^\varepsilon(\partial_\xi^\alpha \partial_x^\beta a) N_d^\varepsilon(\partial_\xi^\beta \partial_x^\alpha b), \quad j \in \{1, 2\},$$

for some constant $C > 0$ independent of a, b and ε .

Remark A.2. When $a = 1$ on the support of b , pushing the Taylor expansion at larger order, one gets for $N \in \mathbb{N}^*$,

$$\text{op}_\varepsilon(a)\text{op}_\varepsilon(b) = \text{op}_\varepsilon(b) + \varepsilon^N R_\varepsilon^{(N)}(a, b)$$

with

$$\|R_\varepsilon^{(N)}(a, b)\|_{\mathcal{L}(L^2(\mathbb{R}^d, \mathbb{C}^2))} \leq C \sup_{|\gamma|=|\gamma'|=N} N_d^\varepsilon(\partial_z^\gamma a) N_d^\varepsilon(\partial_z^{\gamma'} b).$$

Remark A.3. For general (non-commuting) symbols a and b , Lemma A.1 implies

$$[\text{op}_\varepsilon(a), \text{op}_\varepsilon(b)] = \text{op}_\varepsilon([a, b]) + \frac{\varepsilon}{2i}(\text{op}_\varepsilon(\{a, b\}) - \text{op}_\varepsilon(\{b, a\})) + \varepsilon^2(R_\varepsilon^{(2)}(a, b) - R_\varepsilon^{(2)}(b, a)).$$

However, the term of order ε^2 in this expansion has symmetries so that if a and b commutes, for example because a is scalar valued,

$$[\text{op}_\varepsilon(a), \text{op}_\varepsilon(b)] = \frac{\varepsilon}{i}\text{op}_\varepsilon(\{a, b\}) + \mathcal{O}\left(\varepsilon^3 \sup_{|\gamma|=|\gamma'|=3} N_d^\varepsilon(\partial_z^\gamma a) N_d^\varepsilon(\partial_z^{\gamma'} b)\right).$$

Note also that for $1 \leq j \leq d$ the commutation relations between x_j or εD_{x_j} and $\text{op}_\varepsilon(a)$ writes

$$(82) \quad [x_j, \text{op}_\varepsilon(a)] = \varepsilon i \text{op}_\varepsilon(\partial_{\xi_j} a) \quad \text{and} \quad [\varepsilon D_{x_j}, \text{op}_\varepsilon(a)] = -\varepsilon i \text{op}_\varepsilon(\partial_{x_j} a).$$

Using these relations and the estimates in $L^2(\mathbb{R}^d)$, it is possible to prove estimates in Σ_ε^k that are uniform in ε .

Lemma A.4. *Let $\varepsilon \in (0, 1]$ and $k \in \mathbb{N}$. There exist constants $C_{d,k}$ and c_k such that for all $a \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, we have in Σ_ε^k :*

$$(83) \quad \|\text{op}_\varepsilon(a)\|_{\mathcal{L}(\Sigma_\varepsilon^k)} \leq C_{d,k} N_{d+k}^\varepsilon(a).$$

Proof. The proof is based on (82) and a recursive argument. For $a \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, $f \in \mathcal{S}(\mathbb{R}^d)$ and $j \in \{1, \dots, d\}$,

$$\begin{aligned} \|x_j \text{op}_\varepsilon(a) f\|_{\Sigma_\varepsilon^{k-1}} &\leq \|\text{op}_\varepsilon(a)(x_j f)\|_{\Sigma_\varepsilon^{k-1}} + \varepsilon \|\text{op}_\varepsilon(\partial_{\xi_j} a) f\|_{\Sigma_\varepsilon^{k-1}}, \\ \|\varepsilon \partial_{x_j}(\text{op}_\varepsilon(a) f)\|_{\Sigma_\varepsilon^{k-1}} &\leq \|\text{op}_\varepsilon(a)(\varepsilon \partial_{x_j} f)\|_{\Sigma_\varepsilon^{k-1}} + \varepsilon \|\text{op}_\varepsilon(\partial_{x_j} a) f\|_{\Sigma_\varepsilon^{k-1}}. \end{aligned}$$

Therefore, there exists a constant c' such that

$$\begin{aligned} \|\text{op}_\varepsilon(a) f\|_{\Sigma_\varepsilon^k} &\leq c' \|\text{op}_\varepsilon(a)\|_{\mathcal{L}(\Sigma_\varepsilon^{k-1})} \|f\|_{\Sigma_\varepsilon^k} \\ &\quad + c' \sum_j \varepsilon \left(\|\text{op}_\varepsilon(\partial_{\xi_j} a)\|_{\mathcal{L}(\Sigma_\varepsilon^{k-1})} + \|\text{op}_\varepsilon(\partial_{x_j} a)\|_{\mathcal{L}(\Sigma_\varepsilon^{k-1})} \right) \|f\|_{\Sigma_\varepsilon^{k-1}}. \end{aligned}$$

One then concludes by starting the recursive argument from (80) and using (81). \square

APPENDIX B. LOCALIZATION OF WAVE PACKETS

The wave packets defined in (7) enjoy localization properties. We use here the notations introduced in Appendix A and we use the notation \widehat{a} for denoting (non semiclassical) pseudodifferential operators, $\widehat{a} = \text{op}_1(a)$.

