Asymptotic initial value representation of the solutions of semi-classical systems presenting smooth codimension one crossings

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This text is dedicated to the memory of George Hagedorn (1953–2023)

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Abstract

This paper is devoted to the construction of approximations of the propagator associated with a semi-classical matrix-valued Schrödinger operator with symbol presenting smooth eigenvalues crossings. Inspired by the approach of the theoretical chemists Herman and Kluk who propagated continuous superpositions of Gaussian wave-packets for scalar equations, we consider frozen and thawed Gaussian initial value representations that incorporate classical transport and branching processes along a hopping hypersurface. Based on the Gaussian wave-packet frame work, our result relies on an accurate analysis of the solutions of the associated Schrödinger equation for data that are vector-valued wave-packets. We prove that these solutions are asymptotic to wavepackets at any order in terms of the semi-classical parameter.

Key words and phrases. Matrix-valued Hamiltonian, smooth crossings, codimension 1 crossings, wave-packet, Bargmann transform, Herman-Kluk propagators, thawed and frozen Gaussian approximations.

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CHAPTER 1

Introduction

Since the early days of semi-classical analysis, operators that approximate the dynamics of a semi-classical propagator have been the object of major attention. The theory of Fourier integral operators answers to this question by proposing methods for constructing approximative propagators of a scalar semi-classical Schrödinger equation (see [**64**, Chapter 12] or [**14**]). Pioneering work about a semi-classical theory of FIOs is [**7**], extended in [**31**] and [**52**].

Few results exist for systems except for those that are called *adiabatic*, because the eigenvalues of the underlying Hamiltonian matrix are of constant multiplicity. The analysis of such systems can be reduced to those of scalar equations through a diagonalization process using the so-called *super-adiabatic projectors*. The super-adiabatic approach has been carried out by Martinez and Sordoni [**46**] as well as Spohn and Teufel [**55**], see also [**17, 48, 49, 5**] for earlier results or [**4, 51**] for more recent results in a similar direction. The present study gives the first complete construction of an integral representation of the propagator associated to a Hamiltonian generating non-adiabatic dynamics in a very general situation. It focuses on those Hamiltonian matrices that have smooth eigenprojectors, with smooth eigenvalues, though of non constant multiplicity. The framework applies to generic situations where two eigenvalues cross along a hypersurface on points where the Hamiltonian vector fields associated with these eigenvalues are transverse to the crossing hypersurface. This set-up has already been the one of the work of Hagedorn [**26**, Section 5] and Jecko [**35**]. The Fourier integral operators approximating the propagator associated with these non-adiabatic Hamiltonians are based on Gaussian wave-packets and the Bargmann transform, in the spirit of the *Herman–Kluk propagator*.

The Herman–Kluk propagator has been introduced in theoretical chemistry (see [**32, 38, 33, 39**]) for the analysis of molecular dynamics for scalar equations. The mathematical analysis has been performed later by Rousse and Swart [**56**] and Robert [**53**], independently. The action of the Herman–Kluk propagator consists in the continuous decomposition of the initial data into semi-classical Gaussian wave-packets and the implementation of the propagation of the wave-packets as studied in the 70s and 80s by Heller [**32**], Combescure and Robert [**13**], and Hagedorn [**24**]. It involves time-dependent quantities that are called *classical quantities* because they can be interpreted in terms of Newtonian mechanics. Such an approximative description of the propagator in terms of several Gaussian wave packets motivates numerical methods that naturally combine with probabilistic sampling techniques, see [**40**] or more recently [**42, 41**].

We prove the convergence of two types of approximations, respectively called *thawed* and *frozen Gaussian approximations*, both built of continuous superpositions of Gaussian wave-packets, the frozen one in the spirit the original Herman–Kluk propagator. Their difference mainly consists in the way the width matrices resulting from the propagation of the individual semi-classical Gaussian wave packets are treated. The presence of crossings requires to add to the semi-classical Gaussian wave packet propagation some transitions between the crossing hypersurfaces. Therefore, these

Fourier integral operators incorporate classical transport along the Hamiltonian trajectories associated with the eigenvalues of the Hamiltonian and a branching process along the crossing hypersurface. Some of these ideas have been introduced in [**20, 21**], in particular in [**20**] where the propagation of wave-packets through smooth crossings has been studied. Here, we revisit and extend these results, by proving that a wave-packet propagated through a smooth generic crossing remains asymptotically a wave-packet to any order in the semi-classical parameter. We then prove uniform estimates for the associated semi-classical approximations of propagators when acting on families of initial data that are *frequency localized* in the sense that their L^2-mass does not escape in phase space to ∞ when the semi-classical parameter goes to 0, neither in position, nor in momentum. This class of initial data is typically met for the numerical simulation of molecular quantum systems.

Previous results. The analysis of the propagation through smooth eigenvalue crossings has been pioneered by Hagedorn in [**26**, Chapter 5]. He considered Schrödinger operators with matrix-valued potentials and propagated initial data that are known as semi-classical wave packets or generalized coherent states [**13**, Chapter 4]. The core of the wave-packet had to be chosen such that it classically propagates to the crossing. In the same framework adjusted to the context of solid states physics, Watson and Weinstein [**62**] analyze the propagation of wave-packets through a smooth crossing of Bloch bands. The results developed here extend [**26**, Chapter 5] and [**62**] in two ways. The single wave-packet is turned into an initial value representation with uniform control for frequency localized initial data. The Schrödinger and Bloch operators are generalized to Weyl quantized operators with smooth time-dependent symbol.

1.1. First overview

The remainder of the introduction specifies the mathematical setting (assumptions on the Hamiltonian operator and the initial data), discusses the classical quantities involved in the approximation, reviews the known results on the thawed and frozen initial value representations in the adiabatic setting, and then presents the main results of this paper: Theorem 1.18 on the thawed approximation with hopping trajectories, Theorem 1.19 and Theorem 1.20 on the frozen approximation with hopping trajectories, that are pointwise and averaged in time, respectively, and Theorem 1.21 on wave-packet propagation through smooth crossings to arbitrary order.

We prove Theorems 1.18, 1.19 and 1.20 in Chapters 2 and 3. These proofs rely on Theorem 1.21, that is proved in Chapters 4 and 5.

Chapter 2 recalls elementary facts about the Bargmann transform. Then, it introduces the new notion of frequency localization, which will be crucial for controlling the remainder estimates for both the frozen and the thawed initial value representations in Chapter 3.

The refined wave-packet analysis of Chapters 4 and 5 does not depend on the theory of initial value representations and can be read independently from Chapters 2 and 3. It propagates wave-packets through smooth crossings in two steps: using a rough diagonalisation of the Hamiltonian operator in the crossing region and super-adiabatic projectors for the outside. Both constructions rely on pseudo-differential calculus for matrix-valued symbols that is developed in Chapter 4 and complemented by additional technical points in the appendices.

Notations and conventions. All the functional sets that we shall consider in this article can have values in $\mathbb{C}$ (scalar-valued), $\mathbb{C}^m$ (vector-valued) or in $\mathbb{C}^{m,m}$ (matrix-valued). We denote by

$$\langle g, f\rangle = \int_{\mathbb{R}^d} f(x)\overline{g}(x)dx$$

the inner product of $L^2(\mathbb{R}^d, \mathbb{C})$. If π is a projector, then $\pi^\perp$ denotes the projector $\pi^\perp = \mathbb{I} - \pi$. We set $D_x = \frac{1}{i}\partial_x$. In the context of Assumption 1.3, we shall say that a matrix A is diagonal if $A = \pi_1 A\pi_1 + \pi_2 A\pi_2$ and off-diagonal if $A = \pi_1 A\pi_2 + \pi_2 A\pi_1$.

1.2. The setting

1.2.1. The Schrödinger equation. We consider the Schrödinger equation

$$i\varepsilon\partial_t\psi^\varepsilon(t) = \widehat{H}^\varepsilon(t)\psi^\varepsilon(t), \quad \psi^\varepsilon_{|t=t_0} = \psi^\varepsilon_0. \tag{1.1}$$

in $L^2(\mathbb{R}^d, \mathbb{C}^m)$, $m \geq 2$, where $\widehat{H}^\varepsilon(t)$ is the semi-classical quantization of an Hermitian matrix symbol $H^\varepsilon(t, z) \in \mathbb{C}^{m,m}$.

Here, $t \in \mathbb{R}$, $z = (x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d$ and ε is the semi-classical parameter, $\varepsilon \ll 1$. Moreover, for $a \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ being a smooth scalar-, vector- or matrix-valued function with adequate control on the growth of derivatives, the Weyl operator $\widehat{a} = \mathrm{op}^w_\varepsilon(a)$ is defined by

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

for all $f \in \mathcal{S}(\mathbb{R}^d)$.

In full generality, we could assume that the map $(t, z) \mapsto H^\varepsilon(t, z)$ is a semi-classical observable in the sense that the function $H^\varepsilon(t, z)$ is an asymptotic sum of the form $\sum_{j\geq 0}\varepsilon^j H_j(t, z)$. However, in this asymptotic sum, the important terms are the principal symbol $H_0(t, z)$ and the sub-principal one $H_1(t, z)$; the terms $H_j(t, z)$ for $j \geq 2$ only affect the solution at order ε, which is the order of the approximation we are looking for. Therefore, we assume that the self-adjoint matrix H^ε writes

$$H^\varepsilon(t, z) := H_0(t, z) + \varepsilon H_1(t, z).$$

1.2.2. Assumptions on the Hamiltonian. We work on a time interval of the form

$$I := [t_0, t_0 + T], \quad t_0 \in \mathbb{R} \text{ and } T > 0$$

and consider subquadratic matrix-valued Hamiltonians.

Definition 1.1 (Subquadratic). The ε-dependent Hamiltonian

$$H^\varepsilon = H_0 + \varepsilon H_1 \in \mathcal{C}^\infty(I \times \mathbb{R}^{2d}, \mathbb{C}^{m,m})$$

is *subquadratic on the time interval* I if and only if one has the property:

$$\forall j \in \{0, 1\}, \ \forall\gamma \in \mathbb{N}^d, \ \exists C_{j,\gamma} > 0, \quad \sup_{(t,z)\in I\times\mathbb{R}^{2d}} |\partial_z^\gamma H_j(t, z)| \leq C_{j,\gamma}\langle z\rangle^{(2-j-|\gamma|)_+} \tag{1.2}$$

Assuming that H^ε is subquadratic on the time interval I ensures that the system (1.1) is well-posed in $L^2(\mathbb{R}^d, \mathbb{C}^m)$ for $t \in I$, and, more generally (see [**47**]), in the functional spaces

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

endowed with the norm

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

We denote by $\mathcal{U}_H^\varepsilon(t,t_0)$ the unitary propagator defined by

$$i\varepsilon\partial_t\mathcal{U}_H^\varepsilon(t,t_0)=\widehat{H}^\varepsilon(t)\mathcal{U}^\varepsilon(t,t_0),\ \ \mathcal{U}^\varepsilon(t_0,t_0)=\mathbb{I}_{\mathbb{C}^m}.$$

It is a bounded operator of the $\Sigma_\varepsilon^k(\mathbb{R}^d)$ spaces, uniformly in ε (see [**47**]): there exists $C_T>0$ such that

$$\sup_{t\in I}\|\mathcal{U}_H^\varepsilon(t,t_0)\|_{\mathcal{L}(\Sigma_\varepsilon^k)}\ \leq\ C_T.$$

We assume that the principal symbol $H_0(t,z)$ of $H^\varepsilon(t,z)$ has two distinct eigenvalues that present a smooth crossing in the sense of the definitions of [**20**]. Namely, we consider different properties of the crossings.

Definition 1.2. (1) (Smooth crossing). The matrix $H_0\in\mathcal{C}^\infty(I\times\mathbb{R}^{2d},\mathbb{C}^{m,m})$ has a smooth crossing on the set $\Upsilon\subseteq I\times\mathbb{R}^{2d}$ if there exists $h_1,h_2\in\mathcal{C}^\infty(I\times\mathbb{R}^{2d})$ and two orthogonal projectors $\pi_1,\pi_2\in\mathcal{C}^\infty(I\times\mathbb{R}^{2d},\mathbb{C}^{m,m})$ such that $H_0=h_1\pi_1+h_2\pi_2$ and

$$h_1(t,z)=h_2(t,z)\iff(t,z)\in\Upsilon.$$

(2) Set $f(t,z)=\dfrac{1}{2}\left(h_1(t,z)-h_2(t,z)\right)$ and $v(t,z)=\dfrac{1}{2}\left(h_1(t,z)+h_2(t,z)\right)$.

(a) (Non-degenerate crossing). The crossing is non-degenerate at $(t^\flat,\zeta^\flat)\in\Upsilon$ if

$$d_{t,z}\left(H_0-v\,\mathbb{I}_{\mathbb{C}^m}\right)(t^\flat,\zeta^\flat)\neq 0$$

where $d_{t,z}$ is the one differential form in the variables (t,z).

(b) (Generic crossing points). The crossing is generic at $(t^\flat,\zeta^\flat)\in\Upsilon$ if one has

$$\partial_t f+\{v,f\}(t^\flat,\zeta^\flat)\neq 0. \tag{1.3}$$

Note that there then exists an open set $\Omega\subset I\times\mathbb{R}^{2d}$ containing $(t^\flat,\zeta^\flat)$ such that the set $\Upsilon\cap\Omega$ is a manifold.

Above, we denote by $\{f,g\}$ the poisson bracket of the functions f and g defined on $\mathbb{R}^{2d}_{x,\xi}$:

$$\{f,g\}=\nabla_\xi f\cdot\nabla_x g-\nabla_x f\cdot\nabla_\xi g.$$

With these definitions in hands, we introduce one of the main assumptions on the crossing points of the Hamiltonian H^ε.

Assumption 1.3 (Crossing set). The Hamiltonian $H^\varepsilon=H_0+\varepsilon H_1$ has a smooth crossing set Υ and all the points of Υ are non degenerate and generic crossing points.

In order to consider the unitary propagators $\mathcal{U}_{h_1}^{t,t_0}$ and $\mathcal{U}_{h_2}^{t,t_0}$ and be endowed with convenient bounds on the growth of the projectors, we shall make additional assumptions on the growth of the eigenvalues and of their gap function. Our setting will be the following:

Assumption 1.4 (Growth conditions for smooth crossings). Let $H^\varepsilon=H_0+\varepsilon H_1\in\mathcal{C}^\infty(\mathbb{R}\times\mathbb{R}^{2d})$ be subquadratic on the time interval I and have a smooth crossing on the set Υ. We consider the two following assumptions :

(i) The growth of $H_0(t,x)$, $h_1(t,z)$ and $h_2(t,z)$ is driven by the function $v(t,z)$, i.e. for $j\in\{1,2\}$

$$\forall\gamma\in\mathbb{N}^{2d},\ |\gamma|=1,\ \ \exists C_\gamma>0,\ \ \forall(t,z)\in I\times\mathbb{R}^{2d},\ \ |\partial_z^\gamma(H_0-v\,\mathbb{I}_{\mathbb{C}^m})(t,z)|+|f(t,z)|\leq C_\gamma. \tag{1.4}$$

(ii) The eigenvalues h_1 and h_2 are subquadratic, i.e.

$$\forall\gamma\in\mathbb{N}^{2d},\ |\gamma|\geq 2,\ \ \exists C_\gamma>0,\ \ \forall(t,z)\in I\times\mathbb{R}^{2d},\ \ |\partial_z^\gamma h_j(t,z)|\leq C_\gamma. \tag{1.5}$$

(iii) The gap is controlled at infinity, i.e. there exist $R > 0$ and $n_0 \in \mathbb{N}$ such that

$$\forall t \in I, \ \ \forall |z| > R, \ \ |f(t,z)| \geq C\langle z\rangle^{-n_0}, \tag{1.6}$$

and in the case $n_0 \neq 0$, the functions $z \mapsto \pi_1, \pi_2$ are assumed to have bounded derivatives at infinity.

REMARK 1.5. (1) The fact that the eigenvalues $h_1(t,z)$ and $h_2(t,z)$ are of subquadratic growth guarantees the existence of the unitary propagators $\mathcal{U}^\varepsilon_{h_j}(t,t_0)$ for $j \in \{1,2\}$ and of the classical quantities associated with the Hamiltonians h_1 and h_2 that we will introduce below.

(2) The growth conditions of Assumption 1.4 imply that the eigenprojectors $\pi_j(t)$, $j = 1, 2$, and their derivatives have at most polynomial growth. However, when $n_0 \neq 0$, they may actually grow. This is proved in Lemma A.4. It is for this reason that we assume that the projectors have bounded derivatives when $n_0 \neq 0$ in Point (iii).

(3) If one has (1.4) and (1.6) with $n_0 = 0$, then (1.5) holds. However, the examples below contain interesting physical situations for which $n_0 \neq 0$.

EXAMPLE 1.6. (1) Examples of matrix-valued Hamiltonian are given in molecular dynamics (see [Chapter 5] in [**26**]) by Schrödinger operators with matrix-valued potential,

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

When V presents a codimension 1 crossing (as defined in [**26**], then the crossing points (x,ξ) are non degenerate and generic when $\xi \neq 0$.

(2) Another class of examples appear in solid state physics in the context of Bloch band decompositions (see [**62, 12**] for example) with Hamiltonians of the form

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

(3) Finally, in [**21**], the authors have considered the operator

$$\widehat{H}_{k,\theta} = \frac{\varepsilon}{i}\frac{d}{dx}\mathbb{I}_{\mathbb{C}^2} + kx \begin{pmatrix} 0 & \mathrm{e}^{i\theta x} \\ \mathrm{e}^{-i\theta x} & 0 \end{pmatrix},$$

with $d = 1$, $N = 2$, $\theta \in \mathbb{R}_+$, $k \in \mathbb{R}^*$.

1.2.3. Assumptions on the data. We consider vector-valued initial data $\psi_0^\varepsilon \in L^2(\mathbb{R}^d, \mathbb{C}^m)$ of the form

$$\psi_0^\varepsilon = \widehat{\vec{V}}\phi_0^\varepsilon$$

where $z \mapsto \vec{V}(z)$ is a smooth function, bounded together with its derivatives and $\phi_0^\varepsilon \in L^2(\mathbb{R}^d, \mathbb{C})$ is *frequency localized* in the sense of the next definition. For stating it, we denote the Gaussian of expectation q, variance $\sqrt{\varepsilon}$ that oscillates along p according to

$$g_z^\varepsilon(x) = (\pi\varepsilon)^{-d/4}\mathrm{e}^{-\frac{(x-q)^2}{\varepsilon} + \frac{i}{\varepsilon}p\cdot(x-q)}, \ \ \forall x \in \mathbb{R}^d. \tag{1.7}$$

DEFINITION 1.7 (Frequency localized functions). Let $(\phi^\varepsilon)_{\varepsilon>0}$ be a family of functions of $L^2(\mathbb{R}^d)$. The family $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized if the family is bounded in $L^2(\mathbb{R}^d)$ and if there exist $R_0, C_0, \varepsilon_0 > 0$ and $N_0 > d + \frac{1}{2}$ such that for all $\varepsilon \in (0, \varepsilon_0]$,

$$(2\pi\varepsilon)^{-d/2}\,|\langle g_z^\varepsilon, \phi^\varepsilon\rangle| \leq C_0\,\langle z\rangle^{-N_0} \quad \text{for all } z \in \mathbb{R}^d \text{ with } |z| > R_0.$$

One then says that $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized.

We will introduce a more precise definition in Chapter 2. For families that are frequency localized, the set of $z \in \mathbb{R}^{2d}$ in the identity (2.2) can be restricted to a compact set (see Lemma 2.6). The analysis of the examples given below is performed in Lemma 2.9.

EXAMPLE 1.8. (1) The Gaussian wave packets $(g^\varepsilon_{z_0})_{\varepsilon>0}$ are frequency localized families.
(2) Define $(\mathrm{WP}^\varepsilon_{z_0}(u))_{\varepsilon>0}$ by

$$\mathrm{WP}^\varepsilon_{z_0}(u)(x) = \varepsilon^{-d/4} \mathrm{e}^{\frac{i}{\varepsilon} p_0 \cdot (x-q_0)} u\left(\frac{x-q_0}{\sqrt{\varepsilon}}\right), \quad x \in \mathbb{R}^d, \tag{1.8}$$

for $u \in \mathcal{S}(\mathbb{R}^d)$ and $z_0 = (q_0, p_0) \in \mathbb{R}^{2d}$. They are frequency localized families.
(3) Lagrangian (or WKB) states $\varphi^\varepsilon(x) = a(x)\mathrm{e}^{\frac{i}{\varepsilon}S(x)}$ with $a \in \mathcal{C}^\infty_0(\mathbb{R}^d, \mathbb{C})$ and $S \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{R})$, also are frequency localized families.

Our vector-valued initial data will have a scalar part consisting in a frequency localized family.

ASSUMPTION 1.9. The initial data ψ^ε_0 in (1.1) satisfies

$$\psi^\varepsilon_0(x) = \widehat{\vec{V}} \phi^\varepsilon_0(x), \quad x \in \mathbb{R}^d \tag{1.9}$$

where

(i) The family $(\phi^\varepsilon_0)_{\varepsilon>0}$ is frequency localized with constants $R_0, N_0, C_0, \varepsilon_0$ in Definition 1.7.
(ii) The function $z \mapsto \vec{V}(z)$ is a function of $\mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^m)$, bounded together with its derivatives, and valued in the set of normalized vectors.

We point out that any vector-valued bounded family in $L^2(\mathbb{R}^d)$ writes as a sum of data of the form $\widehat{\vec{V}}\phi^\varepsilon_0(x)$ for $(\phi^\varepsilon_0)_{\varepsilon>0}$ bounded. As a consequence, assuming the initial data ψ^ε_0 satisfies 1.9 is not really restrictive. Of course, the vector valued function $\vec{V}$ can be turned into $-\vec{V}$ by changing ϕ^ε_0 into $-\phi^\varepsilon_0$.

1.3. Classical quantities

In this section, we introduce classical quantities associated with the Hamiltonian H^ε. These quantities will be used to construct the approximations of the propagator $\mathcal{U}^\varepsilon_H(t, t_0)$ that are the subject of this text. They are called *classical* because they do not depend on the semi-classical parameter ε and are obtained by solving ε-independent equations that mainly are ODEs instead of PDEs. Thus, the numerical realization of the resulting propagator's approximations avoids the difficulties induced by the $\frac{1}{\varepsilon}$-oscillations and is applicable in a high-dimensional setting, see [**43**] for a recent review on this topic. Besides their definition, we shall also recall well-known results about their role in the description of Schrödinger propagators.