Lemma B.1. *Let $z_0 = (q, p) \in \mathbb{R}^{2d}$, $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and $a \in \mathcal{C}^\infty(\mathbb{R}^{2d})$. Then,*

$$\text{op}_\varepsilon(a) \text{WP}_{z_0}^\varepsilon(\varphi) = \text{WP}_{z_0}^\varepsilon\left(\widehat{a(z_0 + \sqrt{\varepsilon}z)}\varphi\right).$$

Proof. The result comes from change of variables. \square

This Lemma has several important consequences.

Lemma B.2. *Let $\varepsilon \in (0, 1]$, $z_0 = (q, p) \in \mathbb{R}^{2d}$, $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and $a \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ bounded together with its derivatives. Then, we have the following properties:*

(1) For all $n_0, k \in \mathbb{N}$, there exists a constant C_k such that

$$\left\| \text{op}_\varepsilon(a) \text{WP}_{z_0}^\varepsilon(\varphi) - \text{WP}_{z_0}^\varepsilon \left(\widehat{P_a^{(n_0)}}(z\sqrt{\varepsilon})\varphi \right) \right\|_{\Sigma_\varepsilon^k} \leq C_k \varepsilon^{\frac{n_0+1}{2}} N_{d+k+n_0+1}^\varepsilon (d^{n_0+1}a) \|\varphi\|_{\Sigma^{k+n_0+1}}$$

where $z \mapsto P_a^{(n_0)}(z)$ is the Taylor polynomial at order n_0 of a in z_0 :

$$P_a^{(n_0)}(z) = a(z_0) + \nabla a(z_0) \cdot z + \frac{1}{2} \nabla^2 a(z_0) z \cdot z + \dots + \frac{1}{(n_0)!} d^{n_0} a(z_0) [z]^{n_0}.$$

(2) Moreover, assume that $a(z) = 1$ for $|z - z_0| \leq 1$ and $a(z) = 0$ if $|z - z_0| > 2$. Then, for any $n \in \mathbb{N}$, there exists a constant $C'_{k,n}$ such that

$$\|\text{WP}_{z_0}^\varepsilon(\varphi) - \text{op}_\varepsilon(a) \text{WP}_z^\varepsilon(\varphi)\|_{\Sigma_\varepsilon^k} \leq C'_{k,n} \varepsilon^{n/2} N_{d+k+n}^\varepsilon (d^n a) \|\varphi\|_{\Sigma^{k+n}}.$$

Proof. Let us prove Point (1). Applying Lemma B.1,

$$\|\text{op}_\varepsilon(a) \text{WP}_{z_0}^\varepsilon(\varphi) - \text{WP}_{z_0}^\varepsilon(\widehat{P_a^{(n_0)}}(z\sqrt{\varepsilon})\varphi)\|_{\Sigma_\varepsilon^k} = \|\text{WP}_{z_0}^\varepsilon((a(z_0 + \sqrt{\varepsilon}z) - \widehat{P_a^{(n_0)}}(z\sqrt{\varepsilon}))\varphi)\|_{\Sigma_\varepsilon^k}.$$

There exists a constant C'_k such that for all profiles $\varphi \in \mathcal{S}(\mathbb{R}^d)$,

$$\|\text{WP}_{z_0}^\varepsilon(\varphi)\|_{\Sigma_\varepsilon^k} \leq C'_k \|\varphi\|_{\Sigma^k}$$

hence

$$\|\text{WP}_{z_0}^\varepsilon((a(z_0 + \sqrt{\varepsilon}z) - \widehat{P_a^{(n_0)}}(z\sqrt{\varepsilon}))\varphi)\|_{\Sigma_\varepsilon^k} \leq C'_k \|(a(z_0 + \sqrt{\varepsilon}z) - \widehat{P_a^{(n_0)}}(z\sqrt{\varepsilon}))\varphi\|_{\Sigma^k}.$$

We have

$$a(z_0 + \sqrt{\varepsilon}z) - \widehat{P_a^{(n_0)}}(z\sqrt{\varepsilon}) = \varepsilon^{\frac{n_0+1}{2}} r(\sqrt{\varepsilon}z) [z]^{n_0+1}$$

where $r \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ is a smooth tensor of order $n_0 + 1$ that is bounded with bounded derivatives

$$r(z) = \frac{1}{n_0!} \int_0^1 d^{(n_0+1)} a(z_0 + sz) (1-s)^{n_0} ds.$$

We state the following auxiliary claim:

“ Consider a smooth function b that is smooth, bounded with bounded derivatives. Then, for all $k, n \in \mathbb{N}$ there exists a constant $c'_{k,n}$ such that for all $|\alpha| \leq n$,

$$(84) \quad \|\text{op}_1(b(\sqrt{\varepsilon}z)z^\alpha)\|_{\mathcal{L}(\Sigma_\varepsilon^{k+n}, \Sigma_\varepsilon^k)} \leq c'_{k,n} N_{d+k+n}^\varepsilon (b). ”$$

Applying the claim to $r(\sqrt{\varepsilon}z)[z]^{n_0+1}$, with $n = n_0 + 1$, we obtain

$$\|\text{op}_1(r(\sqrt{\varepsilon}z)[z]^{n_0+1})\|_{\mathcal{L}(\Sigma_\varepsilon^{k+n_0+1}, \Sigma_\varepsilon^k)} \leq c'_k N_{d+k+n_0+1}^\varepsilon (d^{n_0+1}a),$$

which is enough to complete the proof of Point (1).

We now turn to the proof of the claim. It relies on a recursive argument on n . When $n = 0$, the estimate (83) gives

$$\|\text{op}_1(b(\sqrt{\varepsilon}z))\|_{\mathcal{L}(\Sigma_\varepsilon^k)} \leq c_k N_{d+k}^1 (b(\sqrt{\varepsilon}\cdot)) \leq c'_{k,0} N_{d+k}^\varepsilon (b).$$

Let us now assume that we have proved the estimate (84) for all indices smaller than some $n \in \mathbb{N}$ and let us consider $\alpha \in \mathbb{N}^{2d}$ with $|\alpha| = n + 1$. Then, α has at least one non-zero component. Let α_j be such a component, with $j \in \{1, \dots, 2d\}$. Either $j \in \{1, \dots, d\}$ and $z^{\mathbf{1}j} = x_j$, or $j \in \{d+1, \dots, 2d\}$ and $z^{\mathbf{1}j} = \xi_j$. We consider the first case and a similar argument will work in the other one. For $\alpha \in \mathbb{N}^{2d}$, we have

$$z^\alpha = x_1^{\alpha_1} \dots x_d^{\alpha_d} \xi_1^{\alpha_{d+1}} \dots \xi_d^{\alpha_{2d}}$$

so that $z^\alpha = z^{\alpha - \mathbf{1}_j} z^{\mathbf{1}_j} = z^{\alpha - \mathbf{1}_j} x_j$. Using (82) and Proposition A.1, we then write for $f \in \mathcal{S}(\mathbb{R}^d)$,

$$\text{op}_1(b(\sqrt{\varepsilon}z)z^\alpha)f = \text{op}_1(b(\sqrt{\varepsilon}z)z^{\alpha - \mathbf{1}_j})(x_j f) - \frac{1}{2i} \text{op}_1(\partial_{\xi_j}(b(\sqrt{\varepsilon}z)z^{\alpha - \mathbf{1}_j}))f.$$

We deduce

$$\begin{aligned} \|\text{op}_1(b(\sqrt{\varepsilon}z)z^\alpha)f\|_{\Sigma_\varepsilon^k} &\leq \|\text{op}_1(b(\sqrt{\varepsilon}z)z^{\alpha - \mathbf{1}_j})\|_{\mathcal{L}(\Sigma_\varepsilon^{k+n}, \Sigma_\varepsilon^k)} \|x_j f\|_{\Sigma_\varepsilon^{k+n}} \\ &\quad + \frac{1}{2} \sqrt{\varepsilon} \|\text{op}_1(\partial_{\xi_j} b(\sqrt{\varepsilon}z)z^{\alpha - \mathbf{1}_j})\|_{\mathcal{L}(\Sigma_\varepsilon^{k+n}, \Sigma_\varepsilon^k)} \|f\|_{\Sigma_\varepsilon^{k+n}} \\ &\quad + \frac{1}{2} \|\text{op}_1(b(\sqrt{\varepsilon}z)z^{\alpha - \mathbf{1}_j - \mathbf{1}_{j+d}})\|_{\mathcal{L}(\Sigma_\varepsilon^{k+n}, \Sigma_\varepsilon^k)} \|f\|_{\Sigma_\varepsilon^{k+n}}, \end{aligned}$$

where the last term is there only if the $(j + d)$ -th component of $\alpha - \mathbf{1}_j$ is non zero. One then deduces the result from the recursive assumption, which concludes the proof of the claim, and thus of Point (1).