In this section, we assume that $H^\varepsilon = H_0 + \varepsilon H_1$ is subquadratic on the time interval I (as defined in Definition 1.1), with smooth eigenprojectors π_1 and π_2, and eigenvalues h_1 and h_2, the latter being subquadratic (as in (ii) of Assumption 1.4).

1.3.1. The flow map. Let $\ell \in \{1, 2\}$, we associate with $h_\ell : I \times \mathbb{R}^{2d} \to \mathbb{R}$, $(t, z) \mapsto h_\ell(t, z)$ the functions

$$z_\ell(t) = (q_\ell(t), p_\ell(t))$$

which denote the *classical Hamiltonian trajectory* issued from a phase space point z_0 at time t_0, that is defined by the ordinary differential equation

$$\dot{z}_\ell(t) = J\partial_z h_\ell(t, z_\ell(t)), \quad z_\ell(t_0) = z_0$$

with

$$J = \begin{pmatrix} 0 & \mathbb{I}_{\mathbb{R}^d} \\ -\mathbb{I}_{\mathbb{R}^d} & 0 \end{pmatrix}. \tag{1.10}$$

We note that J is the matrix associated with the symplectic form

$$\sigma(z,z') = \langle Jz, z' \rangle = p \cdot q' - p' \cdot q, \qquad z = (q,p),\ z' = (q',p') \in \mathbb{R}^{2d}.$$

The trajectory $z_\ell(t) = z_\ell(t,t_0,z_0)$ depends on the initial datum and defines the associated *flow map* $\Phi_{h_\ell}^{t,t_0}$ of the Hamiltonian function h_ℓ via

$$z \mapsto \Phi_{h_\ell}^{t,t_0}(z) := z_\ell(t,t_0,z_0), \qquad z \in \mathbb{R}^{2d}.$$

We will also use the trajectory's *action integral*

$$S_\ell(t,t_0,z_0) = \int_{t_0}^{t} \left(p_\ell(s) \cdot \dot{q}_\ell(s) - h_\ell(s, z_\ell(s))\right) ds, \tag{1.11}$$

and the *Jacobian matrix of the flow map*, also called *stability matrix*

$$F_\ell(t,t_0,z_0) = \partial_z \Phi_{h_\ell}^{t,t_0}(z_0). \tag{1.12}$$

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

$$\partial_t F_\ell(t,t_0,z_0) = J\mathrm{Hess}_z h_\ell(t, z_\ell(t))\, F_\ell(t,t_0,z_0), \quad F_\ell(t_0,t_0,z_0) = \mathbb{I}_{\mathbb{R}^{2d}}. \tag{1.13}$$

We denote its blocks by

$$F_\ell(t,t_0,z_0) = \begin{pmatrix} A_\ell(t,t_0,z_0) & B_\ell(t,t_0,z_0) \\ C_\ell(t,t_0,z_0) & D_\ell(t,t_0,z_0) \end{pmatrix}. \tag{1.14}$$

1.3.2. The metaplectic transform and Gaussian states. It is standard to associate with the time-dependent symplectic map $F_\ell(t,t_0,\cdot)$ a unitary evolution operator, the *metaplectic transformation* that acts on square integrable functions in $L^2(\mathbb{R}^d)$ as a unitary transformation.

$$\mathcal{M}[F_\ell(t,t_0,z_0)] :\ u_0 \mapsto u(t)$$

and associates with an initial datum u_0 the solution at time t of the Cauchy problem

$$i\partial_t u(t) = \mathrm{op}_1^w\left(\mathrm{Hess}_z h_\ell\left(t, \Phi_{h_\ell}^{t,t_0}(z_0)\right) z \cdot z\right) u, \ \ u(t_0) = u_0.$$

This map is called the metaplectic transformation associated with the matrix $F_\ell(t,t_0,z_0)$ (see [**47**]). It satisfies for all $\varepsilon > 0$ and for all symbol a compactly supported or polynomial

$$\mathcal{M}[F_\ell(t,t_0,z_0)]^{-1} \mathrm{op}_\varepsilon(a) \mathcal{M}[F_\ell(t,t_0,z_0)] = \mathrm{op}_\varepsilon(F_\ell(t,t_0,z_0)z). \tag{1.15}$$

All these classical quantities are involved in the description of the propagation of *Gaussian states* by $\mathcal{U}_{h_\ell}^\varepsilon(t,t_0)$, that are a generalization of the Gaussian families $(g_z^\varepsilon)_{\varepsilon>0}$ that we have already seen. Gaussian states are wave packets $\mathrm{WP}_z^\varepsilon(g^\Gamma)$ with complex-valued Gaussian profiles g^Γ, whose covariance matrix Γ is taken in the Siegel half-space $\mathfrak{S}^+(d)$ of $d \times d$ complex-valued symmetric matrices with positive imaginary part,

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

More precisely, g^Γ depends on $\Gamma \in \mathfrak{S}^+(d)$ according to

$$g^\Gamma(x) := c_\Gamma\, \mathrm{e}^{\frac{i}{2}\Gamma x \cdot x}, \quad x \in \mathbb{R}^d, \tag{1.16}$$

where $c_\Gamma = \pi^{-d/4}\det^{1/4}(\mathrm{Im}\Gamma)$ is a normalization constant in $L^2(\mathbb{R}^d)$. It is a non-zero complex number whose argument is determined by continuity according to the working environment. The propagation of Gaussian states by a metaplectic transform is well-known: for $\Gamma_0 \in \mathfrak{S}^+(d)$, we have

$$\mathcal{M}[F_\ell(t,t_0,z_0)]g^{\Gamma_0} = g^{\Gamma_\ell(t,t_0,z_0)}, \tag{1.17}$$

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

$$\begin{aligned} \Gamma_\ell(t,t_0,z_0) &= (C_\ell(t,t_0,z_0) + D_\ell(t,t_0,z_0)\Gamma_0)(A_\ell(t,t_0,z_0) + B_\ell(t,t_0,z_0)\Gamma_0)^{-1} \\ c_{\Gamma_\ell(t,t_0,z_0)} &= c_{\Gamma_0}\det{}^{-1/2}(A_\ell(t,t_0,z_0) + B_\ell(t,t_0,z_0)\Gamma_0). \end{aligned} \tag{1.18}$$

The branch of the square root in $\det^{-1/2}$ is determined by continuity in time. Besides, the action of $\mathcal{U}^\varepsilon_{h_\ell}(t,t_0)$ on Gaussian wave packets $\mathrm{WP}^\varepsilon_z(g^\Gamma)$ obey to

$$\mathcal{U}^\varepsilon_{h_\ell}(t,t_0)\mathrm{WP}^\varepsilon_{z_0}(g^{\Gamma_0}) = \mathrm{e}^{\frac{i}{\varepsilon}S_\ell(t,t_0,z_0)}\mathrm{WP}^\varepsilon_{\Phi^{t,t_0}_{h_\ell}(z_0)}(g^{\Gamma_\ell(t,t_0,z)}) + O(\sqrt{\varepsilon})$$

in any space $\Sigma^k_\varepsilon(\mathbb{R}^d)$ (see [**13**]).

1.3.3. Parallel transport. For systems, the wave function is valued in $L^2(\mathbb{R}^d,\mathbb{C}^m)$ and thus vector-valued. The propagation then involves transformation of the vector part of the eigenfunctions that is called *parallel transport*.

Denoting by $\pi_\ell^\perp$ the projector $\pi_\ell^\perp = \mathbb{I} - \pi_\ell$, we define self-adjoint matrices $H^{\mathrm{adia}}_{\ell,1}$ by

$$\begin{aligned} &\pi_\ell^\perp\, H^{\mathrm{adia}}_{\ell,1}\pi_\ell^\perp = 0, \qquad \pi\, H^{\mathrm{adia}}_{\ell,1}\pi = \pi_\ell\left(H_1 + \frac{1}{2i}\{H_0,\pi_\ell\}\right)\pi_\ell, \\ &\pi_\ell^\perp\, H^{\mathrm{adia}}_{\ell,1}\pi_\ell = \pi_\ell^\perp\left(i\partial_t\pi_\ell + i\{h_\ell,\pi_\ell\}\right)\pi_\ell. \end{aligned} \tag{1.19}$$

One then introduces the map $\mathcal{R}_\ell(t,t_0,z)$ defined for $\ell \in \{1,2\}$ by

$$i\partial_t\mathcal{R}_\ell(t,t_0,z) = H^{\mathrm{adia}}_{\ell,1}\left(t,\Phi^{t,t_0}_{h_\ell}(z)\right)\mathcal{R}_\ell(t,t_0,z), \;\; \mathcal{R}_\ell(t_0,t_0,z) = \mathbb{I}_m. \tag{1.20}$$

The map $t \mapsto H^{\mathrm{adia}}_{\ell,1}\left(t,\Phi^{t,t_0}_{h_\ell}(z)\right)$ is a locally Lipschitz map valued in the set of self adjoint matrices. Therefore, the existence of $\mathcal{R}_\ell(t,t_0,z)$ comes from solving a linear time dependent ODE by the Cauchy Lipschitz Theorem.

LEMMA 1.10. *For all $(t,z) \in I \times \mathbb{R}^{2d}$ and $\ell \in \{1,2\}$, the matrices $\mathcal{R}_\ell(t,t_0,z)$ are unitary matrices. Besides, they satisfy*

$$\mathcal{R}_\ell(t,t_0,z)\pi_\ell(t_0,z) = \pi_\ell\left(t,\Phi^{t,t_0}_\ell(z)\right)\mathcal{R}_\ell(t,t_0,z). \tag{1.21}$$

This Lemma is proved in Appendix A. The relation (1.21) implies that whenever a vector $\vec{V}_0$ is in the eigenspace of $H_0(t_0,z_0)$ for the eigenvalue $h_\ell(t_0,z_0)$, then the vector $\mathcal{R}_\ell(t,t_0,z)\vec{V}_0$ is in the range of $\pi_\ell(t,\Phi^{t,t_0}_\ell(z))$. In other words, we have constructed a map that preserves the eigenspaces along the flow:

$$\mathcal{R}_\ell(t,t_0,z) : \mathrm{Ran}\left(\pi_\ell(t_0,z)\right) \mapsto \mathrm{Ran}\left(\pi_\ell(t,\Phi^{t,t_0}_\ell(z))\right).$$

The matrices $\mathcal{R}_\ell(t,t_0,z)$ are sometimes referred to as Larmor precession (see [**13**]).

The map $\vec{V}_0 \mapsto \mathcal{R}_\ell(t,t_0,z)\pi_\ell(t_0,z)\vec{V}_0$ is a parallel transport in the Hermitian vector fiber bundle $(t,z) \mapsto \mathrm{Ran}(\pi_\ell(t,z))$ over the phase space $I \times \mathbb{R}^{2d} \subset \mathbb{R}^{1+2d}$, associated with the curve $s \mapsto \gamma(s) = \left(s,\Phi^{s,t_0}_{h_\ell}(z_0)\right)_{s\in I}$ and the matrix $H^{\mathrm{adia}}_{\ell,1}$. Indeed, the covariant derivative along the curve $(\gamma(s))_{s\in I}$ is given by

$$\nabla_{\dot\gamma(s)} = \partial_t + Jdh_\ell\cdot\nabla_z$$

and the relation $\vec{X}\left(s, \Phi_{h_\ell}^{s,t_0}(z_0)\right) = \mathcal{R}_\ell(t,t_0,z)\pi_\ell(t_0,z)\vec{V}_0$ defines a smooth section along the path γ that satisfies $\nabla_{\dot\gamma(s)}\vec{X}(t,x) = -iH_{\ell,1}^{\rm adia}(t,x)\vec{X}(t,x)$.

The map $\mathcal{R}_\ell$, $\ell \in \{1,2\}$ plays a role on the quantum side in the adiabatic setting for the propagation of wave packets. The proof of the next statement can be found in [**13**, Chapter 14] and [**20**], and Chapter 5 of this memoir.

PROPOSITION 1.11 (Vector-valued wave packets). Let $k \in \mathbb{N}$ and assume that $H^\varepsilon = H_0 + \varepsilon H_1$ satisfies Assumptions 1.3 and 1.4. Let $\ell \in \{1,2\}$ and $(t_0,z_0) \in I \times \mathbb{R}^d$. Then, for any $\varphi_0 \in \mathcal{S}(\mathbb{R}^d,\mathbb{C})$ and $\vec{V}_0 \in \operatorname{Ran}\pi_\ell(t_0,z_0)$, there exists a constant $C>0$ such that

$$\sup_{t\in J}\left\| \mathcal{U}_H^\varepsilon(t,t_0)\,\vec{V}_0\,\mathrm{WP}_{z_0}^\varepsilon\varphi_0 - \mathrm{e}^{\frac{i}{\varepsilon}S_\ell(t,t_0,z_0)}\,\vec{V}_\ell(t,t_0)\,\mathrm{WP}^\varepsilon_{\Phi_{h_\ell}^{t,t_0}(z_0)}\varphi^\varepsilon(t)\right\|_{\Sigma_\varepsilon^k} \le C\sqrt{\varepsilon},$$

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

$$\varphi^\varepsilon(t) = \mathcal{M}[F_\ell(t,t_0,z_0)]\varphi_0, \quad \text{and} \quad \vec{V}_\ell(t,t_0,z) = \mathcal{R}_\ell\left(t,t_0,\Phi_{h_\ell}^{t,t_0}(z_0)\right)\vec{V}_0.$$

1.4. Thawed and frozen Gaussian approximations

Thawed and frozen Gaussian approximations have been introduced in the 80's in theoretical chemistry [**33, 38, 39**]. The frozen one has become popular as the so-called Herman–Kluk approximation. They rely on the fact that the family of wave packets $(g_z^\varepsilon)_{z\in\mathbb{R}^{2d}}$ forms a continuous frame and provides for all square integrable functions $f \in L^2(\mathbb{R}^d)$ the reconstruction formula

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

The leading idea is then to write the unitary propagation of general, square integrable initial data $\psi_0^\varepsilon \in L^2(\mathbb{R}^d)$ as

$$\mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon = (2\pi\varepsilon)^{-d}\int_{z\in\mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi_0^\varepsilon\rangle\,\mathcal{U}_H^\varepsilon(t,t_0)g_z^\varepsilon\,dz,$$

and to take advantage of the specific properties of the propagation of Gaussian states to obtain an integral representation that allows in particular for an efficient numerical realization of the propagator.

Such a program has been completely accomplished in the scalar case. However, the mathematical proof of the convergence of this approximation is more recent [**56, 53**] and can be easily extended to the adiabatic setting (see [**20**]). We recall in the first subsection these adiabatic results and then we explain how we extend this approach to systems presenting smooth crossings via a hopping process. Surface hopping has been popularized in theoretical chemistry by the algorithm of the fewest switches (see [**60**]) and been combined with frozen Gaussian propagation in various instances, see for example [**63, 44**]. Here, it is the first time that the combination is achieved in a fully rigorous manner.

1.4.1. The adiabatic situation. Whenever the eigenvalues are of constant multiplicity, the classical quantities that we have introduced above are enough to construct an approximation of the propagator. For $\ell \in \{1,2\}$, we define the first order thawed Gaussian approximation for the ℓ-th mode as the operator $\mathcal{J}_{\ell,\rm th}^{t,t_0}$ defined on functions of the form $\psi = \widehat{\vec{V}}f$, $f \in L^2(\mathbb{R}^d)$,

$$\mathcal{J}_{\ell,\rm th}^{t,t_0}(\widehat{\vec{V}}f) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} \mathrm{e}^{\frac{i}{\varepsilon}S_\ell(t,t_0,z)}\langle g_z^\varepsilon, f\rangle\vec{V}_\ell(t,t_0,z)g^{\Gamma_\ell(t,t_0,z),\varepsilon}_{\Phi_\ell^{t,t_0}(t,z)}dz, \tag{1.22}$$

with

$$\vec{V}_\ell(t,t_0,z) = \mathcal{R}_\ell(t,t_0,z)\pi_\ell(t_0,z)\vec{V}(z). \tag{1.23}$$

This family of operators is bounded in $\mathcal{L}\left(L^2(\mathbb{R}^d), \Sigma^k_\varepsilon(\mathbb{R}^d)\right)$ (see Corollary 2.17).

Notice that the operator $f \mapsto \mathcal{J}^{t,t_0}_{\ell,\mathrm{th}}(\widehat{\vec{V}}f)$ has a Schwartz distribution kernel and defines a Fourier integral operator with an explicit complex phase.

THEOREM 1.12 (Thawed Gaussian approximation [**38, 53, 56, 20**]). *Assume h_ℓ is an eigenvalue of constant multiplicity of a matrix $H^\varepsilon = H_0 + \varepsilon H_1$ of subquadratic growth on the time interval I. Let $t_0, T \in \mathbb{R}$ with $[t_0, T] \subset I$. Then, there exists $C_T > 0$ such that for all $\phi^\varepsilon_0 \in L^2(\mathbb{R}^d)$, $\vec{V} \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^m)$ bounded with bounded derivatives, for all $t \in [t_0, t_0 + T]$*

$$\left\| \mathcal{U}^\varepsilon_H(t,t_0)\left(\widehat{\pi}_\ell(t_0)\widehat{\vec{V}}\phi^\varepsilon_0\right) - \mathcal{J}^{t,t_0}_{\ell,\mathrm{th}}(\widehat{\vec{V}}\phi^\varepsilon_0)\right\|_{L^2} \leq C_T\,\varepsilon\,\|\phi^\varepsilon_0\|_{L^2}.$$

REMARK 1.13.
(1) Of course, there is no unicity of the writing $\psi = \widehat{\vec{V}}f$. However, changing $(\vec{V}, f)$ into $(k\vec{V}, \frac{1}{k}f)$ for some constant $k \in \mathbb{C}$ does not affect the result. One can also think to modifying $\vec{V}$ by multiplying it by a non-vanishing function $a \in \mathcal{C}^\infty(\mathbb{R}^{2d})$ such that a and $\frac{1}{a}$ have bounded derivatives. Then, it is enough to turn f into $a^{-1}f$ (see Remark 2.23).
(2) The approach of thawed and frozen approximations that we develop in this text allows to extend the convergence to the spaces Σ^ε_k provided the initial data $(\phi^\varepsilon_0)_{\varepsilon>0}$ is frequency localized and k satisfies $N_0 > k + d + \frac{1}{2}$ (N_0 being associated to $(\phi^\varepsilon_0)_{\varepsilon_0}$ by Definition 1.7).

As first proposed in [**33**], it is also possible to get rid of the time-dependent variance matrices Γ_ℓ by introducing the *Herman-Kluk prefactors for the ℓ-th modes*, a_ℓ, defined by

$$a_\ell(t,t_0,z) = 2^{-d/2}\det{}^{1/2}\left(A_\ell(t,t_0,z) + D_\ell(t,t_0,z) + i(C_\ell(t,t_0,z) - B_\ell(t,t_0,z)\right). \tag{1.24}$$

One then defines the first order frozen Gaussian approximation for the ℓ-th mode as the operator $\mathcal{J}^{t,t_0}_{\ell,\mathrm{fr}}$ defined by

$$\mathcal{J}^{t,t_0}_{\ell,\mathrm{fr}}(\vec{V}f) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} \mathrm{e}^{\frac{i}{\varepsilon}S_\ell(t,t_0,z)}\langle g^\varepsilon_z, f\rangle a_\ell(t,t_0,z)\vec{V}_\ell(t,t_0,z)g^\varepsilon_{\Phi_1^{t,t_0}(z)}dz. \tag{1.25}$$

Here again, this family of operators is bounded in $\mathcal{L}\left(L^2(\mathbb{R}^d), \Sigma^k_\varepsilon(\mathbb{R}^d)\right)$ (see Corollary 2.17). The next result then is a consequence of Theorem 1.12

THEOREM 1.14 (Frozen Gaussians approximation [**38, 53, 56, 20**]). *Assume h_ℓ is an eigenvalue of constant multiplicity of a matrix $H = H_0 + \varepsilon H_1$ of subquadratic growth on the time interval I. Let $t_0, T \in \mathbb{R}$ with $[t_0, T] \subset I$. Then, there exists $C_T > 0$ such that for all $\phi^\varepsilon_0 \in L^2(\mathbb{R}^d)$, $\vec{V} \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^m)$ bounded with bounded derivatives, and for all $t \in [t_0, t_0 + T]$,*

$$\left\| \mathcal{U}^\varepsilon_H(t,t_0)\left(\widehat{\pi}_\ell(t_0)\widehat{\vec{V}}\phi^\varepsilon_0\right) - \mathcal{J}^{t,t_0}_{\ell,\mathrm{fr}}(\widehat{\vec{V}}\phi^\varepsilon_0)\right\|_{L^2} \leq C_T\,\varepsilon\,\|\phi^\varepsilon_0\|_{L^2}.$$

The terminology *thawed/frozen* for these Gaussian approximations was introduced by Heller [**32**] to put emphasis on the fact that, on the first case, the covariance of the matrix was evolving "naturally" by following the classical motion wile, on the other one, the covariance is "frozen" (constant). The possibility of freezing the covariance matrix was realized by Herman and Kluk (see [**33**]) by computing the kernel of the time dependent propagator.

As for Theorem 1.12, one can extend the result to an approximation in Σ^k_ε provided the data $(\phi^\varepsilon_0)_{\varepsilon_0}$ is frequency localized family and $k \in \mathbb{N}$ is chosen so that $N_0 > k+d+\frac{1}{2}$ (N_0 being associated to $(\phi^\varepsilon_0)_{\varepsilon_0}$ by Definition 1.7).

In the next sections, we present our results and an extension of these statements to systems with crossings. The method we develop also allow to prove the approximations of Theorems 1.14 and 1.12 in the spaces $\Sigma^k_\varepsilon(\mathbb{R}^d)$, with additional assumptions on the initial data.

1.4.2. Initial value representations for codimension 1 crossing at order $\sqrt{\varepsilon}$. Our first result consists in an extension of the range of validity of Theorems 1.12 and 1.14 to Hamiltonians presenting smooth crossing and satisfying (1.3) at the prize of a loss in the accuracy of the approximation.