Finally, to prove Point (2), we only need to observe that since a is identically equal to 1 close to z_0 , its Taylor polynomial $P_a^{(n)}(z)$ is equal to 1 for all $n \in \mathbb{N}$. We then apply Point (1) with $n_0 = n - 1$. □

APPENDIX C. MATRICIAL RELATIONS

For $w = (w_1, w_2) \in \mathbb{R}^2$ and $u = (u_1, u_2) \in \mathbb{R}^2$, the matrices $A(u)$ and $A(w)$ defined in (31) satisfy

$$A(w)A(u) = \begin{pmatrix} w \cdot u & w \wedge u \\ -w \wedge u & w \cdot u \end{pmatrix}$$

(recall $w \wedge u = w_1 u_2 - w_2 u_1$).

C.1. The B_\pm matrices. We look more closely at the matrices B_\pm introduced in (13). We recall that for $\xi \in \mathbb{R}^d$, $\xi \cdot \nabla$ denotes the (scalar) operator $\xi \cdot \nabla = \sum_{j=1}^d \xi_j \partial_{\xi_j}$.

Lemma C.1. *For $\xi \in \mathbb{R}^d$ and $w \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{R}^2)$,*

$$\xi \cdot \nabla \Pi_+ = -\frac{\xi \cdot \nabla w(x) \wedge w(x)}{2|w(x)|^3} A(w^\perp(x)), \quad w^\perp = (-w_2, w_1).$$

Therefore, $\Pi_-(x) \xi \cdot \nabla \Pi_+(x) - \Pi_+(x) \xi \cdot \nabla \Pi_+(x) = -\frac{\xi \cdot \nabla w(x) \wedge w(x)}{2|w(x)|^2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

Proof. Since $\Pi_+(x) = \frac{1}{2} \left(\text{Id}_{\mathbb{R}^2} + A\left(\frac{w(x)}{|w(x)|}\right) \right)$, a straightforward computation gives

$$\begin{aligned} \xi \cdot \nabla \Pi_+(x) &= \frac{1}{2|w(x)|} \left(A(\xi \cdot \nabla w(x)) - \frac{w(x) \cdot (\xi \cdot \nabla w(x))}{|w(x)|^2} A(w(x)) \right) \\ &= \frac{1}{2|w(x)|^3} (w_2 \xi \cdot \nabla w_1 - w_1 \xi \cdot \nabla w_2) A(w_2, -w_1) \end{aligned}$$

whence the first formula. Then, we write

$$\begin{aligned}
\Pi_{-}(x)\xi \cdot \nabla \Pi_{+}(x) - \Pi_{+}(x)\xi \cdot \nabla \Pi_{-}(x) &= -\frac{\xi \cdot \nabla w(x) \wedge w(x)}{2|w(x)|^3} (\Pi_{-}(x)A(w^{\perp}(x)) - \Pi_{+}(x)A(w^{\perp}(x))) \\
&= -\frac{\xi \cdot \nabla w(x) \wedge w(x)}{2|w(x)|^4} A(w(x))A(w^{\perp}(x)) \\
&= -\frac{\xi \cdot \nabla w(x) \wedge w(x)}{2|w(x)|^2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.
\end{aligned}$$

□

C.2. Superadiabatic projectors. In this section we use the semi-classical pseudodifferential operators introduced in Appendix A and we denote by $a \#_{\varepsilon} b$ the symbol of the operator $\text{op}_{\varepsilon}(a) \circ \text{op}_{\varepsilon}(b)$.

Lemma C.2. *There exist matrix-valued functions $\mathbb{P}_{\pm}^{(1)}$, $\mathbb{P}_{\pm}^{(2)}$, $\Omega_{\pm}^{(1)}$ and $\Omega_{\pm}^{(2)}$, that are smooth outside Υ and such that the function*

$$\Pi_{\pm}^{\varepsilon}(x, \xi) = \Pi_{\pm}(x) + \varepsilon \mathbb{P}_{\pm}^{(1)}(x, \xi) + \varepsilon^2 \mathbb{P}_{\pm}^{(2)}(x, \xi),$$

satisfies

$$(85) \quad \Pi_{\pm}^{\varepsilon} \#_{\varepsilon} H = (h_{\pm} + \varepsilon \Omega_{\pm}^{(1)} + \varepsilon^2 \Omega_{\pm}^{(2)}) \#_{\varepsilon} \Pi_{\pm}^{\varepsilon} + \varepsilon^3 R_{\varepsilon}(x, \xi).$$

Besides, for all $\alpha, \beta \in \mathbb{N}^d$, there exists constants $C_{\alpha, \beta}$, $p_{\alpha} > 0$ such that for all $(x, \xi) \in \mathbb{R}^{2d} \setminus \Upsilon$,

$$(86) \quad |\partial_x^{\alpha} \partial_{\xi}^{\beta} R_{\varepsilon}(x, \xi)| \leq C_{\alpha, \beta} \langle x \rangle^{(|\alpha|+3)(1+n_0)} |w(x)|^{-|\alpha|-5}$$

(where n_0 controls the gap at infinity, see (5)). Moreover, the following properties hold

(1) One has

$$\mathbb{P}_{\pm}^{(1)}(x, \xi) = \pm \mathbb{P}(x, \xi), \quad \Omega_{\pm}^{(1)}(x, \xi) = \Omega(x, \xi)$$

where \mathbb{P} and Ω are the linear functions in ξ defined respectively in (59) and (56). They are homogeneous functions in w of degree -1 and -2 respectively.

(2) The matrices $\mathbb{P}_{\pm}^{(2)}$ and $\Omega_{\pm}^{(2)}$ are polynomial functions of order 2 of the variable ξ and for $(x, \xi) \in \mathbb{R}^{2d} \setminus \Upsilon$, for all $\alpha, \beta \in \mathbb{N}^d$, there exists $C_{\alpha, \beta} > 0$ such that

$$\begin{aligned}
|\partial_x^{\alpha} \partial_{\xi}^{\beta} \mathbb{P}_{\pm}^{(2)}(x, \xi)| &\leq C_{\alpha, \beta} \langle \xi \rangle^2 \langle x \rangle^{(|\alpha|+2)(1+n_0)} |w(x)|^{-|\alpha|-4}, \\
|\partial_x^{\alpha} \partial_{\xi}^{\beta} \Omega_{\pm}^{(2)}(x, \xi)| &\leq C_{\alpha, \beta} \langle \xi \rangle^2 \langle x \rangle^{(|\alpha|+2)(1+n_0)} |w(x)|^{-|\alpha|-3}.
\end{aligned}$$

Proof. We use the calculus of $a \#_{\varepsilon} b$ detailed in Proposition A.1 and the observations of Remark A.3. We have

$$\begin{aligned}
\Pi_{\pm}^{\varepsilon} \#_{\varepsilon} H &= \Pi_{\pm} H + \varepsilon (\mathbb{P}_{\pm}^{(1)} H + \frac{1}{2i} \{\Pi_{\pm}, H\}) + \varepsilon^2 (\mathbb{P}_{\pm}^{(2)} H + \frac{1}{2i} \{\mathbb{P}_{\pm}^{(1)}, H\} + d_{\pm}) + \varepsilon^3 r^1, \\
(h_{\pm} + \varepsilon \Omega_{\pm}^{(1)} + \varepsilon^2 \Omega_{\pm}^{(2)}) \#_{\varepsilon} \Pi_{\pm}^{\varepsilon} &= h_{\pm} \Pi_{\pm} + \varepsilon (h_{\pm} \mathbb{P}_{\pm}^{(1)} + \frac{1}{2i} \{h_{\pm}, \Pi_{\pm}\} + \Omega_{\pm}^{(1)} \Pi_{\pm}) \\
&\quad + \varepsilon^2 (h_{\pm} \mathbb{P}_{\pm}^{(2)} + \frac{1}{2i} \{h_{\pm}, \mathbb{P}_{\pm}^{(1)}\} + \frac{1}{2i} \{\Omega_{\pm}^{(1)}, \Pi_{\pm}\} + \Omega_{\pm}^{(1)} \mathbb{P}_{\pm}^{(1)} + \Omega_{\pm}^{(2)} \Pi_{\pm} + d_{\pm})
\end{aligned}$$

where r^1 and r^2 involves derivatives of order 3 of Π_{\pm} , of order 2 of $\mathbb{P}_{\pm}^{(1)}$ and of order 1 of $\mathbb{P}_{\pm}^{(2)}$ and d_{\pm} comes from the computations

$$\frac{|\xi|^2}{2} \#_{\varepsilon} \Pi_{\pm} = \frac{|\xi|^2}{2} \Pi_{\pm} + \frac{\varepsilon}{2i} \left\{ \frac{|\xi|^2}{2}, \Pi_{\pm} \right\} + \varepsilon^2 d_{\pm}, \quad \Pi_{\pm} \#_{\varepsilon} \frac{|\xi|^2}{2} = \frac{|\xi|^2}{2} \Pi_{\pm} - \frac{\varepsilon}{2i} \left\{ \frac{|\xi|^2}{2}, \Pi_{\pm} \right\} + \varepsilon^2 d_{\pm}.$$