THEOREM 1.15 (Leading order thawed/frozen Gaussian approximation). *Let $k \in \mathbb{N}$. Assume $H^\varepsilon = H_0 + \varepsilon H_1$ satisfies Assumptions 1.3 and 1.4 on the interval I. Then, there exist constants $C_{T,k} > 0$, such that for all initial data $\psi^\varepsilon_0 = \vec{V}\phi^\varepsilon_0$ that satisfies Assumptions 1.9 with frequency localization index $N_0 > k+d+\frac{1}{2}$, there exists $\varepsilon_0 > 0$ such that for all $t \in I$ and $\varepsilon \in (0, \varepsilon_0]$, we have*

$$\left\| \mathcal{U}^\varepsilon_H(t,t_0) \left(\widehat{\pi_\ell(t_0)\vec{V}}\phi^\varepsilon_0 \right) - \mathcal{J}^{t,t_0}_{\ell,\mathrm{th/fr}}\phi^\varepsilon_0 \right\|_{\Sigma^k_\varepsilon} \leq C_T \sqrt{\varepsilon}\, \left(\|\phi^\varepsilon_0\|_{L^2} + C_0 \right).$$

The remarks below also holds for Theorems 1.18, 1.19 and 1.20.

REMARK 1.16. (1) Of course the result also holds for initial data

$$\psi^\varepsilon_0(x) = \widehat{\vec{V}}\phi^\varepsilon_0(x) + r^\varepsilon_0(x), \quad x \in \mathbb{R}^d$$

when the family $(r^\varepsilon_0)_{\varepsilon>0}$ satisfies $\|r^\varepsilon_0\|_{L^2(\mathbb{R}^d)} = O(\varepsilon)$ in Σ^k_ε for the index k considered in the statement.

(2) The fact of being frequency localized with $N_0 > k+d+\frac{1}{2}$ implies that $(\phi^\varepsilon_0)_{\varepsilon>0}$ is bounded in Σ^k_ε (see Section 2.2.6). Thus, $(\mathcal{U}^\varepsilon_H(t,t_0)\psi^\varepsilon_0)_{\varepsilon>0}$ also is bounded in Σ^k_ε and this space is the natural space where studying the approximation.

(3) The control of the approximation in terms of the initial data by $\|\phi^\varepsilon_0\|_{L^2} + C_0$ instead of $\|\phi^\varepsilon_0\|_{\Sigma^\varepsilon_k}$ is due to the method of the proof, which has to account for the presence of the crossing. The constant C_0 (and the L^2-norm) control the Σ^ε_k-norm.

The loss of accuracy of the approximation, in $\sqrt{\varepsilon}$ instead of ε, is also due to the presence of the crossing set Υ. It induces transitions between the modes that are exactly of order $\sqrt{\varepsilon}$ and cannot be neglected. If the initial data is frequency localized in a domain such that all the classical trajectories issued from its microlocal support at time t_0 do not reach the crossing set before the time $t_0 + T$, then an estimate in ε will hold. However, if these trajectories pass through the crossing, some additional terms of order $\sqrt{\varepsilon}$ have to be added to obtain an approximation at order ε. Let us now introduce the hopping trajectories that we will consider and the branching of classical quantities that we will use above the crossing set.

1.4.3. Hopping trajectories and branching process. Assume $H^\varepsilon = H_0 + \varepsilon H_1$ satisfies Assumptions 1.3 and 1.4 on the interval I. For considering initial data $\psi^\varepsilon_0 = \vec{V}\phi^\varepsilon_0$ that are frequency localized in a compact set $K \subset B(0, R_0)$, we are going to make assumptions on the set K.

We consider sets K that are connected compact subsets of $\mathbb{R}^{2d}$ and that do not intersect the crossing set Υ. If one additionally assumes that the trajectories $\Phi^{t,t_0}_\ell(z)$ issued from points $z \in K$ intersect Υ on generic crossing points, then, because of their transversality to Υ, a given

trajectory $\Phi_\ell^{t,t_0}(z)$ issued from $z \in K$ meets Υ only a finite number of times. We then denote by $(t_\ell^\flat(t_0,z), \zeta_\ell(t_0,z))$ the first crossing point in Υ:

$$\zeta_\ell^\flat(t_0,z) = \Phi_\ell^{t_\ell^\flat(t_0,z),t_0}(z). \tag{1.26}$$

For the ℓ-th mode and the compact K, we define

$$t^\flat_{\ell,\max}(t_0,K) = \max\{t_\ell^\flat(t_0,z),\ z \in K\} \ \text{ and } \ t^\flat_{\ell,\min}(t_0,K) = \min\{t_\ell^\flat(t_0,z),\ z \in K\}.$$

We shall assume that K is well-prepared in the sense that all trajectories issued from K for one of the mode have passed through Υ (if they do) before the ones for the other mode start to reach Υ.

Assumption 1.17 (Well-prepared frequency domain). The set K is a connected compact subset of $\mathbb{R}^{2d}$ that does not intersect the crossing set Υ. The trajectories $\Phi_\ell^{t,t_0}(z)$ issued from points $z \in K$ intersect Υ on generic crossing points and one has

$$t^\flat_{1,\max}(t_0,K) < t^\flat_{2,\min}(t_0,K).$$

A space-time crossing point $(t_\ell^\flat(t_0,z), \zeta_\ell^\flat(t_0,z))$ is characterized by three parameters

$$\mu^\flat \in \mathbb{R}, \qquad (\alpha^\flat, \beta^\flat) \in \mathbb{R}^{2d}$$

given by

$$\mu^\flat(t_0,z) = \frac{1}{2}\left(\partial_t f + \{v,f\}\right)\left(t_\ell^\flat(t_0,z), \zeta_\ell^\flat(t_0,z)\right), \tag{1.27}$$

$$\left(\alpha^\flat(t_0,z), \beta^\flat(t_0,z)\right) = J\nabla_z f\left(t_\ell^\flat(t_0,z), \zeta_\ell^\flat(t_0,z)\right). \tag{1.28}$$

The hopping process is affected with a *transition coefficient* $\tau_{1,2}(t,t_0,z)$ that restrict the space time variables (t,z) to trajectories that have met the crossing set Υ

$$\tau_{1,2}(t,t_0,z) = \mathbb{I}_{t \geq t_1^\flat(t_0,z)} \sqrt{\frac{2i\pi}{\mu^\flat(t_0,z)}}. \tag{1.29}$$

Note that when K satisfies Assumption 1.17, then if $t < t^\flat_{1,\min}(K)$ and $z \in K$, one has $\tau_{1,2}(t,t_0,z) = 0$. Moreover, if $t \in \left(t^\flat_{1,\max}(K), t^\flat_{2,\min}(K)\right)$, $z \mapsto \tau_{1,2}(t,t_0,z)$ is smooth.

One then introduces *hopping trajectories* by setting

$$\Phi_{1,2}^{t,t_0}(z) = \Phi_2^{t,t_1^\flat(t_0,z)}\left(\zeta_1^\flat(t_0,z)\right), \ \ t > t_1^\flat(t_0,z). \tag{1.30}$$

This trajectory $\left(\Phi_{1,2}^{t,t_0}(z)\right)_{t>t^\flat(t_0,z)}$ is the branch of a generalized trajectory that has hopped from the mode $\ell = 1$ to the mode $\ell = 2$ at the crossing point $(t_1^\flat(t_0,z), \zeta_1^\flat(t_0,z))$. One could define similarly trajectories hopping from the mode $\ell = 2$ to $\ell = 1$ by exchanging the role of the indices 1 and 2.

Along these trajectories, one defines classical quantites as follows:

(a) The function $S_{1,2}(t,t_0,z)$ is the action accumulated along the hopping trajectories, i.e. between times t_0 and $t_1^\flat(t_0,z)$ on the mode $\ell = 1$ and then on the mode $\ell = 2$

$$S_{1,2}(t,t_0,z) = S_1(t_1^\flat(t_0,z),t_0,z) + S_2(t,t_1^\flat(t_0,z),\zeta_1^\flat(t_0,z)), \tag{1.31}$$

(b) The matrix $\Gamma_{1,2}(t,t_0,z)$ is generated according to (1.18) for the mode $\ell=2$ along the trajectory $(\Phi_{1,2}(t,t_0,z))_{t>t_1^\flat(t_0,z)}$ starting at time $t_1^\flat=t_1^\flat(t_0,z)$ from the matrix

$$\Gamma^\flat(t_0,z)=\Gamma_1(t_1^\flat,t_0,z)-\frac{(\beta^\flat-\Gamma_1(t_1^\flat,t_0,z)\alpha^\flat)\otimes(\beta^\flat-\Gamma_1(t_1^\flat,t_0,z))}{2\mu^\flat-\alpha^\flat\cdot\beta^\flat+\alpha^\flat\cdot\Gamma_1(t_1^\flat,t_0,z)\alpha^\flat}, \tag{1.32}$$

(c) The vector $\vec{V}_{1,2}(t,t_0,z)$ is obtained by propagating the vector $\vec{V}_1\left(t_1^\flat,t_0,z\right)$ for the mode $\ell=2$ along the trajectory $(\Phi_{1,2}(t,t_0,z))_{t>t^\flat(t_0,z)}$ starting at time $t_1^\flat$ from the vector $\pi_2(t_1^\flat,\zeta_1^\flat)\vec{V}_1\left(t_1^\flat,t_0,z\right)$ with $\zeta_1^\flat=\zeta_1^\flat(t_0,z)$. One has

$$\vec{V}_{1,2}(t,t_0,z)=\mathcal{R}_2(t,t_1^\flat,\zeta_1^\flat)\pi_2\left(t_1^\flat,\zeta_1^\flat\right)\vec{V}_1\left(t_1^\flat,t_0,z\right). \tag{1.33}$$

(d) The matrices $F_{1,2}(t,t_0,z)$ are associated with the flow maps

$$F_{1,2}(t,t_0,z)=\partial_z\Phi_{1,2}^{t,t_0}(z)=\begin{pmatrix}A_{1,2}(t,t_0,z) & B_{1,2}(t,t_0,z)\\ C_{1,2}(t,t_0,z) & D_{1,2}(t,t_0,z)\end{pmatrix}. \tag{1.34}$$

(e) The transitional Herman–Kluk prefactors depend on $\Gamma_{1,2}(t,t_0,z)$ and $\tau_{1,2}(t,t_0,z)$ according to

$$\begin{aligned}a_{1,2}&=\tau_{1,2}\frac{\det^{1/2}(C_{1,2}-iD_{1,2}-i(A_{1,2}-iB_{1,2}))}{\det^{1/2}(C_{1,2}-iD_{1,2}-\Gamma_{1,2}(A_{1,2}-iB_{1,2}))}\\&=\tau_{1,2}\frac{\det^{1/2}(A_{1,2}+D_{1,2}+i(C_{1,2}-B_{1,2}))}{\det^{1/2}(D_{1,2}+iC_{1,2}-i\Gamma_{1,2}(A_{1,2}-iB_{1,2}))}\end{aligned} \tag{1.35}$$

where we have omitted to mark the dependence on (t,t_0,z) for readability.

With these quantities in hands, we can define the correction terms of order $\sqrt{\varepsilon}$ of the thawed & frozen approximations and state our main results.

1.4.4. Thawed Gaussian approximation at order ε. With the notations of the preceding section, one defines the *thawed Gaussian correction term for the mode $\ell=1$* as

$$\mathcal{J}_{1,2,\mathrm{th}}^{t,t_0}(\vec{V}f)=(2\pi\varepsilon)^{-d}\int_{z\in K}\tau_{1,2}(t,t_0,z)\mathrm{e}^{\frac{i}{\varepsilon}S_{1,2}(t,t_0,z)}\langle g_z^\varepsilon,f\rangle\vec{V}_{1,2}(t,t_0,z)g^{\Gamma_{1,2}(t,t_0,z),\varepsilon}_{\Phi_{1,2}^{t,t_0}(z)}dz \tag{1.36}$$

The formula (1.36) defines a family of operators that is bounded in $\mathcal{L}(L^2(\mathbb{R}^d),\Sigma_\varepsilon^k(\mathbb{R}^d))$ (see Corollary 2.17). The restriction $t>t_1^\flat(t_0,z)$ introduces a localization of the domain of integration on one side of the hypersurface $\{t=t_1^\flat(t_0,z)\}$.

The thawed Gaussian correction term for the mode $\ell=2$, denoted by $\mathcal{J}_{2,1,\mathrm{th}}^{t,t_0}$ would be defined by exchanging the roles of the indices 1 and 2. These correction terms allow to ameliorate the accuracy of the thawed gaussian approximation and to obtain an approximation at order ε.

THEOREM 1.18 (Thawed Gaussian approximation with hopping trajectories). *Let $k\in\mathbb{N}$. Assume $H^\varepsilon=H_0+\varepsilon H_1$ satisfies Assumptions 1.3 and* (1.4) *on the interval I. Then, there exists constants $C_{T,k}>0$, such that for all initial data $\psi_0^\varepsilon=\vec{V}\phi_0^\varepsilon$ that satisfies Assumptions 1.9 in a compact K satisfying Assumption 1.17, there exists $\varepsilon_0>0$ such that for all $t\in I$ we have for*

$\varepsilon \in (0, \varepsilon_0]$,

$$\left\| \mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon - \mathcal{J}_{1,\mathrm{th}}^{t,t_0}\left(\widehat{\pi_1(t_0)\vec{V}}\,\phi_0^\varepsilon\right) - \mathcal{J}_{2,\mathrm{th}}^{t,t_0}\left(\widehat{\pi_2(t_0)\vec{V}}\,\phi_0^\varepsilon\right) - \sqrt{\varepsilon}\mathcal{J}_{1,2,\mathrm{th}}^{t,t_0}\left(\widehat{\pi_1(t_0)\vec{V}\phi_0^\varepsilon}\right)\right\|_{\Sigma_\varepsilon^k} \leq C_{T,k}\,\varepsilon\,(C_0 + \|\phi_0^\varepsilon\|_{L^2})\,.$$

This result emphasizes that for systems with smooth crossings, a term of order $\sqrt{\varepsilon}$ is generated by the crossing.

1.4.5. Frozen Gaussian approximation at order ε. In order to freeze the covariance of the Gaussians $\Gamma_{1,2}(t,t_0,z)$ that appear in the formula of the thawed Gaussian correction term (1.36), we use the correction prefactors $a_{1,2}$ and $a_{2,1}$ introduceded in (1.35) and define the frozen Gaussian correction term for the mode $\ell = 1$ as

$$\mathcal{J}_{1,2,\mathrm{fr}}^{t,t_0}(\vec{V}f) = (2\pi\varepsilon)^{-d}\int_{z\in\ K} a_{1,2}(t,t_0,z)\mathrm{e}^{\frac{i}{\varepsilon}S_{1,2}(t,t_0,z)}\langle g_z^\varepsilon, f\rangle \vec{V}_{1,2}(t,t_0,z) g^\varepsilon_{\Phi_{1,2}^{t,t_0}(z)} dz. \tag{1.37}$$

Notice that the map $f \mapsto \mathcal{J}_{1,2,\mathrm{fr}}^{t,t_0}(\vec{V}f)$ defines a Fourier-integral operator with a complex phase associated with the canonical transformations $\Phi_{1,2}^{t,t_0}$ that define the hopping flow. We first state a point-wise approximation.

THEOREM 1.19 (Point-wise time frozen Gaussian approximation with hopping trajectories). *Let $k \in \mathbb{N}$. Assume $H^\varepsilon = H_0 + \varepsilon H_1$ is of subquadratic growth and satisfies Assumptions 1.3 and 1.4 on the interval I. Then, there exists constants $C_{T,k} > 0$, such that for all initial data $\psi_0^\varepsilon = \vec{V}\phi_0^\varepsilon$ that satisfies Assumptions 1.9 in a compact K satisfying Assumption 1.17, there exists $\varepsilon_0 > 0$ such that for all $t \in I$ satisfying*

$$t < t^\flat_{1,\min}(t_0,K) \ \text{ or } \ t^\flat_{1,\max}(t_0,K) \leq t < t^\flat_{2,\min}(t_0,K),$$

we have for $\varepsilon \in (0,\varepsilon_0]$,

$$\left\| \mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon - \mathcal{J}_{1,\mathrm{fr}}^{t,t_0}\left(\widehat{\pi_1(t_0)\vec{V}}\,\phi_0^\varepsilon\right) - \mathcal{J}_{2,\mathrm{fr}}^{t,t_0}\left(\widehat{\pi_2(t_0)\vec{V}}\,\phi_0^\varepsilon\right) - \sqrt{\varepsilon}\mathcal{J}_{1,2,\mathrm{fr}}^{t,t_0}\left(\widehat{\pi_1(t_0)\vec{V}\phi_0^\varepsilon}\right)\right\|_{\Sigma_\varepsilon^k} \leq C_{T,K}\,\varepsilon\,(\|\phi_0^\varepsilon\|_{L^2} + C_0)\,.$$

The proof of Theorem 1.19 is based on integration by parts and requires differentiability. When $t < t^\flat_{1,\min}(K)$, then the transfer coefficient $\tau_{1,2}(t,t_0,z) = 0$ for all $z \in K$. When $t \in [t^\flat_{1,\max}(K), t^\flat_{2,\min}(K))$, then $z \mapsto \tau_{1,2}(t,t_0,z)$ is smooth. It is for that reason, that we have to restrict the time validity of the approximation.

Averaging in time allows to overcome this difficulty and to obtain an approximation result that holds almost everywhere on intervals of time such that the classical trajectories issued from K and associated with the level $\ell = 2$ have not yet reached Υ.

THEOREM 1.20 (Time averaged frozen Gaussians approximation with hopping trajectories). *Let $k \in \mathbb{N}$. Assume $H^\varepsilon = H_0 + \varepsilon H_1$ is of subquadratic growth and satisfies Assumptions 1.3 and 1.4 on the interval I. Then, there exists constants $C_{T,k} > 0$, such that for all initial data $\psi_0^\varepsilon = \vec{V}\phi_0^\varepsilon$*

that satisfies Assumptions 1.9 in a compact K satisfying Assumption 1.17, there exists $\varepsilon_0 > 0$ such that for all $\chi \in \mathcal{C}_0^\infty\left(\left(t_0, t^\flat_{2,\min}(t_0,K)\right)\right)$,

$$\left\| \int_{\mathbb{R}} \chi(t) \Big(\mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon - \mathcal{J}_{1,\mathrm{fr}}^{t,t_0}\left(\widehat{\pi_1(t_0)\vec{V}}\,\phi_0^\varepsilon\right) - \mathcal{J}_{2,\mathrm{fr}}^{t,t_0}\left(\widehat{\pi_2(t_0)\vec{V}}\,\phi_0^\varepsilon\right) - \sqrt{\varepsilon}\mathcal{J}_{1,2,\mathrm{fr}}^{t,t_0}\left(\widehat{\pi_1(t_0)\vec{V}}\phi_0^\varepsilon\right)\Big) dt \right\|_{\Sigma_\varepsilon^k} \leq C_{T,k}\,\varepsilon\,\|\chi\|_{L^\infty}\,\left(\|\phi_0^\varepsilon\|_{L^2} + C_0\right).$$

To go beyond the time $t^\flat_{2,\min}(t_0,K)$, one has to consider new transitions that would now go from the level $\ell = 2$ to the level $\ell = 1$, each time a trajectory for the level $\ell = 2$ hits Υ. The process can be understood as a random walk: each time a trajectory passes through Υ a new trajectory arises on the other mode with a transition rate of order $\sqrt{\varepsilon}$.

The averaging in time can be understood as the result of a non-pointwise observation, that takes place over some time interval, that might even be a short one.

For proving Theorem 1.19, 1.20 we use an accurate analysis for the propagation of individual wave-packets. We prove that a Gaussian wave-packet stays a generalized Gaussian wave packet modulo an error term of order ε^μ, for any $\mu \in \mathbb{N}$, and in any space Σ_ε^k, $k \in \mathbb{N}$, as well before, or after, hitting the crossing hypersurface Υ.

The proof consists first in proving the thawed approximations and in then deriving the frozen approximation from the thawed one. The arguments developed in Section 3.3 will show that one can "freeze" the Gaussian on any state $g_z^{\Gamma_0,\varepsilon}$. The choice of some Γ_0 instead of $i\mathbb{I}$ will imply a slight modification of the definition of the Herman–Kluk prefactors a_ℓ, and the transitional ones $a_{\ell,\ell'}$, $\ell, \ell' \in \{1,2\}$.

1.5. Wave packets propagation at any order through generic smooth crossings

Our results crucially rely on the analysis of the propagation of wave-packets (including the ones with Gaussian amplitude functions) through smooth crossings. We consider a Hamiltonian $H^\varepsilon = H_0 + \varepsilon H_1$ that satisfies Assumptions 1.4 on the time interval I and presents a smooth crossing on a set Υ. We fix a point $z_0 = (q_0, p_0) \notin \Upsilon$ and times t_0, T such that

$$t_0 < t_1^\flat(t_0,z_0) < t_0 + T < t_2^\flat(t_0,z_0). \tag{1.38}$$

We assume that the point $\Phi_{h_1}^{t_1^\flat(t_0,z_0),t_0}(z_0)$ is a non degenerate generic crossing point (see Definition 1.2) that we denote by $\Phi_{h_1}^{t_1^\flat,t_0}(z_0)$ for simplicity. We use the notations introduced in Section 1.4.4 (namely equations (1.26), (1.27), (1.28), (1.30) and (1.31)). For $\ell \in \{1,2\}$, we set

$$z_\ell(t) = \Phi_\ell^{t,t_0}(z_0).$$

THEOREM 1.21. *Let (t_0,z_0) satisfy (1.38), let ψ_0^ε be a polarized wave packet*

$$\psi_0^\varepsilon = \vec{V}_0 \mathrm{WP}_{z_0}^\varepsilon(f_0) \;\; \textit{with} \;\; f_0 \in \mathcal{S}(\mathbb{R}^d) \;\; \textit{and} \;\; \vec{V}_0 \in \mathbb{C}^m. \tag{1.39}$$

Let $\psi^\varepsilon(t)$ be the solution of (1.1) with initial data ψ_0^ε. There exist $\kappa_0 \in \mathbb{N}$ and three families of differential operators $\left(\vec{B}_{\ell,j}(t)\right)_{j\in\mathbb{N}}$, $\ell \in \{1,2\}$ and $\left(\vec{B}_{1\to 2,j}(t)\right)_{j\in\mathbb{N}}$ such that setting for $\delta > 0$ and

$$
\begin{aligned}
t \in I_\delta = [t_0, t_1^\flat(t_0,z_0) - \delta] \cup [t_1^\flat(t_0,z_0) + \delta, t_0 + T]\\
\psi_1^{\varepsilon,N}(t) = \mathrm{e}^{\frac{i}{\varepsilon}S_1(t,t_0,z_0)}\mathrm{WP}^\varepsilon_{z_1(t)}\left(f_1^\varepsilon(t)\right),\\
\psi_2^{\varepsilon,N}(t) = \mathrm{e}^{\frac{i}{\varepsilon}S_2(t,t_0,z_0)}\mathrm{WP}^\varepsilon_{z_2(t)}\left(f_2^\varepsilon(t)\right) + \mathbb{I}_{t>t^\flat}\mathrm{e}^{\frac{i}{\varepsilon}S_{1,2}(t,t_0,z_0)}\mathrm{WP}^\varepsilon_{\Phi_{1,2}(t,t_0,z_0)}\left(f_{1\to 2}^\varepsilon(t)\right),
\end{aligned}
$$

with

$$
\begin{aligned}
f_\ell^\varepsilon(t) = \mathcal{R}_\ell(t,t_0)\,\mathcal{M}[F_\ell(t,t_0)] \sum_{0\le j\le N} \varepsilon^{j/2}\,\vec{B}_{\ell,j}(t) f_0, \quad \ell \in \{1,2\},\\
f_{1\to 2}^\varepsilon(t) = \mathcal{R}_2(t,t_1^\flat)\,\mathcal{M}[F_2(t,t_1^\flat)] \sum_{1\le j\le N} \varepsilon^{j/2}\,\vec{B}_{1\to 2,j}(t) f_0,
\end{aligned}
$$

one has the following property: for all $k, N, M \in \mathbb{N}$, there exists $C_{M,N,k} > 0$ such for all $t \in I_\delta$

$$
\left\| \psi^\varepsilon(t) - \left(\psi_1^{\varepsilon,N}(t) + \psi_2^{\varepsilon,N}(t)\right)\right\|_{\Sigma^k_\varepsilon} \le C_{M,N,k}\left(\left(\frac{\sqrt{\varepsilon}}{\delta}\right)^{N+1}\delta^{-\kappa_0} + \delta^M\right).
$$

Moreover, the operators $\vec{B}_{\ell,j}(t)$ are differential operators of degree $\le 3j$ with time dependent smooth vector-valued coefficients and satisfy for $\ell \in \{1,2\}$,

$$
\vec{B}_{\ell,0}(t) = \pi_\ell(t_0,z_0)\vec{V}_0 \quad \textit{and} \quad \vec{B}_{\ell,j}(t_0) = 0 \ \ \forall j \ge 1, \tag{1.40}
$$

$$
\begin{aligned}
\vec{B}_{\ell,1}(t) = \Bigg(\sum_{|\alpha|=3} \frac{1}{\alpha!}\frac{1}{i}\int_{t_0}^t \partial_z^\alpha h_\ell(s, z_\ell(s))\,\mathrm{op}_1^w[(F_\ell(s,t_0,z_0)z)^\alpha]\,ds\\
+ \frac{1}{i}\int_{t_0}^t \nabla_z H_1^{\mathrm{adia},\ell}(s,z_s)\cdot \mathrm{op}_1(F_\ell(t_0,s)z)ds\Bigg)\pi_\ell(t_0,z_0)\vec{V}_0,
\end{aligned} \tag{1.41}
$$

$$
\vec{B}_{1\to 2}(t) = W_1(t_1^\flat,\zeta_1^\flat)^*\,\mathcal{T}^\flat_{1\to 2}\,\mathcal{M}[F_1(t_1^\flat,t_0)]\pi_1(t_0,z_0)\vec{V}_0 \tag{1.42}
$$

where the scalar transfer operator $\mathcal{T}^\flat_{1\to 2}$ is defined by

$$
\mathcal{T}^\flat_{1\to 2}\varphi(y) = \int_{-\infty}^{+\infty} \mathrm{e}^{i(\mu^\flat - \alpha^\flat\cdot\beta^\flat/2)s^2}\mathrm{e}^{is\beta^\flat\cdot y}\varphi(y - s\alpha^\flat)ds, \quad \forall \varphi \in \mathcal{S}(\mathbb{R}^d) \tag{1.43}
$$

and the transfer matrix $W_1(t^\flat,\zeta^\flat)$ is given by

$$
W_1 = \pi_1 H_1 \pi_2 + i\pi_1\left(\partial_t\pi_1 + \frac{1}{2}\{h_1+h_2,\pi_1\}\right)\pi_2. \tag{1.44}
$$

In other words, Theorem 1.21 says that if ψ_0^ε a polarized wave packet, then, for $t \in I$, $t \ne t_1^\flat(t_0,z_0)$, the solution $\psi^\varepsilon(t)$ of (1.1) is asymptotic at any order to an asymptotic sum of wave packets. Indeed, if $n \in \mathbb{N}$ is fixed, choosing $\delta = \varepsilon^\alpha$ and M, N large enough will give an approximation in $\mathcal{O}(\varepsilon^n)$.

The polarization of the wave packets $\psi_\ell^{\varepsilon,N}(t)$ is first described by the vectors $\vec{B}_{\ell,j}(t_0)$ that evolves through $\mathcal{R}_\ell(t,t_0)\,\mathcal{M}[F_\ell(t,t_0)]$. Such evolution preserves the eigenmode. Secondly, in $\psi_2^{\varepsilon,N}(t)$, one sees a $\sqrt{\varepsilon}$ contribution that comes from a transfer from the mode 1 to the mode 2. The change of polarization is performed by the matrix W_1^* which maps $\mathrm{Ran}(\pi_1)$ to $\mathrm{Ran}(\pi_2)$. Indeed, one has

$$
\begin{aligned}
W_1^* &= \pi_2 H_1 \pi_1 - i\pi_2\left(\partial_t\pi_1 + \frac{1}{2}\{h_1+h_2,\pi_1\}\right)\pi_1\\
&= \pi_2 H_1 \pi_1 + i\pi_2\left(\partial_t\pi_2 + \frac{1}{2}\{h_1+h_2,\pi_2\}\right)\pi_1.
\end{aligned}
$$

The latter equation shows that the result is symmetric with respect to the modes and one can exchange their roles.

Theorem 1.21 was proved in [**20**] up to order $o(\varepsilon)$. The notations are compatible. However, in [**20**], a coefficient $\gamma^\flat$ appears in the definition of the transfer operator. It corresponds to a normalization process that we avoid here by using the projector $\pi_2(t_1^\flat, \zeta_1^\flat)$ instead of taking the scalar product with a normalized eigenvector.

For proving the initial value representations of $\mathcal{U}_H^\varepsilon$ of Theorems 1.15 to 1.20, we shall use two consequences of Theorem 1.21:

(i) the wave packet structure up to any order in ε of $\mathcal{U}_H^\varepsilon \vec{V}_0 \mathrm{WP}_{z_0}^\varepsilon(g^{i\mathbb{I}})$,

(ii) the exact value of the action of $\vec{B}_{1,0}$, $\vec{B}_{2,0}$, and of $\vec{B}_{1\to 2}(t)$ when f_0 is the Gaussian $g^{i\mathbb{I}}$.

We recall that the action of the operators $\mathcal{R}_\ell(t,s)\,\mathcal{M}[F_\ell(t,s)]$ on focalized Gaussians preserves the Gaussian structure and the focalization: in view of (1.17) and (1.23),

$$\mathcal{R}_\ell(t,s)\,\mathcal{M}[F_\ell(t,s,z)]\pi_\ell(s,z)\vec{V}_0 g^{i\mathbb{I}} = \vec{V}_\ell(t,s,z) g^{\Gamma_\ell(t,s,z)}$$

where $\vec{V}_\ell \in \mathrm{Ran}(\pi_\ell(t, \Phi_\ell^{t,s}(z)))$ and the matrix $\Gamma_\ell(t,s,z)$ is given by (1.18) with $\Gamma_0 = i\mathbb{I}$. Besides, regarding the transfer term, with the notations of Corollary 3.9 of [**20**] and those of (1.27), (1.28), (1.32) and (1.33)

$$\vec{B}_{1\to 2}(t_1^\flat) g^{i\mathbb{I}} = \sqrt{\frac{2i\pi}{\mu^\flat(t_0,z_0)}}\, \vec{V}_{1,2}(t_1^\flat, t_0, z_0) g^{\Gamma^\flat(t_1^\flat, t_0, z_0)}.$$

These elements may enlighten the construction of the operator $\mathcal{J}^\ell_{\ell,\mathrm{fr/th}}$ and $\mathcal{J}^{t,t_0}_{\ell,\ell',\mathrm{fr/th}}$ for indices $\ell, \ell' \in \{1,2\}$, $\ell \neq \ell'$.

1.6. Detailed overview

The main results of this paper are Theorems 1.18, 1.19, 1.20, and 1.21.

We prove Theorems 1.18, 1.19 and 1.20 in Chapters 2 and 3. These proofs rely on Theorem 1.21 that is proved later. Chapter 2 starts with Section 2.1 that recalls elementary facts about the Bargmann transform. Then, in Section 2.2, we analyze the notion of frequency localization that we have first introduced in this text and that is crucial in the setting of frozen and thawed initial value representations. Indeed, these approximations rely on a class of operators that is studied in Section 2.3. Endowed with these results, we are able to prove the approximations of Theorems 1.18, 1.19, 1.20 in Chapter 3. We describe the general proof strategy in Section 3.1 and develop the proof of Theorem 1.18 in Section 3.2. We explain in Section 3.3 how to pass from a thawed to a frozen approximation, and thus obtain Theorems 1.19 and 1.20.

Chapters 4 and 5 are devoted to the proof of Theorem 1.21. These two chapters are independent of the preceding ones, and one can start reading them, skipping Chapters 2 and 3. In Chapter 4, we construct the different diagonalisations of the Hamiltonian H^ε that we are going to use. In the crossing region, we use a rough diagonalisation (see Section 4.2), and outside this region we use super-adiabatic projectors as proposed in [**5, 46, 58**] (see Section 4.3). These constructions rely on a symbolic calculus that we present in Section 4.1. The analysis of the propagation of wave-packets is then performed in Chapter 5.

The Appendices are devoted to the proof of some technical points used in the proofs of Chapters 4 and 5.

Part 1

Initial value representations

CHAPTER 2

Frequency localized families

In this chapter, we study frequency localized families as introduced in the Introduction. We shall use the more precise following definition.

DEFINITION 2.1 (Frequency localized functions of order β). Let $\beta \geq 0$. Let $(\phi^\varepsilon)_{\varepsilon>0}$ be a family of functions of $L^2(\mathbb{R}^d)$. The family $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized of order β if the family is bounded in $L^2(\mathbb{R}^d)$ and if there exist $R_\beta, C_\beta, \varepsilon_\beta > 0$ and $N_\beta > d + \frac{1}{2}$ such that for all $\varepsilon \in (0, \varepsilon_\beta]$,

$$(2\pi\varepsilon)^{-d/2} \, |\langle g_z^\varepsilon, \phi^\varepsilon \rangle| \leq C_\beta \, \varepsilon^\beta \, \langle z \rangle^{-N_\beta} \quad \text{for all } z \in \mathbb{R}^d \text{ with } |z| > R_\beta.$$

One then says that $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized of order β on the ball $B(0, R_\beta)$.

Above, $\langle g, f \rangle = \int_{\mathbb{R}^d} f(x)\overline{g}(x)dx$ denotes the inner product of $L^2(\mathbb{R}^d)$. In this chapter, we first recall some facts about the Bargmann transform, then we study frequency localized families and, finally, the class of operators built by use of Bargmann transform and to which the thawed/frozen Gaussian approximations belong.

2.1. The Bargmann transform

The thawed/frozen approximations that we aim at studying are constructed thanks to the Bargmann transform. They belong to a class of operators obtained by integrating the Bargmann transform against adapted families.

Recall that the Bargman transform is the map $\mathcal{B}$

$$\mathcal{B}: \;\; L^2(\mathbb{R}^d) \ni f \mapsto \mathcal{B}[f] \in L^2(\mathbb{R}^{2d}),$$

defined by

$$\mathcal{B}[f](z) = (2\pi\varepsilon)^{-\frac{d}{2}} \langle g_z^\varepsilon, f \rangle, \;\; z \in \mathbb{R}^{2d}. \tag{2.1}$$

The Bargmann transform is an isometry and one has

$$\int_{\mathbb{R}^{2d}} |\mathcal{B}[f](z)|^2 dz = \|f\|_{L^2}^2.$$

Indeed, the Gaussian frame identity writes

$$f(x) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, f \rangle g_z^\varepsilon(x) dz = (2\pi\varepsilon)^{-\frac{d}{2}} \int_{\mathbb{R}^{2d}} \mathcal{B}[f] g_z^\varepsilon(x) dz, \tag{2.2}$$

where the function g_z^ε is introduced in (1.7), $g_z^\varepsilon = \mathrm{WP}_z^\varepsilon(g^{i\mathbb{I}})$ with the notation (1.16). Equation (2.2) is equivalent to

$$f(x) = (2\pi\varepsilon)^{-\frac{d}{2}} \int_{\mathbb{R}^{2d}} \mathcal{B}[f](z) g_z^\varepsilon(x) dz, \;\; \forall f \in L^2(\mathbb{R}^d).$$

More generally, the Bargmann transform characterizes the Σ_ε^k spaces according to the next result that we prove in Section 2.2.6 below.

LEMMA 2.2. *Let $k \in \mathbb{N}$, there exists a constant c_k such that for all $f \in \mathcal{S}(\mathbb{R}^d)$,*

$$\|f\|_{\Sigma^k_\varepsilon} \leq c_k \|\langle z\rangle^k \mathcal{B}[f]\|_{L^2(\mathbb{R}^{2d})}.$$

The condition of *spectral localization* introduced in Definition 2.1 expresses in terms of the Bargmann transform: The family $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized at the scale $\beta \geq 0$ if there exists constants $R_\beta, C_\beta, , \varepsilon_\beta > 0$, $N_\beta \in \mathbb{N}$, $N_\beta > 2d$ such that for $|z| > R_\beta$ and $\varepsilon \in (0, \varepsilon_\beta]$,

$$|B[\phi^\varepsilon](z)| \leq C_\beta\, \varepsilon^\beta\, \langle z\rangle^{-N_\beta}.$$

In other words, the Bargmann transform of $(\phi^\varepsilon)_{\varepsilon>0}$ has polynomial decay at infinity and is controlled by ε^β outside a ball $B(0, R_\beta)$.

The operators in which we are interested are built on the Bargmann transform. Consider a smooth family of the form

$$(z \mapsto \theta^\varepsilon_z) \in \mathcal{C}^\infty(\mathbb{R}^{2d}_z, L^2(\mathbb{R}^d)).$$

We then denote by $\mathcal{J}[\theta^\varepsilon_z]$ the operator acting on $\phi \in L^2(\mathbb{R}^d)$ according to

$$\mathcal{J}[\theta^\varepsilon_z](\phi)(x) = (2\pi\varepsilon)^{-\frac{d}{2}} \int_{\mathbb{R}^{2d}} \mathcal{B}[\phi](z)\theta^\varepsilon_z(x)dz = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g^\varepsilon_z, \phi\rangle \theta^\varepsilon_z(x)dz, \quad x \in \mathbb{R}^d. \tag{2.3}$$

The thawed/frozen operators of equations (1.22), (1.25), (1.36) and (1.37) are of that form. The Gaussian frame identity (2.2) also writes with these notations

$$\mathcal{J}[g^\varepsilon_z] = \mathbb{I}_{L^2(\mathbb{R}^d)}.$$

Note that the formal adjoint of $\mathcal{J}[\theta^\varepsilon_z]$ is

$$\mathcal{J}[\theta^\varepsilon_z]^* : \phi \mapsto (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle \theta^\varepsilon_z, \phi\rangle g^\varepsilon_z dz. \tag{2.4}$$

In the first Section 2.2, we study the properties of frequency localized families, which is the type of data we consider in our main results. Then, in Section 2.3, we analyze some properties of the operators of the form (2.3). Finally, we prove Theorems 1.15 and 1.18 in Section 3.2, and Theorems 1.19 and 1.20 in Section 3.3.

Along the next sections of this chapter, we shall use properties of wave packets that we sum-up here.

LEMMA 2.3. *if $f, g \in \mathcal{S}(\mathbb{R}^d)$ and $z, z' \in \mathbb{R}^{2d}$, then*

$$\langle \mathrm{WP}^\varepsilon_z(f), \mathrm{WP}^\varepsilon_{z'}(g)\rangle = \mathrm{e}^{\frac{i}{\varepsilon}p'\cdot(q-q')} W[f,g]\left(\frac{z'-z}{\sqrt{\varepsilon}}\right) \tag{2.5}$$

where the function $W[f,g]$ is the Schwartz function on $\mathbb{R}^{2d}$ defined by

$$W[f,g](\zeta) = \int_{\mathbb{R}^d} \overline{f}(x) g(x-q) \mathrm{e}^{ip\cdot x} dx, \quad \zeta = (q,p).$$

Moreover, for all $n \in \mathbb{N}$, there exists a constant $C_n > 0$ such that

$$\forall \zeta \in \mathbb{R}^{2d}, \quad \langle\zeta\rangle^n\, |W[f,g](\zeta)| \leq C_n \sum_{0\leq n'\leq n} \|f\|_{\Sigma^{n'}} \|g\|_{\Sigma^{n-n'}}. \tag{2.6}$$

PROOF. The formula for $\langle \mathrm{WP}_z^\varepsilon(f), \mathrm{WP}_{z'}^\varepsilon(g)\rangle$ comes from a simple computation. Then, for $\alpha, \gamma \in \mathbb{N}^d$ and $z = (q,p) \in \mathbb{R}^{2d}$, we observe

$$\begin{aligned}|q^\gamma p^\alpha W[f,g](z)| &= \left| q^\gamma \int_{\mathbb{R}^d} D_x^\alpha(\overline{f}(x) g(x-q)) \mathrm{e}^{ix\cdot p} dx \right| \\ &\leq \langle q\rangle^{|\gamma|} \int_{\mathbb{R}^d} \left| D_x^\alpha(\overline{f}(x) g(x-q))\right| dx \\ &\leq 2^{\frac{|\gamma|}{2}} \int_{\mathbb{R}^d} \langle x\rangle^{|\gamma|} \langle x-q\rangle^{|\gamma|} \left| D_x^\alpha(\overline{f}(x) g(x-q))\right| dx\end{aligned}$$

where we have used Peetre inequality

$$\forall t \in \mathbb{R}, \quad \forall \ell \in \mathbb{Z}, \quad \frac{\langle t\rangle^\ell}{\langle t'\rangle^\ell} \leq 2^{\frac{\ell}{2}} \langle t - t'\rangle^{|\ell|}. \tag{2.7}$$

The conclusion then follows. □

2.2. Frequency localized families

We investigate here the properties of families that are frequency localized in the sense of Definition 2.1 and we use the notation (2.1).

We point out that Definition 2.1 is enough to treat vector-valued families by saying that a vector-valued family is frequency localized at the scale $\beta \geq 0$ if and only if all its coordinates are frequency localized at the scale β. For this reason, we focus below on scalar-valued frequency localized families.

2.2.1. First properties of frequency localized functions. It is interesting to investigate the properties of this notion. The first properties are straightforward.

PROPOSITION 2.4. The set of frequency localized function is a subspace of $L^2(\mathbb{R}^d)$. Moreover, we have the following properties:

(1) If $(\phi_1^\varepsilon)_{\varepsilon>0}$ and $(\phi_2^\varepsilon)_{\varepsilon>0}$ are two frequency localized families at the scales β_1 and β_2 respectively, then for all $a, b \in \mathbb{C}$, the family $(a\phi_1^\varepsilon + b\phi_2^\varepsilon)_{\varepsilon>0}$ is frequency localized at the scale $\min(\beta_1, \beta_2)$.
(2) If $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized at the scale $\beta \geq 0$, then it is also frequency localized at the scale β' for all $\beta' \in [0, \beta]$.

This notion is microlocal. Indeed, defining the ε-Fourier transform by

$$\mathcal{F}^\varepsilon f(\xi) = (2\pi\varepsilon)^{-\frac{d}{2}} \int_{\mathbb{R}^d} \mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot x} \phi^\varepsilon(x) dx = (2\pi\varepsilon)^{-\frac{d}{2}} \widehat{f}\left(\frac{\xi}{\varepsilon}\right), \quad f \in \mathcal{S}^2(\mathbb{R}^d).$$

PROPOSITION 2.5. Let $(\phi^\varepsilon)_{\varepsilon>0}$ be a bounded family in $L^2(\mathbb{R}^d)$. Then, $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized family at the scale $\beta \geq 0$ if and only if $(\mathcal{F}^\varepsilon \phi^\varepsilon)_{\varepsilon>0}$ is frequency localized at the scale $\beta \geq 0$.

PROOF. This comes from the observation that for all $z \in \mathbb{R}^{2d}$,

$$|\langle g_z^\varepsilon, \phi^\varepsilon\rangle| = |\langle g_{Jz}^\varepsilon, \mathcal{F}^\varepsilon \phi^\varepsilon\rangle|$$

where J is the matrix defined in (1.10). Thus it is equivalent to state the fact of being frequency localized for a family or for the family of its ε-Fourier transform. □

2.2.2. Frequency localized families and Bargmann transform. The Gaussian frame identity (2.2) allows to decompose a function of $L^2(\mathbb{R}^d)$ into a (continuous) sum of Gaussians. After discretization of the integral, this sum may be turned into a finite one, which opens the may to approximation's strategies (see [**42**] where this observation is used for numerical purposes). It is thus important to identify assumptions that allow to compactify the set of integration in z. The notion of frequency localized families plays this role according to the next result.

LEMMA 2.6. *Let $(\phi^\varepsilon)_{\varepsilon>0}$ be a frequency localized family at the scale $\beta \geq 0$. Let R_β, C_β and N_β be the constants associated to $(\phi^\varepsilon)_{\varepsilon>0}$ according to Definition 2.1. Let $k \in \mathbb{N}$ with $N_\beta > d + k$. Then, for all $\chi \in L^\infty(\mathbb{R})$ supported in $[0,2]$ and equal to 1 on $[0,1]$, there exists $C > 0$ such that for $R > R_\beta$,*

$$\left\| \phi^\varepsilon - \mathcal{J}\left[g_z^\varepsilon \chi\left(\frac{|z|}{R}\right)\right](\phi^\varepsilon) \right\|_{\Sigma_\varepsilon^k(\mathbb{R}^d)} \leq C\, C_\beta\, \varepsilon^\beta \left(\int_{|z|>R} \langle z\rangle^{-2(N_\beta - k)} dz \right)^{1/2}.$$

In the following, we will use the notation

$$\phi^\varepsilon_{R,<} := \mathcal{J}\left[g_z^\varepsilon \chi\left(\frac{|z|}{R}\right)\right](\phi^\varepsilon) = \mathcal{B}^{-1}\left(\mathbb{I}_{|z|<R} \mathcal{B}[\phi^\varepsilon](z)\right). \tag{2.8}$$

REMARK 2.7. Lemma 2.6 can be used in different manners.