We deduce that in order to realize equation (85), we only need to equalize the terms of order ε and ε^2 on both developments (indeed $\Pi_{\pm}H = h_{\pm}\Pi_{\pm}$). We obtain two equations that it is convenient to put on the form

$$(87) \quad [\mathbb{P}_{\pm}^{(1)}, H] - (h_{\pm} - H)\mathbb{P}_{\pm}^{(1)} - \Omega_{\pm}^{(1)}\Pi_{\pm} = \mp i\xi \cdot \nabla \Pi_{\pm},$$

$$(88) \quad [\mathbb{P}_{\pm}^{(2)}, H] - (h_{\pm} - H)\mathbb{P}_{\pm}^{(2)} - \Omega_{\pm}^{(2)}\Pi_{\pm} = F_{\pm}$$

where F_{\pm} depends on $\mathbb{P}_{\pm}^{(1)}$ and $\Omega_{\pm}^{(1)}$

$$F_{\pm} = \frac{1}{2i}\{h_{\pm}, \mathbb{P}_{\pm}^{(1)}\} + \frac{1}{2i}\{\Omega_{\pm}^{(1)}, \Pi_{\pm}\} + \Omega_{\pm}^{(1)}\mathbb{P}_{\pm}^{(1)} - \frac{1}{2i}\{\mathbb{P}_{\pm}^{(1)}, H\}.$$

For solving these equations, we multiply them on both sides by Π_{+} or Π_{-} , which gives four relations each time.

Let us perform the computation for the *plus*-mode. Multiplying (87) on the right by Π_{+} and on the left successively by Π_{+} and Π_{-} , we obtain two relations

$$\Pi_{+}\Omega_{+}^{(1)}\Pi_{+} = 0, \quad \Pi_{-}\Omega_{+}^{(1)}\Pi_{+} = i\Pi_{-}\xi \cdot \nabla \Pi_{+}\Pi_{+}.$$

Using that we want to find $\Omega_{+}^{(1)}$ self-adjoint, we deduce that we can choose

$$\Omega_{+}^{(1)} = i\Pi_{-}\xi \cdot \nabla \Pi_{+}\Pi_{+} - i\Pi_{+}\xi \cdot \nabla \Pi_{+}\Pi_{-} = \Omega.$$

Similarly, for the *minus*-mode

$$\Omega_{-}^{(1)} = -i\Pi_{+}\xi \cdot \nabla \Pi_{+}\Pi_{-} + i\Pi_{-}\xi \cdot \nabla \Pi_{+}\Pi_{+} = \Omega.$$

Multiplying (87) on the left by Π_{+} and on the right by Π_{-} , we end up with

$$(h_{+} - h_{-})\mathbb{P}_{+}^{(1)} = i\Pi_{+}\xi \cdot \nabla \Pi_{+}\Pi_{-}.$$

Choosing $\mathbb{P}_{+}^{(1)}$ self-adjoint, we obtain

$$\mathbb{P}_{+}^{(1)} = \frac{i}{2|w(x)|}(\Pi_{+}\xi \cdot \nabla \Pi_{+}\Pi_{-} - \Pi_{-}\xi \cdot \nabla \Pi_{+}\Pi_{+}) = \mathbb{P}.$$

We argue in a similar way for the *minus*-mode and find

$$\mathbb{P}_{-}^{(1)} = -\frac{i}{2|w(x)|}(\Pi_{-}\xi \cdot \nabla \Pi_{+}\Pi_{+} - \Pi_{+}\xi \cdot \nabla \Pi_{+}\Pi_{-}) = -\mathbb{P}.$$

Let us now determine $\mathbb{P}_{+}^{(2)}$ and $\Omega_{+}^{(2)}$. We first decompose F_{+} as the sum of a self-adjoint matrix and a skew-symmetric one: $F_{+} = F_{+,aa} + F_{+,ss}$ with

$$\begin{aligned} F_{+,aa} &= \frac{1}{2}(F_{+} + F_{+}^*), & F_{+,ss} &= \frac{1}{2}(F_{+} - F_{+}^*) \\ F_{+}^* &= -\frac{1}{2i}\{h_{+}, \mathbb{P}\} + \frac{1}{2i}\{\Pi_{+}, \Omega\} + \Omega\mathbb{P} - \frac{1}{2i}\{H, \mathbb{P}\}. \end{aligned}$$