(1) If $\beta > 0$, then $\mathcal{J}[g_z^\varepsilon \chi(|z|/R)](\phi^\varepsilon)$ approximates ϕ^ε in $L^2(\mathbb{R}^d)$ as ε goes to 0 in any space $\Sigma_\varepsilon^k(\mathbb{R}^d)$ with $k \in \mathbb{N}$ such that $N_\beta > k + d + \frac{1}{2}$, and uniformly with respect to $R > R_\beta$.
(2) If $\beta \geq 0$ (which includes $\beta = 0$), then the same approximation holds by letting R go to $+\infty$, and it is uniform with respect to ε. In particular, when $\beta = 0$ we have

$$\limsup_{\varepsilon\to 0} \left\| \phi^\varepsilon - \mathcal{J}\left[g_z^\varepsilon \chi\left(\frac{|z|}{R}\right)\right](\phi^\varepsilon) \right\|_{\Sigma_\varepsilon^k(\mathbb{R}^d)} \leq C R^{-(N_\beta - k - d - \frac{1}{2})}.$$

PROOF. We set

$$r^\varepsilon(x) = (2\pi\varepsilon)^{-d} \int_{|z|\geq R} \langle g_z^\varepsilon, \varphi^\varepsilon\rangle g_z^\varepsilon(x) dz$$

and consider $k \in \mathbb{N}$. For $R > R_\beta$, $\alpha, \gamma \in \mathbb{N}^d$ with $|\alpha| + |\gamma| = k$, we have

$$\begin{aligned} &\|x^\alpha (\varepsilon D_x)^\gamma r^\varepsilon\|^2_{L^2(\mathbb{R}^d)} \\ &\quad \leq (2\pi\varepsilon)^{-2d} \int_{\mathbb{R}^d} \int_{|z|>R} \int_{|z'|>R} \langle g_z^\varepsilon, \varphi^\varepsilon\rangle \, \overline{\langle g_{z'}^\varepsilon, \varphi^\varepsilon\rangle} g_{\varepsilon,z}^{\alpha,\gamma}(x)\, \overline{g_{\varepsilon,z'}^{\alpha,\gamma}(x)}\, dx\, dz\, dz'. \end{aligned}$$

where

$$g_{\varepsilon,z}^{\alpha,\gamma} = x^\alpha (\varepsilon D_x)^\gamma g_z^\varepsilon = \mathrm{WP}_z^\varepsilon\left((q + \sqrt{\varepsilon} y)^\alpha (p + \sqrt{\varepsilon} D_y)^\gamma g^{i\mathbb{I}}) \right), \quad z = (q,p). \tag{2.9}$$

We will use that for all $n \in \mathbb{N}$, there exists $c_{n,k} > 0$ such that for all $z \in \mathbb{R}^{2d}$

$$\|g_{\varepsilon,z}^{\alpha,\gamma}\|_{\Sigma^n} \leq c_{n,k} \langle z\rangle^k. \tag{2.10}$$

By (2.5), we obtain

$$\begin{aligned} &\|x^\alpha (\varepsilon D_x)^\gamma r^\varepsilon\|^2_{L^2(\mathbb{R}^d)} \\ &\quad \leq C_\beta^2\, \varepsilon^{2\beta}\, (2\pi\varepsilon)^{-d} \int_{|z|>R} \int_{|z'|>R} \langle z\rangle^{-N_\beta} \langle z'\rangle^{-N_\beta}\, W[g_{\varepsilon,z}^{\alpha,\gamma}, g_{\varepsilon,z'}^{\alpha,\gamma}]\left(\frac{z-z'}{\sqrt{\varepsilon}}\right) dz\, dz'. \end{aligned}$$

Besides, by (2.6), there exists a constant $C'_{n,k}$ such that

$$\left|W[g^{\alpha,\gamma}_{\varepsilon,z}, g^{\alpha,\gamma}_{\varepsilon,z'}](\zeta)\right| \leq C'_{n,k}\,\langle\zeta\rangle^{-n}\langle z\rangle^{k}\langle z'\rangle^{k}.$$

We deduce the existence of $c>0$ such that

$$\begin{aligned}\|x^\alpha(\varepsilon D_x)^\gamma r^\varepsilon\|^2_{L^2(\mathbb{R}^d)} &\leq c\,C_\beta^2\,\varepsilon^{2\beta}\,\varepsilon^{-d}\int_{|z|>R}\int_{|z'|>R}\langle z\rangle^{-N_\beta+k}\langle z'\rangle^{-N_\beta+k}\left\langle\frac{z-z'}{\sqrt{\varepsilon}}\right\rangle^{-n}dzdz'\\ &\leq c\,C_\beta^2\,\varepsilon^{2\beta}\int_{|z|>R}\int\langle z\rangle^{-N_\beta+k}\langle z+\sqrt{\varepsilon}\zeta\rangle^{-N_\beta+k}\langle\zeta\rangle^{-n}dzd\zeta.\end{aligned}$$

Since $-N_\beta+k\leq 0$, Peetre inequality gives

$$\langle z+\sqrt{\varepsilon}\zeta\rangle^{-N_\beta+k}\leq 2^{\frac{N_\beta-k}{2}}\langle\sqrt{\varepsilon}\zeta\rangle^{N_\beta-k}\langle z\rangle^{-N_\beta+k}\leq 2^{\frac{N_\beta-k}{2}}\langle\zeta\rangle^{N_\beta-k}\langle z\rangle^{-N_\beta+k},$$

by restricting ourselves to $\varepsilon\leq 1$. Therefore, there exists a constant $c>0$ such that

$$\|x^\alpha(\varepsilon D_x)^\gamma r^\varepsilon\|^2_{L^2(\mathbb{R}^d)}\leq c\,C_\beta^2\,\varepsilon^{2\beta}\left(\int_{\mathbb{R}^{2d}}\langle\zeta\rangle^{-n+N_\beta-k}d\zeta\right)\left(\int_{|z|>R}\langle z\rangle^{-2(N_\beta-k)}dz\right)$$

and we conclude the proof by choosing $n=N_\beta+k+2d+1$. □

2.2.3. Examples. A first fundamental example consists in bounded families in $L^2(\mathbb{R}^d)$ that are compactly supported.

LEMMA 2.8. *Let $(\phi_0^\varepsilon)_{\varepsilon>0}$ be a bounded family in $L^2(\mathbb{R}^d)$ such that $\phi_0^\varepsilon=\mathbb{I}_{|x|\leq M}\phi_0^\varepsilon$ for some $M>0$. Then, $(\phi_0^\varepsilon)_{\varepsilon>0}$ is frequency localised at any scale $\beta\geq 0$.*

PROOF. There exists a constant $C>0$ such that for all $z=(q,p)\in\mathbb{R}^{2d}$

$$|\mathcal{B}[\phi_0^\varepsilon](z)|\leq C\|g_z^\varepsilon\mathbb{I}_{|x|\leq M}\|_{L^2}.$$

Besides, one can find a smooth real-valued function χ compactly supported in $\{|x|\leq 2\}$ such that

$$\|g_z^\varepsilon\mathbb{I}_{|x|\leq M}\|^2_{L^2}=(\pi\varepsilon)^{-\frac{d}{2}}\int_{\mathbb{R}^{2d}}\chi(\frac{x}{M})\chi(\frac{y}{M})g_z^\varepsilon(x)\overline{g_z^\varepsilon}(y)dxdy.$$

We set

$$L=(|p|^2+|q-x|^2)^{-1}(-ip+q-x)\cdot\nabla_x$$

and we observe that $\varepsilon Lg_z^\varepsilon(x)=g_z^\varepsilon(x)$ for all $x\in\mathbb{R}^d$.

Besides, if $|z|>8M$, either $|q|>4M$ and if $|x|\leq 2M\leq\frac{|q|}{2}$, then $|x-q|>\frac{|q|}{2}>4M$, or $|q|\leq 4M$ and $|p|>2M$. In any case, $(|p|^2+|q-x|^2)^{-1}>2|z|^{-1}$ and for all $N\in\mathbb{N}$, there exists a constant $c_{N,M}$ such that

$$\left|(L^*)^N\,\chi(\frac{x}{M})\right|\leq c_{N,M}|z|^{-N},$$

Using the vector field L, we perform N integration by parts, and we obtain the existence of a constant $C>0$ such that

$$\|g_z^\varepsilon\mathbb{I}_{|x|\leq M}\|^2_{L^2}\leq C\,\varepsilon^{N-\frac{d}{2}}|z|^{-N}\int_{\mathbb{R}^{2d}}\mathbb{I}_{|x|,|y|\leq M}dxdy,$$

whence the boundedness of $\varepsilon^{-\beta}\langle z\rangle^{N_\beta}\|g_z^\varepsilon\mathbb{I}_{|x|\leq M}\|_{L^2}$ for all $\beta\geq 0$ and $N_\beta\in\mathbb{N}$. □

An important consequence of this result is related with the notiont notion of compacity and of ε-oscillation that are often considered in semi-classical analysis. We recall that the uniformly bounded family $(\phi^\varepsilon)_{\varepsilon>0}$ is said to be compact if

$$\limsup_{\varepsilon\to 0}\int_{|x|>R}|\phi^\varepsilon(x)|^2dx \underset{R\to+\infty}{\longrightarrow} 0.$$

It is said ε-oscillating when

$$\limsup_{\varepsilon\to 0}\int_{|\xi|>\frac{R}{\varepsilon}}|\widehat{\phi^\varepsilon}(\xi)|^2d\xi \underset{R\to+\infty}{\longrightarrow} 0,$$

or, equivalently, when its ε-Fourier transform $(\mathcal{F}^\varepsilon\phi^\varepsilon)_{\varepsilon>0}$ is compact. Therefore, a compact family or an ε-oscillatory family can be approached by frequency-localized families. Note however that The notion of compacity or ε-oscillation is weaker than being frequency localized. For example, the family

$$u^\varepsilon(x) = |\ln\varepsilon|^{\frac{d}{2}}a(x|\ln\varepsilon|),\quad x\in\mathbb{R}^d, \tag{2.11}$$

is a compact and ε-oscillating family which has no scale of frequency localization.

Let us now analyze the examples given in the Introduction.

LEMMA 2.9. (1) *Let $u\in\mathcal{S}(\mathbb{R}^d)$ and $z_0=(q_0,p_0)\in\mathbb{R}^{2d}$. Then, the family $(\mathrm{WP}^\varepsilon_{z_0}(u))_{\varepsilon>0}$ is frequency localized at the scale β for any $\beta\geq 0$.*

(2) *Let $a\in\mathcal{C}^\infty_0(\mathbb{R}^d)$ and $S\in\mathcal{C}^\infty(\mathbb{R}^d)$. Then, the family $(\mathrm{e}^{\frac{i}{\varepsilon}S(x)}a)_{\varepsilon>0}$ is frequency localized at the scale β for any $\beta\geq 0$.*

PROOF. 1- By (2.5), we have for $z\in\mathbb{R}^{2d}$

$$\mathcal{B}[\mathrm{WP}^\varepsilon_{z_0}(u)](z) = (2\pi\varepsilon)^{-\frac{d}{2}}\langle \mathrm{WP}^\varepsilon_z(g^{i\mathbb{I}}),\mathrm{WP}^\varepsilon_{z_0}(u)\rangle = (2\pi\varepsilon)^{-\frac{d}{2}}\,\mathrm{e}^{\frac{i}{\varepsilon}p_0\cdot(q-q_0)}\,W[g^{i\mathbb{I}},u]\left(\frac{z_0-z}{\sqrt{\varepsilon}}\right).$$

Let $N\in\mathbb{N}$, the estimate (2.6) implies the existence of a constant C'_N such that

$$|\mathcal{B}[\mathrm{WP}^\varepsilon_{z_0}(u)](z)|\leq C'_N\,\varepsilon^{-\frac{d}{2}}\left\langle\frac{z_0-z}{\sqrt{\varepsilon}}\right\rangle^{-N}.$$

Choosing $|z|>\max(2|z_0|,1)$, we have $2|z_0-z|\geq 2(|z|-|z_0|)\geq|z|$ and we deduce

$$\left\langle\frac{z_0-z}{\sqrt{\varepsilon}}\right\rangle^{-N} = \left(\frac{\varepsilon}{\varepsilon+|z-z_0|^2}\right)^{\frac{N}{2}}\leq\left(\frac{4\varepsilon}{4\varepsilon+|z|^2}\right)^{\frac{N}{2}}\leq(4\varepsilon)^{\frac{N}{2}}\,|z|^{-N},$$

whence the existence of a constant $c_N>0$ such that for all $z\in\mathbb{R}^{2d}$ and $N\in\mathbb{N}$,

$$|\mathcal{B}[\mathrm{WP}^\varepsilon_{z_0}(u)](z)|\leq c_N\,\varepsilon^{\frac{N-d-1}{2}}\,\langle z\rangle^{-N}.$$

2- One has

$$\begin{aligned}\mathcal{B}[\mathrm{e}^{\frac{i}{\varepsilon}S(x)}a](z) = (2\pi)^{-d/2}\pi^{-d/4}\varepsilon^{-d/4}\mathrm{e}^{\frac{i}{\varepsilon}S(q)}\int_{\mathbb{R}^d}a(q+\sqrt{\varepsilon}y)\\ \times\mathrm{Exp}\left(-\frac{i}{\sqrt{\varepsilon}}p\cdot y+\frac{i}{\varepsilon}S(q+y\sqrt{\varepsilon})\right)\mathrm{e}^{-\frac{|y|^2}{2}}dy.\end{aligned}$$

This term has a very specific structure involving the symbol $y \mapsto a(y)$, a rapidly decaying function $y \mapsto \mathrm{e}^{-\frac{|y|^2}{2}}$ and an oscillating phase

$$y \mapsto \Lambda^\varepsilon(y) := -\frac{1}{\sqrt{\varepsilon}} p \cdot y + \frac{1}{\varepsilon} S(q + y\sqrt{\varepsilon}).$$

We are going to show that the terms defined for $j \in \{1, \cdots, d\}$ by

$$A_j^\varepsilon := q_j \int_{\mathbb{R}^d} a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} \mathrm{e}^{i\Lambda^\varepsilon(y)} dy \quad \text{and} \quad B_j^\varepsilon := p_j \int_{\mathbb{R}^d} a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} \mathrm{e}^{i\Lambda^\varepsilon(y)} dy,$$

have the same structure. Then, it will be enough to consider only one of these terms and to prove that they are controlled by a power of ε, this will implies the adequate control on $|\mathcal{B}[\mathrm{e}^{\frac{i}{\varepsilon}S(x)} a](z)|$.

Let us first transform A_j^ε and B_j^ε. Indeed, we have

$$A_j^\varepsilon = \int_{\mathbb{R}^d} (q_j + \sqrt{\varepsilon} y_j) a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} \mathrm{e}^{i\Lambda^\varepsilon(y)} dy - \sqrt{\varepsilon} \int_{\mathbb{R}^d} a(q + \sqrt{\varepsilon} y) \left(y_j \mathrm{e}^{-\frac{|y|^2}{2}} \right) \mathrm{e}^{i\Lambda^\varepsilon(y)} dy.$$

The first integral of the right hand side has the same structure with the symbol $y \mapsto a(y)$ and the second one with the rapidly decaying function $y \mapsto y_j \mathrm{e}^{-\frac{|y|^2}{2}}$. Besides, observing

$$p_j \mathrm{e}^{i\Lambda^\varepsilon(y)} = -i\sqrt{\varepsilon} \partial_{y_j} (\mathrm{e}^{i\Lambda^\varepsilon(y)}) - \partial_{y_j} S(q + \sqrt{\varepsilon} y) \mathrm{e}^{i\Lambda^\varepsilon(y)},$$

we obtain with an integration by parts

$$\begin{aligned} B_j^\varepsilon = &- \int_{\mathbb{R}^d} \partial_{y_j} S(q + \sqrt{\varepsilon} y) a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} \mathrm{e}^{i\Lambda^\varepsilon(y)} dy \\ &+ i\sqrt{\varepsilon} \int_{\mathbb{R}^d} \partial_{y_j} \left(a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} \right) \mathrm{e}^{i\Lambda^\varepsilon(y)} dy. \end{aligned}$$

Here again the right hand side has the same structure with different symbols and rapidly decaying term.

We now focus in proving that one typical term

$$L^\varepsilon := \int_{\mathbb{R}^d} a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} \mathrm{e}^{i\Lambda^\varepsilon(y)} dy \tag{2.12}$$

is of order ε^N for all $N \in \mathbb{N}$. The decay of $y \mapsto \mathrm{e}^{-\frac{|y|^2}{2}}$ allows to reduce the set of integration. Indeed, we have

$$\left| \int_{|y| > \varepsilon^{-\frac{1}{4}}} a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} \mathrm{e}^{i\Lambda^\varepsilon(y)} dy \right| \leq \mathrm{e}^{-\frac{\sqrt{\varepsilon}}{4}} \|a\|_{L^\infty} \int_{\mathbb{R}^d} \mathrm{e}^{-\frac{|y|^2}{4}} dy.$$

Therefore, there exists a constant $c > 0$ such that

$$|L^\varepsilon| \leq c \left(\left| \int_{|y| \leq \varepsilon^{-\frac{1}{4}}} a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} \mathrm{e}^{i\Lambda^\varepsilon(y)} dy \right| + \mathrm{e}^{-\frac{1}{4\sqrt{\varepsilon}}} \right).$$

We now use the oscillations of the phase for treating the integral in $|y| \leq \varepsilon^{-\frac{1}{4}}$. We observe that there exists $R_0 > 0$ such that if $|z| > R_0$, then

$$z \notin \{ |p - \nabla S(q)| \leq 1, \ \mathrm{dist}(q, \mathrm{supp}(a)) \leq 1 \}.$$

We choose $|z| > R_0$ and we have the following alternative:

$$\text{either } \mathrm{dist}(q, \mathrm{supp}(a)) > 1, \ \text{ or } \ (\mathrm{dist}(q, \mathrm{supp}(a)) \leq 1 \ \text{ and } |p - \nabla S(q)| > 1).$$

If $\mathrm{dist}(q, \mathrm{supp}(a)) > 1$, there exists $\varepsilon_0 > 0$ such that if $\varepsilon \in (0, \varepsilon_0]$ and $|y| \leq \varepsilon^{1/4}$, then $q + \sqrt{\varepsilon} y \notin \mathrm{supp}(a)$. The integral thus is zero and we are reduced to the case where $\mathrm{dist}(q, \mathrm{supp}(a)) \leq 1$ and $|p - \nabla S(q)| > 1$. One can find $\varepsilon_1 > 0$ such that for $\varepsilon \in (0, \varepsilon_1]$ and $|y| \leq \varepsilon^{\frac{1}{4}}$,

$$\left|\nabla S(q + y\sqrt{\varepsilon}) - p\right| > \frac{1}{2}.$$

We then consider the differential operator

$$L^\varepsilon = \sqrt{\varepsilon} \frac{\nabla S(q + y\sqrt{\varepsilon}) - p}{|\nabla S(q + y\sqrt{\varepsilon}) - p|^2} \cdot \nabla_y$$

and we write

$$\begin{aligned}
&\int_{|y| \leq \varepsilon^{-\frac{1}{4}}} a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} \mathrm{e}^{i\Lambda^\varepsilon(y)} dy \\
&= \int_{|y| \leq \varepsilon^{-\frac{1}{4}}} a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} (L^\varepsilon)^N \left(\mathrm{e}^{i\Lambda^\varepsilon(y)}\right) dy \\
&= \int_{|y| \leq \varepsilon^{-\frac{1}{4}}} (L^\varepsilon)^{N*} \left(a(q + \sqrt{\varepsilon} y) |\nabla S(q + y\sqrt{\varepsilon}) - p|^{-2N} \mathrm{e}^{-\frac{|y|^2}{2}}\right) \mathrm{e}^{i\Lambda^\varepsilon(y)} dy.
\end{aligned}$$

There exists a constant $C > 0$ independent of z such that for all $\varepsilon \in (0, \varepsilon_1]$ and $|y| \leq \varepsilon^{\frac{1}{4}}$,

$$\left|(L^\varepsilon)^{N*} \left(a(q + \sqrt{\varepsilon} y) |\nabla S(q + y\sqrt{\varepsilon}) - p|^{-2N} \mathrm{e}^{-\frac{|y|^2}{2}}\right)\right| \leq C \varepsilon^{\frac{N}{2}} \mathrm{e}^{-\frac{|y|^2}{2}}.$$

We deduce

$$\left|\int_{|y| \leq \varepsilon^{-\frac{1}{4}}} a(q + \sqrt{\varepsilon} y) \mathrm{e}^{-\frac{|y|^2}{2}} \mathrm{e}^{i\Lambda^\varepsilon(y)} dy\right| \leq C \varepsilon^{\frac{N}{2}}$$

and (2.12) writes

$$|L^\varepsilon| \leq c \left(\varepsilon^{\frac{N}{2}} + \mathrm{e}^{-\frac{1}{4\sqrt{\varepsilon}}}\right)$$

for some constant $c > 0$. This terminates the proof. □

2.2.4. Characterization of frequency localized families. The characterization of frequency localized families can be done by using other families of wave packets than Gaussian ones and the cores z can be distributed in different manners.

Proposition 2.10. The family $(\phi^\varepsilon)_{\varepsilon > 0}$ is frequency localized at the scale $\beta \geq 0$ if and only if for all $\mathcal{C}^1$-diffeomorphism Φ satisfying

$$\exists a, b > 0, \ \ \forall z \in \mathbb{R}^{2d}, \ \ a|z| \leq \Phi(z) \leq b|z|,$$

for all $\theta \in \mathcal{S}(\mathbb{R}^d)$, there exists C_β, N_β, R_β and ε_β such that for all $\varepsilon \in (0, \varepsilon_\beta]$ and for $|z| > R_\beta$

$$(2\pi\varepsilon)^{-\frac{d}{2}} |\langle \mathrm{WP}^\varepsilon_{\Phi(z)}(\theta), \phi^\varepsilon \rangle| \leq C_\beta \, \varepsilon^\beta \, \langle z \rangle^{-N_\beta} \, \max\left(1, \frac{1}{a}\right)^{N_\beta} \|\theta\|_{\Sigma^{2d+1+N_\beta}}.$$

Moreover, for all family $(\lambda^\varepsilon)_{\varepsilon > 0}$ bounded in $L^\infty(\mathbb{R}^{2d})$, $\varepsilon \in (0, \varepsilon_\beta]$ and $R > R_\beta$,

$$\left\|\mathcal{J}\left[\mathrm{e}^{\frac{i}{\varepsilon}\lambda^\varepsilon(z)} \mathrm{WP}^\varepsilon_{\Phi(z)}(\theta) \mathbb{I}_{|z| > R}\right](\phi^\varepsilon)\right\|_{\Sigma^k_\varepsilon} \leq C \, C_\beta \, \varepsilon^\beta \left(\int_{|z| > R} \langle z \rangle^{-N_\beta} dz\right).$$

PROOF. We only have to prove that if $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized at the scale $\beta \geq 0$, then the property holds for some given profile θ and diffeomorhism Φ. Then, the equivalence will follow. We consider the constants C_β, N_β, R_β and ε_β given by Definition 2.1 and we take $\varepsilon \in (0, \varepsilon_\beta]$. We observe

$$(2\pi\varepsilon)^{-\frac{d}{2}} \langle \mathrm{WP}^\varepsilon_{\Phi(z)}(\theta), \phi^\varepsilon \rangle = (2\pi\varepsilon)^{-\frac{3d}{2}} \int_{\mathbb{R}^d} \langle \mathrm{WP}^\varepsilon_{\Phi(z)}(\theta), g^\varepsilon_{z'} \rangle \langle g^\varepsilon_{z'}, \phi^\varepsilon \rangle dz' = I_1 + I_2$$

with

$$I_1 = (2\pi\varepsilon)^{-\frac{3d}{2}} \int_{|z'|>R_\beta} \langle \mathrm{WP}^\varepsilon_{\Phi(z)}(\theta), g^\varepsilon_{z'} \rangle \langle g^\varepsilon_{z'}, \phi^\varepsilon \rangle dz'.$$

Let us study I_1. Using (2.5), (2.6) and that $(\phi^\varepsilon)_{\varepsilon>0}$ is frequency localized at the scale $\beta \geq 0$, we deduce the existence of $c_\beta, N_\beta > 0$ such that we have

$$\begin{aligned}
|I_1| &\leq c_\beta\, \varepsilon^\beta\, (2\pi\varepsilon)^{-d} \int_{|z'|>R_\beta} \left| W[\theta, g^{i\mathbb{I}}] \left(\frac{z' - \Phi(z)}{\sqrt{\varepsilon}} \right) \right| \langle z' \rangle^{-N_\beta} dz' \\
&\leq c_\beta\, \|\theta\|_{\Sigma^n}\, \varepsilon^\beta\, (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^d} \left\langle \frac{z' - \Phi(z)}{\sqrt{\varepsilon}} \right\rangle^{-n} \langle z' \rangle^{-N_\beta} dz' \\
&\leq c_\beta\, \|\theta\|_{\Sigma^n}\, \varepsilon^\beta \int_{\mathbb{R}^d} \langle \zeta \rangle^{-n} \langle \Phi(z) + \sqrt{\varepsilon}\zeta \rangle^{-N_\beta} d\zeta,
\end{aligned}$$

where the constant c_β may have changed between two successive lines. We observe that Peetre's inequality (2.7) yields

$$\langle \Phi(z) + \sqrt{\varepsilon}\zeta \rangle^{-N_\beta} \leq 2^{\frac{N_\beta}{2}} \langle \Phi(z) \rangle^{-N_\beta} \langle \sqrt{\varepsilon}\zeta \rangle^{N_\beta} \leq 2^{\frac{N_\beta}{2}} \langle \Phi(z) \rangle^{-N_\beta} \langle \zeta \rangle^{N_\beta},$$

whence by choosing $n > 2d + 1 + N_\beta$,

$$|I_1| \leq c_\beta\, \|\theta\|_{\Sigma^{2d+1+N_\beta}}\, \varepsilon^\beta\, \langle \Phi(z) \rangle^{-N_\beta} \int_{\mathbb{R}^d} \langle \zeta \rangle^{-(2d+1)}\, d\zeta,$$

for some new constant $c_\beta > 0$. We conclude by observing that

$$\langle \Phi(z) \rangle^{-N_\beta} \leq \max\left(1, \frac{1}{a}\right)^{N_\beta} \langle z \rangle^{-N_\beta},$$

whence, by modifying c_β,

$$|I_1| \leq c_\beta\, \|\theta\|_{\Sigma^{2d+1+N_\beta}}\, \varepsilon^\beta\, \max\left(1, \frac{1}{a}\right)^{N_\beta} \langle z \rangle^{-N_\beta}.$$

We now study I_2. Using (2.5), (2.6), we write for $n \in \mathbb{N}$

$$|I_2| \leq \|\phi^\varepsilon\|_{L^2} (2\pi\varepsilon)^{-\frac{3d}{2}} \int_{|z'|\leq R_\beta} \left\langle \frac{z' - \Phi(z)}{\sqrt{\varepsilon}} \right\rangle^{-n} dz'.$$

We observe that if $|z| > 2aR_\beta$, then for $|z'| \leq R_\beta \leq \frac{1}{2a}|z|$, we have

$$|z' - \Phi(z)| \geq |\Phi(z)| - |z'| \geq \frac{1}{2a}|z|.$$

Therefore

$$\left\langle \frac{z' - \Phi(z)}{\sqrt{\varepsilon}} \right\rangle^{-n} = \left(\frac{\varepsilon}{\varepsilon + |z' - \Phi(z)|^2} \right)^{\frac{n}{2}} \leq (2a)^n \varepsilon^{\frac{n}{2}} |z|^{-n}.$$

Using that $(\phi^\varepsilon)_{\varepsilon>0}$ is a bounded family in L^2, we obtain that there exists a constant c' such that for $|z| > 2aR_\beta$ and any $n \in \mathbb{N}$,

$$|I_2| \leq c' \varepsilon^{\frac{n-3d}{2}} |z|^{-n}.$$

The proof of the last property follows the line of the proof of Lemma 2.6 combined with adapted change of variables. This terminates the proof. □

2.2.5. Frequency localized families and semi-classical pseudodifferential calculus. With these elements in hands, we can prove some properties that frequency localized families enjoy with respect to pseudodifferential calculus.

PROPOSITION 2.11. Let $(\phi^\varepsilon)_{\varepsilon>0}$ be a frequency localized family at the scale $\beta \geq 0$.

(1) For all semi-classical symbol $a \in \mathcal{C}_c^\infty(\mathbb{R}^{2d})$, the family $\left(\widehat{a}\,\phi^\varepsilon\right)_{\varepsilon>0}$ is frequency localized at the scale $\beta \geq 0$.
(2) For all subquadratic Hamiltonian $h \in \mathcal{C}^\infty(\mathbb{R} \times \mathbb{R}^{2d})$, for all $t, t_0 \in \mathbb{R}$, the vector-valued family $\left(\mathcal{U}_h^\varepsilon(t,t_0)\phi^\varepsilon\right)_{\varepsilon>0}$ is frequency localized at the scale $\beta \geq 0$.

PROOF. (1) We can assume without loss of generality that a is real-valued. We write

$$\mathcal{B}[\widehat{a}\phi^\varepsilon] = (2\pi\varepsilon)^{-d/2} \langle \widehat{a} g_z^\varepsilon, \phi^\varepsilon \rangle.$$

Since g_z^ε is a wave packet, we have

$$\widehat{a} g_z^\varepsilon = \widehat{a}\, \mathrm{WP}_z^\varepsilon(g^{i\mathbb{I}}) = \mathrm{WP}_z^\varepsilon(\mathfrak{g}_a^\varepsilon), \quad \mathfrak{g}_a^\varepsilon = \widehat{a(\sqrt{\varepsilon}\cdot + z)} g^{i\mathbb{I}}.$$

The function $\mathfrak{g}_a^\varepsilon$ is of Schwartz class on $\mathbb{R}^d$ and its Schwartz semi-norms are uniformly bounded in ε because a is compactly supported. We deduce from Proposition 2.10,

$$|\mathcal{B}[\widehat{a}\phi^\varepsilon]| \leq C_\beta\, \varepsilon^\beta\, \langle z \rangle^{-N_\beta} \|\mathfrak{g}_a^\varepsilon\|_{2d+1+N_\beta},$$

which concludes the proof.

(2) We write

$$\mathcal{B}\left[\mathcal{U}_h^\varepsilon(t,t_0)\phi^\varepsilon\right] = (2\pi\varepsilon)^{-d/2} \langle \mathcal{U}_h^\varepsilon(t,t_0) g_z^\varepsilon, \phi^\varepsilon \rangle.$$

Since g_z^ε is a wave packet, we have

$$\mathcal{U}_h^\varepsilon(t,t_0) g_z^\varepsilon = \mathrm{e}^{\frac{i}{\varepsilon}S(-t,z)} \mathrm{WP}^\varepsilon_{\Phi_h^{-t,0}(z)}(g^{\Gamma(-t,z)} + \sqrt{\varepsilon}\, r_z^\varepsilon(t)) \tag{2.13}$$

with the notations of the introduction. Besides, for all $n \in \mathbb{N}$, there exists a constant $C = C(n,t)$ such that $\|r_z^\varepsilon(t)\|_{\Sigma^n} \leq C(n,t)$. We deduce from Proposition 2.10,

$$|\mathcal{B}\left[\mathcal{U}_h^\varepsilon(t,t_0)\phi^\varepsilon\right]| \leq C_\beta\, \varepsilon^\beta\, \langle z \rangle^{-N_\beta} \|g^{\Gamma(t,z)} + \sqrt{\varepsilon} r_z^\varepsilon(t)\|_{2d+1+N_\beta},$$

which concludes the proof. □

REMARK 2.12. (1) The proof of Proposition 2.11 (1) extends to smooth functions a with polynomial growth

$$\exists N_0 \in \mathbb{N}, \ \ \forall \gamma \in \mathbb{N}^d, \ \ \forall z \in \mathbb{R}^{2d}, \ \ |\partial^\gamma a(z)| \leq \langle z \rangle^{N_0 - |\gamma|}$$

provided the integer N_β associated with the frequency localisation at the scale $\beta \geq 0$ of the family $(\phi_0^\varepsilon)_{\varepsilon>0}$ verifies $N_\beta > 2d + 1 + N_0$.

(2) The proof of Proposition 2.11 (2) also extends to adiabatic smooth matrix-valued Hamiltonian H that are subquadratic according to Definition 1.1. However, it is not clear whether the same result holds for Hamiltonians with crossings, either they are smooth as in this article or conical as in the Appendix of [**18**]. Indeed, even though one knows that $\mathcal{U}_H^\varepsilon(t,t_0)(g_z^\varepsilon \vec{V})$ is asymptotic to a wave packet, it is not clear that the remainder of the approximation has a wave-packet structure as in (2.13).

2.2.6. Frequencies localized families and Σ_ε^k-regularity. The size of N_β in Definition 2.1 gives an information about the regularity of the family.

LEMMA 2.13. *Let $(\phi^\varepsilon)_{\varepsilon>0}$ a frequency localized family at the scale $\beta \geq 0$, let $C_\beta, N_\beta, \varepsilon_\beta$ are the constants associated by Definition 2.1. Assume such that $k \in \mathbb{N}$ is such that $N_\beta > d + k + \frac{1}{2}$, then $(\phi^\varepsilon)_{0<\varepsilon<\varepsilon_\beta}$ is uniformly bounded in Σ_ε^k and there exists $c > 0$ independent of ε*

$$\|\phi^\varepsilon\|_{\Sigma_\varepsilon^k} \leq c(C_\beta + \|\phi_0^\varepsilon\|_{L^2}).$$

This Lemma is a simple consequence of Lemma 2.2 that we are going to prove now.

PROOF OF LEMMA 2.2. Let $k \in \mathbb{N}$ and $\alpha, \gamma \in \mathbb{N}^d$ such that $|\alpha| + |\gamma| = k$. we consider the operator

$$T_{\alpha,\gamma} = \mathcal{B} \circ (x^\alpha (\varepsilon D_x)^\gamma) \circ \mathcal{B}^{-1} \circ \langle z \rangle^{-k}.$$

The kernel of this operator is the function

$$\mathbb{R}^{4d} \ni (X,Y) \mapsto k^\varepsilon(X,Y) = (2\pi\varepsilon)^{-d} \langle g_X^\varepsilon, x^\alpha (\varepsilon D_x)^\gamma g_Y^\varepsilon \rangle \langle Y \rangle^{-k}.$$

Therefore, by (2.5), there exists a constant c_k such that

$$\int_{Y\in\mathbb{R}^{2d}} \sup_{X\in\mathbb{R}^{2d}} |k^\varepsilon(X,Y)| dY = (2\pi\varepsilon)^{-d} \int_{Y\in\mathbb{R}^{2d}} \sup_{X\in\mathbb{R}^{2d}} \left| W[g_{i\mathbb{I}}, g_{\varepsilon,Y}^{\alpha,\gamma}] \left(\frac{X-Y}{\sqrt{\varepsilon}} \right) \right| \langle Y \rangle^{-k} dY.$$

We deduce from (2.6) and (2.5) the existence of a constant $c_k > 0$ such that

$$\int_{Y\in\mathbb{R}^{2d}} \sup_{X\in\mathbb{R}^{2d}} |k^\varepsilon(X,Y)| dY \leq c_k.$$

Similarly, we have

$$\int_{X\in\mathbb{R}^{2d}} \sup_{Y\in\mathbb{R}^{2d}} |k^\varepsilon(X,Y)| dX = (2\pi\varepsilon)^{-d} \int_{X\in\mathbb{R}^{2d}} \sup_{Y\in\mathbb{R}^{2d}} \left| W[g_{i\mathbb{I}}, g_{\varepsilon,Y}^{\alpha,\gamma}] \left(\frac{X-Y}{\sqrt{\varepsilon}} \right) \right| \langle Y \rangle^{-k} dX \leq c_k.$$

Therefore, the Schur test yields the boundedness of $T_{\alpha,\gamma}$. One then deduces that for $f \in \mathcal{S}(\mathbb{R}^d)$, one has

$$\begin{aligned} \|x^\alpha (\varepsilon D_x)^\gamma f\|_{L^2(\mathbb{R}^d)} &= \|\mathcal{B}[x^\alpha (\varepsilon D_x)^\gamma f\|_{L^2(\mathbb{R}^{2d})} \\ &= \left\| T^{\alpha,\gamma} \left(\langle z \rangle^k \mathcal{B}[f] \right) \right\|_{L^2(\mathbb{R}^{2d})} \leq c_k \|\langle z \rangle^k \mathcal{B}[f]\|_{L^2(\mathbb{R}^{2d})}, \end{aligned}$$

which concludes the proof. □

Let us now prove Lemma 2.13

PROOF OF LEMMA 2.13. Since $N_\beta > d + k$, we have for $|z| > R_\beta$,

$$\langle z \rangle^k |\mathcal{B}[\phi^\varepsilon](z)| \leq \varepsilon^\beta C_\beta \langle z \rangle^{-N_\beta + k} \in L^2(\mathbb{R}^{2d}).$$

Moreover, $z \mapsto \langle z\rangle^{2k}|\mathcal{B}[\phi^\varepsilon](z)|^2$ is locally integrable and we can write

$$\begin{aligned}\|\langle z\rangle^k \mathcal{B}[\phi^\varepsilon](z)\|^2_{L^2(\mathbb{R}^{2d})} &\leq \langle R_\beta\rangle^{2k}\int_{|z|\leq R_\beta}|\mathcal{B}[\phi^\varepsilon](z)|^2dz + \varepsilon^{2\beta}C_\beta^2\int_{\mathbb{R}^{2d}}\langle z\rangle^{-2(N_\beta-k)}dz\\ &\leq \langle R_\beta\rangle^{2k}\|\mathcal{B}[\phi^\varepsilon](z)\|^2_{L^2(\mathbb{R}^{2d}} + \varepsilon^{2\beta}C_\beta^2\int_{\mathbb{R}^{2d}}\langle z\rangle^{-2(N_\beta-k)}dz\\ &\leq \langle R_\beta\rangle^{2k}\|\phi^\varepsilon\|^2_{L^2(\mathbb{R}^d)} + \varepsilon^{2\beta}C_\beta^2\int_{\mathbb{R}^{2d}}\langle z\rangle^{-2(N_\beta-k)}dz,\end{aligned}$$

whence the conclusion since the right hand side is bounded for $2(N_\beta - k) - 2d > 1$. □

2.3. Operators built on Bargmann transform

We investigate here the properties of the operators defined in (2.3). We shall investigate two cases :

(a) The case where the family $(\theta_z^\varepsilon)_{\varepsilon>0}$ is only uniformly bounded in $L^2(\mathbb{R}^d)$, which is a light assumption, but with uniform bounds in z on adequate semi-norms or norms.
(b) The case where the family $(\theta_z^\varepsilon)_{\varepsilon>0}$ is a wave packet (up to a phase), which is a stronger assumption on the family.

The thawed/frozen approximation operators belong to the type (b). We will consider operators of type (a) in the proofs of Theorems 1.15 and 1.18, when taking for the family $(\theta_z^\varepsilon)_{\varepsilon>0}$ a term of rest appearing in the expansion of the action of the propagator on a Gaussian wave packet. The Theorems 1.19 and 1.20 are consequences of Theorem 1.18.

In the Subsection 2.3.1, we analyze the action of these operators on Σ^k_ε spaces. In Subsection 2.3.2, we prove special properties of the operators corresponding to families of the type (b) involving classical quantities linked with the propagation of Gaussian wave packets by Schrödinger evolution.

2.3.1. Action in Σ^k_ε of operators built on Bargmann transform. This section is devoted to the proof of the following result.

THEOREM 2.14. *Let $\varepsilon_0 > 0$.*

(1) *Let $R > 0$. There exists $c_0 > 0$ such that for all measurable z-dependent family $(\theta_z^\varepsilon)_{\varepsilon>0}$, for all $k \in \mathbb{N}$, $\varepsilon \in (0, \varepsilon_0]$, for all $\phi \in L^2(\mathbb{R}^d)$*

$$\|\mathcal{J}[\theta_z^\varepsilon \mathbb{I}_{|z|<R}](\phi)\|_{\Sigma^k_\varepsilon} \leq (2\pi\varepsilon)^{-d}\, c_0\|\phi\|_{L^2}\, R^{2d}\sup_{|z|\leq R}\|\theta_z^\varepsilon\|_{\Sigma^k_\varepsilon}.$$

(2) *Assume $\theta_z^\varepsilon = \lambda^\varepsilon(z)\mathrm{WP}^\varepsilon_{\Phi(z)}(\theta)$ with $\theta \in \mathcal{S}(\mathbb{R}^d)$, $(\lambda^\varepsilon)_{\varepsilon>0}$ a bounded family in $L^\infty(\mathbb{R}^{2d}, \mathbb{C})$ and Φ a smooth diffeomorphism of $\mathbb{R}^{2d}$ such that*

$$\exists c > 0,\ \exists \ell \in \mathbb{N},\ \ \forall z \in \mathbb{R}^{2d},\ \ |J_\Phi(z)| + |J_\Phi(z)^{-1}| \leq c\langle z\rangle^\ell.$$

Then, there exists $c_0' > 0$ such that for all $\phi \in L^2(\mathbb{R}^d)$, $k \in \mathbb{N}$, $\varepsilon \in (0, \varepsilon_0]$,

$$\|\mathcal{J}[\theta_z^\varepsilon](\phi)\|_{\Sigma^k_\varepsilon} \leq c_0'\,\|\lambda_\varepsilon\|_{L^\infty}\|\phi\|_{L^2}\|\theta\|_{\Sigma^{k+\ell+2d+1}}.$$

The properties of the operators $\mathcal{J}[\theta_z^\varepsilon]$ extend to its adjoint (see (2.4)).

COROLLARY 2.15. Under the assumptions of Theorem 2.14, the family of operators $\mathcal{J}[\theta_z^\varepsilon]^*$ (see (2.4)) satisfies the same kind of estimates than the family $\mathcal{J}[\theta_z^\varepsilon]$.

A straightforward consequence of Theorem 2.14 and of Lemme 2.6 is given in the next statement.

COROLLARY 2.16. Assume $(\theta_z^\varepsilon)_{\varepsilon>0}$ satisfies the assumptions of Theorem 2.14 (2). Let $(\Phi^\varepsilon)_{\varepsilon>0}$ be a frequency localized family at the scale $\beta \geq 0$ and $C_\beta > 0$, $N_\beta \in \mathbb{N}$ be the constants associated with Definition 2.1. Then, for all $k > 0$ such that $N_\beta > k + d$, there exists a constant c_k such that for all $R > 0$,

$$\|\mathcal{J}[\theta_z^\varepsilon](\phi^\varepsilon - \phi^\varepsilon_{R,<})\|_{\Sigma^\varepsilon_k} \leq c_k\, C_\beta\, \varepsilon^\beta R^{-(N_\beta - k - d - \frac{1}{2})}.$$

where the family $(\phi^\varepsilon_{R,<})_{\varepsilon>0}$ is introduced in (2.8).

PROOF OF THEOREM 2.14. (1) The proof is similar to the first part of the proof of (1). By Cauchy-Schwartz inequality, for $x \in \mathbb{R}^d$, we have

$$\begin{aligned}
\|\mathcal{J}[\theta_z^\varepsilon \mathbb{I}_{|z|\leq R}](\phi^\varepsilon)\|_{L^2}^2 &\leq (2\pi\varepsilon)^{-2d}\|\phi^\varepsilon\|_{L^2}^2 \int_{|z|,|z'|\leq R} \left| \int_{x\in\mathbb{R}^d} \theta_z^\varepsilon(x)\overline{\theta_{z'}^\varepsilon}(x)dx \right| dz\, dz' \\
&\leq (2\pi\varepsilon)^{-2d}\|\phi^\varepsilon\|_{L^2}^2 \int_{|z|,|z'|\leq R} \|\theta_z^\varepsilon\|_{L^2}\|\theta_{z'}^\varepsilon\|_{L^2}\, dz\, dz' \\
&\leq c_1 R^{4d}(2\pi\varepsilon)^{-2d}\|\phi^\varepsilon\|_{L^2}^2 \sup_{|z|\leq 2R} \|\theta_z^\varepsilon\|_{L^2}^2
\end{aligned}$$

where $c_1 > 0$ is a universal constant.