We have used $\{M, N\}^* = -\{N, M\}$ for smooth matrix-valued function M and N . We also obtain

$$(89) \quad \Pi_{\pm}F_{+,ss}\Pi_{\pm} = 0,$$

which is required from (88) (when multiplied on both side by Π_{\pm}). These relations come from $\mathbb{P}\Omega = \Omega\mathbb{P}$,

$$\Pi_{\pm} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \Pi_{\pm} = 0_{\mathbb{C}^{2,2}} \quad \text{and} \quad A(u) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} A(u) = 0, \quad \forall u \in \mathbb{R}^2.$$

Then, multiplying (88) by Π_+ on the right, we deduce

$$\Omega_{\pm}^{(2)}\Pi_+ = -F_+\Pi_+.$$

One then chooses

$$(90) \quad \Omega_{\pm}^{(2)} = -\Pi_+F_{+,aa}\Pi_+ - \Pi_-F_+\Pi_+ - \Pi_+F_+\Pi_-.$$

For determining $\mathbb{P}_+^{(2)}$, we multiply (88) by Π_- on the right

$$(h_+ - h_-)\mathbb{P}_+^{(2)}\Pi_- = -F_+\Pi_-,$$

and we obtain

$$(91) \quad \mathbb{P}_+^{(2)} = -\frac{1}{2|w(x)|}(\Pi_+F_+\Pi_- + \Pi_-F_+\Pi_+ + \Pi_-F_{+,aa}\Pi_-).$$

The polynomial features of these matrices in the variable ξ and their properties as functions of w come from their explicit formula. These aspects determine their behavior at ∞ and close to Υ . \square

Remark C.3. As already observed in the literature ([1, 33, 36, 37, 41]), it is possible to push these asymptotics at any order by constructing a sequence of matrices $(\Omega_{\pm}^{(j)}, \mathbb{P}_{\pm}^{(j)})_{j \in \mathbb{N}}$ that will satisfy controls of the form

$$\begin{aligned} |\partial_x^\alpha \partial_\xi^\beta \mathbb{P}_{\pm}^{(j)}(x, \xi)| &\leq C_{\alpha, \beta} \langle \xi \rangle^j \langle x \rangle^{(|\alpha|+j)(1+n_0)} |w(x)|^{-|\alpha|-2j}, \\ |\partial_x^\alpha \partial_\xi^\beta \Omega_{\pm}^{(j)}(x, \xi)| &\leq C_{\alpha, \beta} \langle \xi \rangle^j \langle x \rangle^{(|\alpha|+j)(1+n_0)} |w(x)|^{-|\alpha|-2j+1}. \end{aligned}$$

As a consequence of the computations above, we also have the following result.

Lemma C.4. *Let $\Phi_{\pm}^{t^b, t}(z^b)$ be a trajectory reaching the point $z^b \in \Upsilon$ at time t^b with the conditions of (1.1). Then, we have for t close to t^b ,*

$$\begin{aligned} \Omega_{\pm}^{(1)}(\Phi_{\pm}^{t^b, t}(z^b)) &= \mathcal{O}(1), \quad \mathbb{P}_{\pm}^{(1)}(\Phi_{\pm}^{t^b, t}(z^b)) = \mathcal{O}(|t - t^b|), \\ \Omega_{\pm}^{(2)}(\Phi_{\pm}^{t^b, t}(z^b)) &= \mathcal{O}(|t - t^b|^2), \quad \mathbb{P}_{\pm}^{(2)}(\Phi_{\pm}^{t^b, t}(z^b)) = \mathcal{O}(|t - t^b|^3). \end{aligned}$$

APPENDIX D. GENERALIZATION TO TIME-DEPENDENT HAMILTONIAN

We consider a Hamiltonian

$$H(t, z) = v(t, z)\text{Id}_{\mathbb{C}^2} + A(w(t, z)), \quad w(t, z) = {}^t(w_1(t, z), w_2(t, z)) \in \mathbb{R}^2$$

with subquadratic growth and polynomial control of the gap at infinity (as in (5)). The crossing set is the subset of $\mathbb{R} \times \mathbb{R}^d$ given by

$$\Upsilon = \{(t, z) \in \mathbb{R} \times \mathbb{R}^{2d}, \quad w(t, z) = 0\}.$$

We denote as before by h_+ and h_- the eigenvalues of H and Π_+ and Π_- the associated eigenprojectors. Following [13], a point $(t^b, z^b) \in \Upsilon$ is a non-degenerate crossing point if and only if

$$\text{Rk } dw(t^b, z^b) = 2 \quad \text{and} \quad E(t^b, z^b) := \partial_t w(t^b, z^b) + \{v, w\}(t^b, z^b) \neq 0.$$

With such a point, we associate the vector

$$\omega = \frac{E(t^b, z^b)}{|E(t^b, z^b)|} \quad \text{and} \quad r = |E(t^b, z^b)|.$$

By Proposition 1 in [13], there exists a pair of generalized trajectories passing through non-degenerate crossing points and we denote them by $\Phi_{\pm}^{t^b, t}(z^b)$.