(2) Let us first prove the L^2-estimate ($k = 0$). Let $(x, y) \mapsto k^\varepsilon(x, y)$ be the integral kernel of the operator $\mathcal{J}[\theta_z^\varepsilon]$. Since the Bargmann transform is an isometry, it is equivalent to consider the operator $\mathcal{B} \circ \mathcal{J}[\theta_z^\varepsilon] \circ \mathcal{B}^{-1}$, the kernel of which is the function $(\mathbb{R}^{2d})^2 \ni (X, Y) \mapsto k^\varepsilon_{\mathcal{B}}(X, Y)$ defined by

$$k^\varepsilon_{\mathcal{B}}(X,Y) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \overline{g}^\varepsilon_X(x) g^\varepsilon_Y(y) k^\varepsilon(x,y)dxdy = (2\pi\varepsilon)^{-2d} \int_{z\in\mathbb{R}^{2d}} \langle g^\varepsilon_z, g^\varepsilon_Y\rangle\langle g^\varepsilon_X, \theta^\varepsilon_z\rangle dz.$$

Therefore, by (2.5), $k^\varepsilon_{\mathcal{B}}(X, Y)$ satisfies

$$|k^\varepsilon_{\mathcal{B}}(X,Y)| \leq (2\pi\varepsilon)^{-2d} \int_{z\in\mathbb{R}^{2d}} \left| \lambda^\varepsilon(z) W[g^{i\mathbb{I}}, g^{i\mathbb{I}}]\left(\frac{Y-z}{\sqrt{\varepsilon}}\right) W[g^{i\mathbb{I}}, \theta]\left(\frac{\Phi(z)-X}{\sqrt{\varepsilon}}\right)\right| dz.$$

We deduce

$$\begin{aligned}
\int_{\mathbb{R}^{2d}} |k^\varepsilon_{\mathcal{B}}(X,Y)|dX &\leq M\|\lambda^\varepsilon\|_{L^\infty} \left(\int_{\mathbb{R}^{2d}} |W[g^{i\mathbb{I}}, g^{i\mathbb{I}}](z)|dz\right)\left(\int_{\mathbb{R}^{2d}} |W[g^{i\mathbb{I}}, \theta](X)|dX\right), \\
\int_{\mathbb{R}^{2d}} |k^\varepsilon_{\mathcal{B}}(X,Y)|dY &\leq M\|\lambda^\varepsilon\|_{L^\infty} \left(\int_{\mathbb{R}^{2d}} |W[g^{i\mathbb{I}}, g^{i\mathbb{I}}](Y)|dY\right)\left(\int_{\mathbb{R}^{2d}} |W[g^{i\mathbb{I}}, \theta](z) J_\Phi^{-1}(z)|dz\right),
\end{aligned}$$

with $M = \sup_{\varepsilon\in(0,1]} \|\lambda^\varepsilon\|_{L^\infty}$, and, by equations (2.6) and (2.10), we deduce the existence of $C > 0$ such that

$$\int_{\mathbb{R}^{2d}} |k^\varepsilon_{\mathcal{B}}(X,Y)|dX + \int_{\mathbb{R}^{2d}} |k^\varepsilon_{\mathcal{B}}(X,Y)|dY \leq CM\|\theta\|_{\Sigma^{2d+\ell+1}}.$$

We then conclude by Schur Lemma and obtain

$$\|\mathcal{B} \circ \mathcal{J}[\theta_z^\varepsilon] \circ \mathcal{B}^{-1}\|_{\mathcal{L}(L^2(\mathbb{R}^{2d}))} \leq CM\ \|\lambda^\varepsilon\|_{L^\infty}\, \|\theta\|_{\Sigma^{2d+\ell+1}},$$

and so it is for $\mathcal{J}[\theta_z^\varepsilon]$.

For concluding the proof when $k \neq 0$, we again use that for $\alpha, \gamma \in \mathbb{N}^d$ and $\phi \in \mathcal{S}(\mathbb{R}^d)$,

$$x^\alpha(\varepsilon\partial_x)^\gamma \mathcal{J}[\theta_z^\varepsilon] = \mathcal{J}[x^\alpha(\varepsilon\partial_x)^\gamma \theta_z^\varepsilon],$$

and the additional observation

$$x^\alpha(\varepsilon\partial_x)^\gamma \mathrm{WP}_z^\varepsilon(\theta) = \mathrm{WP}^\varepsilon\left((q + \sqrt{\varepsilon}x)^\alpha(p + \sqrt{\varepsilon}D_x)^\gamma\theta\right).$$

We then conclude by observing that, as in the estimate (2.10), we have for all $n \in \mathbb{N}$,

$$\|(q+\sqrt{\varepsilon}x)^\alpha(p+\sqrt{\varepsilon}D_x)^\gamma\theta\|_{\Sigma^n} \leq \langle z\rangle^k \|\theta\|_{\Sigma^{n+k}}.$$

This finishes the proof. □

Theorem 2.14 has consequences for the thawed/frozen approximation operators introduced in Chapter 1.

COROLLARY 2.17. Assume the Hamiltonian $H^\varepsilon = H_0 + \varepsilon H_1$ satisfies Assumptions 1.3 and 1.4. Let $k \in \mathbb{N}$ and $t \in I$.

(1) The families of operators $\left(\mathcal{J}^{t,t_0}_{\ell,\mathrm{th/fr}}\right)_{\varepsilon>0}$ defined in (1.22) and (1.25) are bounded families in $\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^m),\Sigma^k_\varepsilon(\mathbb{R}^d,\mathbb{C}^m))$.
(2) Assume moreover that the compact K satisfies Assumptions 1.17. Then, the family of operators $\left(\mathcal{J}^{t,t_0}_{1,2,\mathrm{th/fr}}\right)_{\varepsilon>0}$ defined in (1.36) and (1.37) are bounded families in the space $\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^m),\Sigma^k_\varepsilon(\mathbb{R}^d,\mathbb{C}^m))$.

REMARK 2.18. If one assumes that $(t,z) \mapsto \partial_t f + \{v,f\}$ is bounded from below and $\partial_t f$ is bounded, then one can replace the compact K by $\mathbb{R}^{2d}$ in the definition of $\mathcal{J}^{t,t_0}_{1,2,\mathrm{th}}$ and one obtains a bounded family in $\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^m),\Sigma^k_\varepsilon(\mathbb{R}^d,\mathbb{C}^m))$.

PROOF. Let $\ell \in \{1,2\}$. Let us first discuss $\mathcal{J}^{t,t_0}_{\ell,\mathrm{th}}$. We write $\mathcal{J}^{t,t_0}_{\ell,\mathrm{th}} = \mathcal{J}[\theta^\varepsilon_z]$ with

$$\theta^\varepsilon_z = \lambda^\varepsilon(z)\mathrm{WP}^\varepsilon_{\Phi^{t,t_0}_\ell(z)}(g^\Gamma_\ell(t,t_0,z)) \text{ and } \lambda^\varepsilon(z) = \mathrm{e}^{\frac{i}{\varepsilon}S_\ell(t,t_0,z)}\vec{V}_\ell(t,t_0,z).$$

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

$$\|\vec{V}_\ell(t,t_0,z)\|_{\mathbb{C}^m} = \|\vec{V}_\ell(t_0,t_0,z)\|_{\mathbb{C}^m} = \|\pi_\ell(t_0)\vec{V}\|_{\mathbb{C}^m} \leq \|\vec{V}\|_{\mathbb{C}^{m,m}}$$

which is independent of z. Therefore, the family $(\lambda^\varepsilon)_{\varepsilon>0}$ is bounded in $L^\infty(\mathbb{R}^{2d})$.

Besides, by Proposition A.4, the flow map $(t,z) \mapsto \Phi^{t,t_0}_\ell(z)$ satisfies the assumptions of (2) of Theorem 2.14. Similarly, the map $(t,z) \mapsto \Gamma_\ell(t,t_0,z)$ is bounded on $I \times \mathbb{R}^{2d}$. Therefore, for any $N \in \mathbb{N}$, there exists $c_{N,t_0,T} > 0$ such that

$$\forall t \in I, \ \ \|x^\alpha \partial^\beta_x g^\Gamma_\ell(t,t_0,\cdot)\|_{\Sigma^N} \leq c_{N,t_0,T}.$$

We then conclude by (2) of Theorem 2.14. The proof for $\mathcal{J}^{t,t_0}_{\ell,\mathrm{fr}}$ follows exactly the same lines.

The proof for $\mathcal{J}^{t,t_0}_{1,2,\mathrm{th/fr}}$ requires additional observations. We need to consider the transition coefficient map $(t,z) \mapsto \tau_{1,2}(t,t_0,z)$ (see (1.29)) and the matrix-valued maps $z \mapsto \Gamma^\flat(t_0,z)$ (see (1.32)), which requires the analysis of the function parametrizing the crossing (see (1.27) and (1.28)),

$$z \mapsto \left(\alpha^\flat(t_0,z), \beta^\flat(t_0,z), \mu^\flat(t_0,z)\right). \tag{2.14}$$

By the condition (1.4) of Assumption 1.3, with $n_0 = 0$, the derivatives of $(t,z) \mapsto f(t,z)$ are uniformly bounded in z. Moreover, if one takes z in a compact K that satisfies Assumptions 1.17, one has the additional properties that $\partial_t f$ and $\mu^\flat$ are bounded below. As a consequence $z \mapsto \alpha^\flat(t_0,z)$, $z \mapsto \beta^\flat(t_0,z)$ and $z \mapsto \mu^\flat(t_0,z)$ are bounded functions on $\mathbb{R}^{2d}$ for all $t \in I$, the map defined in (2.14) is smooth. One then argues as before by including the coefficient $\tau_{1,2}(t,t_0,z)$ in the definition of λ^ε and the result follows from Theorem 2.14 (2). □

2.3.2. Some properties of operators built on Bargmann transform via families with wave packet structure. In this section we analyze the properties of the operators $\mathcal{J}[\theta_z^\varepsilon]$ when $(\theta_z^\varepsilon)_{\varepsilon>0}$ is of the form

$$\theta_z^\varepsilon = \mathrm{e}^{\frac{i}{\varepsilon}S(z)}u(z)\mathrm{WP}^\varepsilon_{\Phi(z)}(\theta(z,\cdot)), \tag{2.15}$$

where $\theta \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathcal{S}(\mathbb{R}^d))$, $S \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{R})$, $u \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C})$ and Φ a smooth diffeomorphism sarisfying the assumptions of Theorem 2.14. We are interested in the case where S and Φ are linked in the same manner as when they are the flow map and the action associated with classical trajectories. Therefore, we consider the following set of Assumptions.

Assumption 2.19. Let $S \in \mathcal{C}^\infty(\mathbb{R}^{2d}_z, \mathbb{R})$, $u \in \mathcal{C}^\infty(\mathbb{R}^{2d}_z, \mathbb{C})$ and Φ a smooth diffeomorphism. We assume the following properties:

(i) There exists $c > 0$ and $\ell \in \mathbb{N}$ such that

$$\forall z \in \mathbb{R}^{2d}, \ \ |J_\Phi(z)| + |J_\Phi(z)^{-1}| \leq c\langle z\rangle^\ell.$$

(ii) Setting $\Phi(z) = (\Phi_q(z), \Phi_p(z))$ and

$$\partial_z\Phi = \begin{pmatrix} A(z) & B(z) \\ C(z) & D(z) \end{pmatrix},$$

we have

$$\nabla_q S(z) = -p + A(z)\Phi_p(z) \ \text{ and } \ \nabla_p S(z) = B(z)\Phi_p(z), \ \ z = (q,p).$$

(iii) For all $k \in \mathbb{N}$, the z-dependent seminorms $\|u(z)\|_{\Sigma^k}$ and $\sup_{|\alpha|\leq k}\|\partial_z^\alpha S\|_{L^\infty}$ are uniformly bounded in z.

The next technical lemma will be useful for proving our main results. It contains all the information needed to pass from the thawed approximation to the frozen one.

Lemma 2.20. *Let $\mathfrak{d} = \partial_q - i\partial_p$. Let $\theta \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathcal{S}(\mathbb{R}^d))$, $S \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{R})$, $u \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C})$ and Φ be a smooth diffeomorphism satisfying Assumptions 2.19. Then, the following equality between operators in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma^k_\varepsilon)$ holds for $k \in \mathbb{N}$:*

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left((\mathfrak{d}\Phi_p x - \mathfrak{d}\Phi_q D_x)\theta\right)\right] = -i\sqrt{\varepsilon}\,\mathcal{J}\left[\mathfrak{d}u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi(\theta)\right] - i\sqrt{\varepsilon}\,\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi(\mathfrak{d}\theta)\right].$$

Note that with the notation of Lemma 2.20, we have

$$\mathfrak{d}\Phi_p(z) = C(z) - iD(z) \ \text{ and } \ \mathfrak{d}\Phi_q(z) = A(z) - iB(z). \tag{2.16}$$

Besides, if condition (ii) of Assumption 2.19 is satisfied, then the equality of Remark 2.20 holds formally. The condition (i) ensures the boundedness of the operators involved in the estimates.

Proof. The integral kernel of the operator $\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi(\theta)\right]$ is the function

$$(x,y) \mapsto \int_{z\in\mathbb{R}^{2d}} k(z,x,y)dz$$

defined by

$$k(z,x,y) = u(z,x)\mathrm{e}^{\frac{i}{\varepsilon}S(z)}\overline{g^\varepsilon_z(y)}\mathrm{WP}^\varepsilon_{\Phi(z)}(\theta(z,\cdot))(x), \ \ (x,y) \in \mathbb{R}^d, \ \ z \in \mathbb{R}^{2d}.$$

We aim at calculating $\mathfrak{d}k$. We observe for $z=(q,p)\in\mathbb{R}^{2d}$, $y\in\mathbb{R}^d$ and

$$\begin{aligned}\mathfrak{d}S(z)&=-p+(A(z)-iB(z))\mathfrak{d}\Phi_p(z),\\ \mathfrak{d}\left(\overline{g_z^\varepsilon(y)}\right)&=\frac{i}{\varepsilon}[(\mathfrak{d}p+i\mathfrak{d}q)(y-q)+p\mathfrak{d}q]g_z^\varepsilon(y)=\frac{i}{\varepsilon}p\,g_z^\varepsilon(y),\\ \mathfrak{d}\left(\mathrm{WP}^\varepsilon_{\Phi(z)}(\theta(z,\cdot))\right)&=\mathrm{WP}^\varepsilon_{\Phi(z)}(\mathfrak{d}\theta(z,\cdot))+\frac{i}{\sqrt{\varepsilon}}\mathrm{WP}^\varepsilon_{\Phi(z)}\left((\mathfrak{d}\Phi_p(z)x-\mathfrak{d}\Phi_q(z)D_x)\theta(z,\cdot)\right)\\ &\quad-\frac{i}{\varepsilon}\mathrm{WP}^\varepsilon_{\Phi(z)}\left((A(z)-iB(z))\mathfrak{d}\Phi_p(z)\theta(z,\cdot)\right).\end{aligned}$$

We obtain

$$\begin{aligned}\mathfrak{d}k(z,x,y)=\mathrm{e}^{\frac{i}{\varepsilon}S(z)}\Big(&\mathfrak{d}u(z,x)\,\overline{g_z^\varepsilon(y)}\,\mathrm{WP}^\varepsilon_{\Phi(z)}(\theta(z,\cdot))(x)+u(z,x)\,\overline{g_z^\varepsilon(y)}\,\mathrm{WP}^\varepsilon_{\Phi(z)}(\mathfrak{d}\theta(z,\cdot))(x)\\ &+\frac{i}{\sqrt{\varepsilon}}u(z,x)\,\overline{g_z^\varepsilon(y)}\,\mathrm{WP}^\varepsilon_{\Phi(z)}\left((\mathfrak{d}\Phi_p(z)x-\mathfrak{d}\Phi_q(z)D_x)\theta(z,\cdot)\right)(x)\Big)\end{aligned}$$

The result then follows from the integration in $z\in\mathbb{R}^{2d}$. □

The case of Gaussian functions θ is of particular interest. Indeed, if $\theta(z,\cdot)=g^{\Theta(z)}$ with $\Theta\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathfrak{S}^+(d))$, we have for $x\in\mathbb{R}^d$ and $z\in\mathbb{R}^{2d}$,

$$(\mathfrak{d}\Phi_p(z)x-\mathfrak{d}\Phi_q(z)D_x)g^{\Theta(z)}(x)=(\mathfrak{d}\Phi_p(z)-\mathfrak{d}\Phi_q(z)\Theta(z))x\,g^{\Theta(z)}(x). \tag{2.17}$$

We set

$$M_\Theta(z):=\mathfrak{d}\Phi_p(z)-\mathfrak{d}\Phi_q(z)\Theta(z).$$

By (2.16), we have the equality between matrix-valued functions

$$M_\Theta=(C-iD)-(A-iB)\Theta=(A-iB)\left[(A-iB)^{-1}(C-iD)-\Theta\right]. \tag{2.18}$$

Note that this matrix M_Θ is invertible because $(A+iB)^{-1}(C+iD)-\overline{\Theta}\in\mathfrak{S}^+(d)$ (as the sum of two elements of $\mathfrak{S}^+(d)$). These observations are in the core of the proof of the next result which is a corollary of Lemma 2.20, when applied to Gaussian profiles.

Corollary 2.21. Let $k\in\mathbb{N}$. Let $\Theta\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathfrak{S}^+(d))$ such that M_Θ is bounded together with its inverse, let $S\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{R})$, $u\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{C})$ and Φ a smooth diffeomorphism satisfying Assumptions 2.19. Then, in $\mathcal{L}(L^2(\mathbb{R}^d),\Sigma^k_\varepsilon(\mathbb{R}^d))$, we have

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left(xg^\Theta\right)\right]=O(\sqrt{\varepsilon}). \tag{2.19}$$

Besides, for all $L\in\mathcal{C}^\infty(\mathbb{R}^{2d},\mathbb{C}^{d,d})$, in $\mathcal{L}(L^2(\mathbb{R}^d),\Sigma^k_\varepsilon(\mathbb{R}^d))$, we have

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left(Lx\cdot xg^\Theta\right)\right]=\frac{1}{i}\,\mathcal{J}\left[u\,\mathrm{Tr}\left(L\,M_\Theta^{-1}\,\mathfrak{d}\Phi_q\right)\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^\varepsilon_\Phi\left(g^\Theta\right)\right]+O(\varepsilon). \tag{2.20}$$

with

$$LM_\Theta^{-1}\mathfrak{d}\Phi_q=L\left[(A-iB)^{-1}(C-iD)-\Theta\right]^{-1}.$$

Remark 2.22. (1) This result has an interesting consequence concerning the pseudodifferential calculus. Indeed, for a real-valued and with bounded derivatives, in view of (2.4)

$$\widehat{a}=\mathcal{J}(\widehat{a}g_z^\varepsilon)=\mathcal{J}[a(z)g_z^\varepsilon]+\sqrt{\varepsilon}\widetilde{\mathcal{J}}\left(\mathrm{WP}^\varepsilon_z\left(\nabla a(z)\cdot\begin{pmatrix}x\\D_x\end{pmatrix}g^{i\mathbb{I}}\right)\right)+O(\varepsilon),$$

where we have used the properties of wave packets. Using $\nabla g^{i\mathbb{I}} = xg^{i\mathbb{I}}$ allows to conclude by Corollary 2.21

$$\widehat{a} = \mathcal{J}[a(z)g_z^\varepsilon] + O(\varepsilon)$$

in any space Σ_ε^k. This was already proved in [**56**].

(2) More can be said about the $\sqrt{\varepsilon}$-order term on the right-hand side of (2.19). By revisiting the proof below, one sees that there exists a real-valued smooth function $z \mapsto c(z)$ such that

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}_\Phi^\varepsilon\left(xg^\Theta\right)\right] = -i\sqrt{\varepsilon}\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}_\Phi^\varepsilon\left(c(z)g^\Theta\right)\right] + O(\varepsilon).$$

Remark 2.23. The latter remark allows to prove Remark 1.13 (1). We observe that in L^2,

$$\psi = \widehat{a\vec{V}}(\widehat{(a^{-1})}f) + O(\varepsilon) \text{ and } \mathcal{U}_H^\varepsilon(t,t_0)\psi = \mathcal{U}_H^\varepsilon(t,t_0)\left(\widehat{a\vec{V}}(\widehat{(a^{-1})}f)\right) + O(\varepsilon)$$

Turning the pair $(\vec{V}, f)$ into $(\widehat{a\vec{V}}, \widehat{(a^{-1})}f)$ consists in replacing $\vec{V}_\ell(t,t_0,z)$ by

$$\vec{V}_{\ell,a}(t,t_0,z) := \mathcal{R}_\ell(t,t_0,z)\pi_\ell(t_0,z)(a(z)\vec{V}(z)) = a(z)\vec{V}_\ell(t,t_0,z).$$

The two thawed Gaussian approximation constructed in that two different manner then differs one from the other by $O(\varepsilon)$: the analysis developed in Section 2.3 (in particular, the arguments of Remark 2.22) shows that in $\Sigma_\varepsilon^k(\mathbb{R}^d)$,

$$\mathcal{J}_{\ell,\mathrm{th}}^{t,t_0}(\widehat{\vec{V}}f) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} \mathrm{e}^{\frac{i}{\varepsilon}S_\ell(t,t_0,z)}\langle g_z^\varepsilon, \widehat{(a^{-1})}f\rangle \vec{V}_{\ell,a}(t,t_0,z) g_{\Phi_\ell^{t,t_0}(t,z)}^{\Gamma_\ell(t,t_0,z),\varepsilon} dz + O(\varepsilon).$$

Proof of Corollary 2.21. One uses (2.17) and the first relation of Lemma 2.20 that we apply to $\theta = g^\Theta$. It gives that in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma_\varepsilon^k(\mathbb{R}^d))$,

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}_\Phi^\varepsilon\left(xg^\Theta\right)\right] = \mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}_\Phi^\varepsilon\left(M_\Theta^{-1}(\mathfrak{d}\Phi_p x - \mathfrak{d}\Phi_q D_x)g^\Theta\right)\right] = O(\sqrt{\varepsilon}),$$

whence (2.19).