Time-dependent eigenvectors along the trajectories. Starting from a point $(t_0, z_0) \in \mathbb{R} \times \mathbb{R}^{2d}$ such that $\Phi_{\pm}^{t_0, t_0}(z_0) = z^b$, we associate with these trajectories time-dependent eigenvectors by solving the differential equation

$$\frac{d}{dt} \vec{Y}_{\pm}(t) = B_{\pm}(\Phi_{\pm}^{t, t^b}(z^b)) \vec{Y}_{\pm}(t), \quad \vec{Y}_{\pm}(t_0) = \vec{Y}_0$$

where

$$B_{\pm} = \Pi_{\mp}(\partial_t \Pi_{\pm}(t, z) + \{v, \Pi_{\pm}\}) \Pi_{\pm},$$

and \vec{Y}_0 is an eigenvector of $H(t_0, z_0)$ for the \pm -mode. One can then prove that the vectors $\vec{Y}_{\pm}(t)$, $t < t^b$ can be continued up to $t = t^b$.

Profile equations. The profile equations associated with the trajectory $\Phi_{\pm}^{t, t_0}(z_0)$ write

$$i\partial_t u_{\pm} = \text{Hess } H(t, \Phi_{\pm}^{t, t_0}) \begin{pmatrix} y \\ D_y \end{pmatrix} \cdot \begin{pmatrix} y \\ D_y \end{pmatrix} u_{\pm}, \quad u_{\pm}(t_0) = \varphi_{\pm}.$$

Close to t^b , we have the asymptotics

$$\text{Hess } H(t, \Phi_{\pm}^{t, t_0}) \sim_{t \rightarrow t^b} \pm \frac{1}{r|t - t^b|} ({}^t dw(t^b, z^b)(\text{Id}_{\mathbb{R}^2} - \omega \otimes \omega) dw(t^b, z^b))$$

which allow to define ingoing profiles u_{\pm}^{in} by

$$u_{\pm}(t) \sim e^{\pm \frac{i}{2} \widehat{\Gamma}_0 \ln |t - t^b|} u_{\pm}^{\text{in}} \quad \text{as } t \rightarrow t^b, \quad t < t^b$$

with

$$\widehat{\Gamma}_0 = \frac{1}{r} {}^t dw(t^b, z^b)(\text{Id}_{\mathbb{R}^2} - \omega \otimes \omega) dw(t^b, z^b) \begin{pmatrix} y \\ D_y \end{pmatrix} \cdot \begin{pmatrix} y \\ D_y \end{pmatrix}.$$

Note that in the case we have studied, the function w only depends on x and thus the operator $\widehat{\Gamma}_0$ is an operator of multiplication.

Transition formulas. The transitions formula are now operator-valued. The function $\eta(y)$ inside the coefficients of Theorem 1.9 have to be replaced by the operator

$$\eta(y, D_y) = \left(\omega \cdot (d_z w(t^b, z^b))^t(y, D_y), \omega^{\perp} \cdot (d_z w(t^b, z^b))^t(y, D_y) \right).$$

Then, the transition rules are the same as in Theorem 1.9.

The Hermitian case. Such an approach extends to Hermitian Hamiltonians with crossings that have the geometric feature of [13], the so-called *generic involutive codimension 3 crossing* (see also [6]). Assume

$$H(t, z) = v(t, z) \mathbf{1}_{\mathbb{C}^2} + \begin{pmatrix} w_1(t, z) & w_2(t, z) + iw_3(t, z) \\ w_2(t, z) - iw_3(t, z) & -w_1(t, z) \end{pmatrix},$$

with $w(t, z) = ({}^t(w_1(t, z), w_2(t, z), w_3(t, z))) \in \mathbb{R}^3$.

Set

$$E(t, z) = (\partial_t w(t, z) + \{v, w\})(t, z) \quad \text{and} \quad B(t, z) = ({}^t(\{w_2, w_3\}, \{w_3, w_1\}, \{w_1, w_2\}))(t, z).$$

The strategy developed in this article extends to crossing points (t^b, z^b) close to Υ , where the latter is a codimension 2 or 3 manifold, with $E(t, z) \cdot B(t, z)$ identically equal to 0 in a neighborhood of (t^b, z^b) and $|E(t^b, z^b)| > |B(t^b, z^b)|$. Even though this situation is not generic, it contains for example the case where $w = w(x)$. More intricate phenomena appear in the generic setting (see [9])

and [10] for example). Note however that a special attention has to be attached to the diabatic basis used at the crossing point because the eigenvectors are now complex-valued.

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