Secondly, if l $L \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^{d,d})$, we consider the matrix L' such that $L = {}^tL'M_\Theta$. We observe that

$$(\mathfrak{d}\Phi_p x - \mathfrak{d}\Phi_q D_x)\cdot(L'xg^\Theta) = \left(({}^tL'(\mathfrak{d}\Phi_p - \mathfrak{d}\Phi_q\Theta))x\cdot x - \mathrm{Tr}({}^tL'\mathfrak{d}\Phi_q)\right)g^\Theta.$$

It remains to prove that in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma_\varepsilon^k(\mathbb{R}^d))$, we have

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}_\Phi^\varepsilon\left((\mathfrak{d}\Phi_p x - \mathfrak{d}\Phi_q D_x)\cdot(L'xg^\Theta)\right)\right] = O(\varepsilon). \tag{2.21}$$

We first apply Lemma 2.20 to the function $\theta = L'xg^\Theta$ and we write

$$\begin{aligned}&\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}_\Phi^\varepsilon\left((\mathfrak{d}\Phi_p x - \mathfrak{d}\Phi_q D_x)\cdot(L'xg^\Theta)\right)\right]\\ &\quad = -i\sqrt{\varepsilon}\mathcal{J}\left[\mathfrak{d}u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}_\Phi^\varepsilon\left(L'xg^\Theta\right) + u\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}_\Phi^\varepsilon\left(L'x\,\mathfrak{d}(g^\Theta)\right)\right].\end{aligned}$$

We use the relation (2.19) and obtain in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma_\varepsilon^k(\mathbb{R}^d))$,

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}_\Phi^\varepsilon\left((\mathfrak{d}\Phi_p x - \mathfrak{d}\Phi_q D_x)\cdot(L'xg^\Theta)\right)\right] = -i\sqrt{\varepsilon}\mathcal{J}\left[u\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}_\Phi^\varepsilon\left(L'x\,\mathfrak{d}(g^\Theta)\right)\right] + O(\varepsilon). \tag{2.22}$$

We calculate

$$\mathfrak{d}(g^\Theta) = \frac{\mathfrak{d}c_\Theta}{c_\Theta}g^\Theta + (\mathfrak{d}\Theta x\cdot x)g^\Theta,$$

with

$$(\mathfrak{d}\Theta x\cdot x)\,x\,g^{\Theta} = (\mathfrak{d}\Theta x\cdot x)M_{\Theta}^{-1}(\mathfrak{d}\Phi_p x-\mathfrak{d}\Phi_q D_x)g^{\Theta}$$
$$= M_{\Theta}^{-1}(\mathfrak{d}\Phi_p x-\mathfrak{d}\Phi_q D_x)\left((\mathfrak{d}\Theta x\cdot x)g^{\Theta}\right) - 2M_{\Theta}^{-1}\mathfrak{d}\Phi_q\mathfrak{d}\Theta\, x\, g^{\Theta}.$$

Therefore, there exists matrices L_1 and L_2 such that, setting $\tilde{\theta}=(\mathfrak{d}\Theta x\cdot x)g^{\Theta}$, we have

$$L'x\,\mathfrak{d}(g^{\Theta}) = L_1 x g^{\Theta} + L_2(\mathfrak{d}\Phi_p x-\mathfrak{d}\Phi_q D_x)\tilde{\theta}.$$

We deduce

$$\mathcal{J}\left[u\,\mathrm{e}^{\frac{i}{\varepsilon}S}\,\mathrm{WP}^{\varepsilon}_{\Phi}\left((\mathfrak{d}\Phi_p x-\mathfrak{d}\Phi_q D_x)\cdot(L'xg^{\Theta})\right)\right] = -i\sqrt{\varepsilon}\mathcal{J}[L_1 x g^{\Theta}] - i\sqrt{\varepsilon}\mathcal{J}[L_2(\mathfrak{d}\Phi_p x-\mathfrak{d}\Phi_q D_x)\tilde{\theta}]$$

and we obtain (2.21) by Lemma 2.20 applied to the function $\tilde{\theta}$, and by the relation (2.19), which concludes the proof □

2.3.3. Operators built on Bargmann transform via classical quantities. We now apply the results of the preceding section to the diffeomorphism Φ given by a flow map associated to a Hamiltonian h. We are going to derive the results induced by Lemma 2.20 and Corollary 2.21 for time dependent quantities after integration in time. We will use the resulting formula for the Hamiltonians h_1 and h_2 associated with the matrix-valued Hamiltonian H^{ε}.

LEMMA 2.24. *Let $k\in\mathbb{N}$. Let h be a subquadratic Hamiltonian on $I\times\mathbb{R}^{2d}$, $I=[t_0,t_0+T]$. We consider*

1. *the classical quantities associated to h as in Section 1.3 on the interval I:*
$$z\mapsto S(t,z),\Phi^{t,t_0}(z),F(t,t_0,z),$$
2. *a smooth function defined on $I\times\mathbb{R}^{2d}$, bounded and with bounded derivatives, $(t,z)\mapsto u(t,z)$,*
3. *a smooth map from $I\times\mathbb{R}^{2d}$ into $\mathcal{S}(\mathbb{R}^d)$, $(t,z)\mapsto\theta(t,z)$,*
4. *a smooth function from $\mathbb{R}^{2d}$ into I, $z\mapsto t^{\flat}(z)$.*

Then, for all $\chi\in\mathcal{C}_0^{\infty}(I)$, we have the following equality between operators in $\mathcal{L}(L^2(\mathbb{R}^d),\Sigma^k_{\varepsilon}(\mathbb{R}^d))$,

$$\int_{\mathbb{R}}\chi(t)\mathcal{J}\left[\mathbb{I}_{t>t^{\flat}(z)}u(t)\,\mathrm{e}^{\frac{i}{\varepsilon}S(t)}\,\mathrm{WP}^{\varepsilon}_{\Phi^{t,t_0}}\left((\mathfrak{d}\Phi^t_p x-\mathfrak{d}\Phi^{t,t_0}_q D_x)\theta(t)\right)\right]dt$$
$$= i\sqrt{\varepsilon}\int_{\mathbb{R}}\mathcal{J}\left[\mathbb{I}_{t>t^{\flat}(z)}\mathfrak{d}u(t)\,\mathrm{e}^{\frac{i}{\varepsilon}S(t)}\,\mathrm{WP}^{\varepsilon}_{\Phi^{t,t_0}}(\theta(t))\right]dt$$
$$+ i\sqrt{\varepsilon}\int_{\mathbb{R}}\chi(t)\mathcal{J}\left[\mathbb{I}_{t>t^{\flat}(z)}u(t)\,\mathrm{e}^{\frac{i}{\varepsilon}S(t)}\,\mathrm{WP}^{\varepsilon}_{\Phi^{t,t_0}}(\mathfrak{d}\theta(t))\right]dt$$
$$- i\sqrt{\varepsilon}\mathcal{J}\left[\chi(t^{\flat})\,\mathfrak{d}t^{\flat}\,u(t^{\flat})\;\mathrm{e}^{\frac{i}{\varepsilon}S(t^{\flat})}\,\mathrm{WP}^{\varepsilon}_{\Phi^{t^{\flat},t_0}}(\theta(t^{\flat}))\right].$$

Note that the result of this lemma is an equality. Thus, we have not emphasized assumptions that make these operators bounded. One could for example assume global boundedness of all the quantities involve and of their derivatives, or, what would be enough, that θ is compactly supported in z.

We also emphasize that the functions denoted by $(\chi\circ t^{\flat})\,u(t^{\flat})\;\mathrm{e}^{\frac{i}{\varepsilon}S(t^{\flat})}\,\mathrm{WP}^{\varepsilon}_{\Phi^{t^{\flat}}}(\theta(t^{\flat}))$ is the map

$$z\mapsto\chi\left(t^{\flat}(z)\right)\;u\left(t^{\flat}(z),z\right)\;\mathrm{e}^{\frac{i}{\varepsilon}S\left(t^{\flat}(z),z\right)}\,\mathrm{WP}^{\varepsilon}_{\Phi^{t^{\flat}(z),t_0(z)}}\left(\theta\left(t^{\flat}(t),z\right)\right).$$

Note also that, by construction, the flow map Φ^{t,t_0} and the action S satisfy Assumptions 2.19 (see [**13, 53, 43**]).

PROOF. The proof follows the lines of the one of Lemma 2.20, using the relation

$$\mathfrak{d}\left(\mathbb{I}_{t>t^\flat(z)}\right) = \mathfrak{d}t^\flat(z)\delta(t-t^\flat(z)) \tag{2.23}$$

that produces an additional term. □

As a Corollary, for Gaussian profiles, we have the following Corollary.

COROLLARY 2.25. With the same assumptions as in Lemma 2.24, we additionally assume $\theta(t) = g^{\Theta(t)}$, with $\Theta \in \mathcal{C}^\infty(I \times \mathbb{R}^{2d}, \mathcal{S}^+(d))$. Then, for all $L \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^{d,d})$, we have the following equality in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma^k_\varepsilon(\mathbb{R}^d))$,

$$\begin{aligned}&\int \chi(t)\mathcal{J}\left[\mathbb{I}_{t>t^\flat(z)} u\, \mathrm{e}^{\frac{i}{\varepsilon}S(t,t_0)}\, \mathrm{WP}^\varepsilon_{\Phi^{t,t_0}}\left(Lx\cdot x g^{\Theta(t,t_0)}\right)\right] dt\\ &\quad = \frac{1}{i}\int \chi(t)\mathcal{J}\left[1_{t>t^\flat(z)}\tilde{u}(t,t_0)\, \mathrm{e}^{\frac{i}{\varepsilon}S(t,t_0)}\, \mathrm{WP}^\varepsilon_{\Phi^{t,t_0}}\left(g^{\Theta(t,t_0)}\right)\right] dt + O(\varepsilon)\end{aligned}$$

with $\widetilde{u}(t,t_0) = \mathrm{Tr}\left(L\left[(A(t,t_0)-iB(t,t_0))^{-1}(C(t,t_0)-iD(t,t_0)) - \Theta(t,t_0)\right]^{-1}\right)$.

PROOF. The proof follows the lines of the one of Corollary 2.21, using the relation (2.23). □

CHAPTER 3

Convergence of the thawed and the frozen Gaussian approximations

3.1. Strategy of the proofs

Our aim in this section is to prove the initial value representations of Theorems 1.15. We also explain the overall strategy that is also used for proving Theorems 1.18, 1.19 and 1.20.

Let $k \in \mathbb{N}$. Let $\psi_0^\varepsilon = \widehat{\vec{V}}\phi_0^\varepsilon$ be as in Assumption 1.9 with $\phi_0^\varepsilon \in L^2$ frequency localized at the scale $\beta \geq 0$ with $N_\beta > d + k + \frac{1}{2}$ (which implies $\phi_0^\varepsilon \in \Sigma_\varepsilon^k$. Without loss of generality, we assume $\vec{V} = \pi_\ell(t_0)\vec{V}$ for some $\ell \in \{1, 2\}$ that is now fixed.

We start with the Gaussian frame equality (2.2)

$$\psi_0^\varepsilon = (2\pi\varepsilon)^{-d} \int_{z\in\mathbb{R}^{2d}} \langle g_z^\varepsilon, \widehat{\vec{V}}\phi_0^\varepsilon\rangle g_z^\varepsilon \, dz.$$

Writing $\langle g_z^\varepsilon, \widehat{\vec{V}}\phi_0^\varepsilon\rangle = \langle \widehat{\overline{\vec{V}}} g_z^\varepsilon, \phi_0^\varepsilon\rangle$ and using Remark 2.22, we have in Σ_ε^k,

$$\psi_0^\varepsilon = \mathcal{J}[\widehat{\overline{\vec{V}}}(z)g_z^\varepsilon]^*(\phi_0^\varepsilon) + O(\varepsilon) = \mathcal{J}[\widehat{\vec{V}}(z)g_z^\varepsilon](\phi_0^\varepsilon) + O(\varepsilon\|\phi_0^\varepsilon\|_{L^2}).$$

Corollary 2.16 yields that, in Σ_ε^k, we have

$$\begin{aligned}\psi_0^\varepsilon &= \mathcal{J}[\mathbb{I}_{|z|<R}\widehat{\vec{V}}(z)g_z^\varepsilon](\phi_0^\varepsilon) + O(\varepsilon\|\phi_0^\varepsilon\|_{L^2}) + O(\varepsilon^\beta C_\beta R^{-n_\beta}) \\ &= \mathcal{J}[\widehat{\vec{V}}(z)g_z^\varepsilon]((\phi_0^\varepsilon)_{R,<}) + O(\varepsilon\|\phi_0^\varepsilon\|_{L^2}) + O(\varepsilon^\beta C_\beta R^{-n_\beta})\end{aligned}$$

with the notations of Corollary 2.16 and setting $n_\beta = N_\beta - k - d - \frac{1}{2} > 0$.

Now that the data has been written in a convenient form, we apply the propagator $\mathcal{U}_H^\varepsilon(t, t_0)$ and we take advantage of its boundedness in $\mathcal{L}(\Sigma_\varepsilon^k)$ to write

$$\begin{aligned}\mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon &= (2\pi\varepsilon)^{-d} \int_{|z|\leq R} \langle g_z^\varepsilon, \phi_0^\varepsilon\rangle \left(\mathcal{U}_H^\varepsilon(t,t_0)\vec{V}(z)g_z^\varepsilon\right) dz + O(\varepsilon\|\phi_0^\varepsilon\|_{L^2}) + O(\varepsilon^\beta\, C_\beta\, R^{-n_\beta}) \\ &= \mathcal{J}\left[\mathbb{I}_{|z|\leq R}\mathcal{U}_H^\varepsilon(t,t_0)\vec{V}(z)g_z^\varepsilon\right](\phi_0^\varepsilon) + O(\varepsilon\|\phi_0^\varepsilon\|_{L^2}) + O(\varepsilon^\beta\, C_\beta\, R^{-n_\beta}).\end{aligned}$$

We then use the description of the propagation of wave packets by $\mathcal{U}_H^\varepsilon(t, t_0)$, as stated in Theorem 1.21: for $N \geq d + 1$, in $\Sigma_\varepsilon^k(\mathbb{R}^d)$, we have

$$\mathcal{U}_H^\varepsilon(t,t_0)\vec{V}(z)g_z^\varepsilon = \psi_\ell^{\varepsilon,N}(t) + O(\varepsilon^N).$$

Therefore, by (1) of Theorem 2.14 in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma_\varepsilon^k(\mathbb{R}^d, \mathbb{C}^m))$,

$$\mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon = \mathcal{J}\left[\mathbb{I}_{|z|\leq R}\ \psi_\ell^{\varepsilon,N}(t)\right] + O(\varepsilon^{N-d}\, R^d\, \|\phi_0^\varepsilon\|_{L^2}) + O(\varepsilon^\beta\, C_\beta\, R^{-n_\beta}) \tag{3.1}$$

Besides, using that $\psi_\ell^{\varepsilon,N}(t)$ is a linear combination of wave packets and considering the explicit formula of Theorem 1.21, (2) of Theorem 2.14 implies that in $\mathcal{L}(\Sigma^k_\varepsilon(\mathbb{R}^d,\mathbb{C}^m))$,

$$\begin{aligned}\mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon &= \mathcal{J}^{t,t_0}_{\ell,\mathrm{th}}\left(\widehat{\vec{V}}(\phi_0^\varepsilon)_{R,<}\right) + O(\sqrt{\varepsilon}\|\phi_0^\varepsilon\|_{L^2}) + O(\varepsilon^{N-d}\,R^d\,\|\phi_0^\varepsilon\|_{L^2}) + O(\varepsilon^\beta\,C_\beta\,R^{-n_\beta})\\ &= \mathcal{J}^{t,t_0}_{\ell,\mathrm{th}}\left(\widehat{\vec{V}}\phi_0^\varepsilon\right) + O(\sqrt{\varepsilon}\|\phi_0^\varepsilon\|_{L^2}) + O(\varepsilon^{N-d}\,R^d\,\|\phi_0^\varepsilon\|_{L^2}) + O(\varepsilon^\beta\,C_\beta\,R^{-n_\beta})\end{aligned}$$

where we have used again Corollary 2.16. If $\beta < \frac{1}{2}$, we perform an appropriate choice of R and N: we choose $R = \varepsilon^{-\gamma}$ with $\gamma \geq \frac{1}{n_\beta}(\frac{1}{2}-\beta)$ and $N \geq \frac{1}{2} + d(1+\gamma)$.

At this stage of the description, the thawed Gaussian approximation of Theorem (1.15) is proved. For obtaining the frozen one, we shall argue as in the scalar case considered in [**53**] (Lemma 3.2 and Lemma 3.4). We will detail this argument later in Section 3.3 below.

The proofs of the order ε approximations of Theorems 1.18, 1.19 and 1.20 start with the same lines. However, one includes in the approximation the two first terms of the asymptotic expansion of $\psi_\ell^{\varepsilon,N}(t)$: the one of order ε^0 and the one of order $\varepsilon^{\frac{1}{2}}$. The terms of order $\sqrt{\varepsilon}$ are twofold:

(i) The one along the same mode as the initial data, here denoted by ℓ. This term will be proved to be of lower order because its structure allows to use the first part of Corollary 2.21.

(ii) The one generated by the crossing along the other mode. This one is not negligible.

At that stage of the proofs, one will be left with the thawed approximation. The derivation of the frozen approximation from the thawed one involves the second part of Corollary 2.21. However, complications are induced in the treatment of term described in (ii) above because of the singularity in time that it contains. This difficulty is overcome by averaging in time and using Corollary 2.25. We implement this strategy in the next sections.

3.2. Thawed Gaussian approximations with transfers terms

We prove here the higher order approximation of Theorem 1.18 for initial data $\psi_0^\varepsilon = \vec{V}\phi_0^\varepsilon$ with $(\phi_0^\varepsilon)_{\varepsilon>0}$ frequency localized at the scale $\beta \geq 0$ in a compact set K. As in the preceding section, we assume $\vec{V} = \pi_\ell(t_0)\vec{V}$ and, without loss of generality, we suppose $\ell = 1$.

We start as in the preceding section and transform equation (3.1) by taking the terms of order ε^0 and $\varepsilon^{\frac{1}{2}}$ in the expansion of $\psi_\ell^{\varepsilon,N}$. We obtain

$$\mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon(x) = \mathcal{J}\left[\mathbb{I}_{|z|<R}(\psi_1^{\varepsilon,1}(t)+\psi_2^{\varepsilon,1}(t))\right](\phi_0^\varepsilon) + O\left(\varepsilon^\beta\,C_\beta\,R^{-n_\beta}\right) + O(\varepsilon^{N-d}R^d\|\psi_0^\varepsilon\|_{L^2}).$$

The rest in $O(\varepsilon^{N-d}R^d\|\psi_0^\varepsilon\|_{L^2})$ comes from the remainder of the approximation of $\mathcal{U}_H^\varepsilon(t,t_0)g_z^\varepsilon$ while the term $O(\varepsilon\|\psi_0^\varepsilon\|_{L^2})$ comes from the terms of order ε^j for $j \geq 1$ of the approximation, these terms having a wave packet structure while the rest is just known as bounded in Σ^k_ε.

We write for $\ell \in \{1,2\}$

$$\psi_\ell^{\varepsilon,1}(t) = \sum_{j=0}^{1}\varepsilon^{\frac{j}{2}}\psi_{\ell,j}^{\varepsilon,1}(t).$$

Because the assumptions on K induce that there is only one passage through the crossing, Theorem 1.21 implies that $\psi_{2,0}^{\varepsilon,1}(t) = 0$ and $\psi_{2,1}^{\varepsilon,1}(t)$ only depends on the transfer profile $f_{1\to2}^\varepsilon$ (indeed, we

have assumed $\vec{V} = \pi_1(t_0)\vec{V}$). Moreover, for the mode 1, we have for $\ell \in \{1,2\}$ and $j \in \{0,1\}$

$$\psi^{\varepsilon,1}_{\ell,j}(t) = \mathrm{e}^{\frac{i}{\varepsilon}S_\ell(t,t_0,z_0)}\mathrm{WP}^\varepsilon_{z_\ell(t)}\left(\mathcal{R}_\ell(t,t_0)\,\mathcal{M}[F_\ell(t,t_0)]\,\vec{B}_{\ell,j}(t)g^{i\mathbb{I}}\right).$$

We recall that $\vec{B}_{\ell,1}$ is given by (1.41). We use the structure of the term

$$\mathcal{R}_\ell(t,t_0)\,\mathcal{M}[F_\ell(t,t_0)]\,\vec{B}_{\ell,1}(t)g^{i\mathbb{I}}$$

(see [**54**] section 3 or the book [**13**]): it writes

$$\mathcal{R}_\ell(t,t_0)\,\mathcal{M}[F_\ell(t,t_0)]\,\vec{B}_{\ell,1}(t)g^{i\mathbb{I}}(x) = \vec{a}(t)xg^{\Gamma_\ell(t,t_0,z_0)}(x)$$

for some smooth and bounded vector-valued map $(t,z)\mapsto\vec{a}(t,z)$. Therefore, Corollary 2.21 yields

$$\mathcal{J}\left[\mathbb{I}_{|z|<R}\psi^{\varepsilon,1}_{1,1}(t)\right](\phi^\varepsilon_0) = O(\sqrt{\varepsilon}\|\phi^\varepsilon_0\|_{L^2})$$

and we are left with

$$\begin{aligned}\mathcal{U}^\varepsilon_H(t,t_0)\psi^\varepsilon_0(x) &= \mathcal{J}\left[\mathbb{I}_{|z|<R}(\psi^{\varepsilon,1}_{1,0}(t)+\sqrt{\varepsilon}\,\psi^{\varepsilon,1}_{2,1}(t))\right](\phi^\varepsilon_0) + O\left(\varepsilon^\beta\,C_\beta\,R^{-n_\beta}\right) + O(\varepsilon^{N-d}R^d\|\psi^\varepsilon_0\|_{L^2})\\ &= \mathcal{J}\left[\psi^{\varepsilon,1}_{1,0}(t)+\sqrt{\varepsilon}\,\psi^{\varepsilon,1}_{2,1}(t)\right]((\phi^\varepsilon_0)_{R,<}) + O\left(\varepsilon^\beta\,C_\beta\,R^{-n_\beta}\right) + O(\varepsilon^{N-d}R^d\|\psi^\varepsilon_0\|_{L^2})\\ &= \mathcal{J}\left[\psi^{\varepsilon,1}_{1,0}(t)+\sqrt{\varepsilon}\,\psi^{\varepsilon,1}_{2,1}(t)\right](\phi^\varepsilon_0) + O\left(\varepsilon^\beta\,C_\beta\,R^{-n_\beta}\right) + O(\varepsilon^{N-d}R^d\|\psi^\varepsilon_0\|_{L^2})\end{aligned}$$

by Corollary 2.16. Identifying the terms, we deduce

$$\mathcal{U}^\varepsilon_H(t,t_0)\psi^\varepsilon_0(x) = \mathcal{J}^{t,t_0}_{1,\mathrm{th}}\left(\widehat{\vec{V}}\,\phi^\varepsilon_0\right) + \sqrt{\varepsilon}\,\mathcal{J}^{t,t_0}_{1,2,\mathrm{th}}\left(\widehat{\vec{V}}\phi^\varepsilon_0\right) + O\left(\varepsilon^\beta\,C_\beta\,R^{-n_\beta}\right) + O(\varepsilon^{N-d}R^d\|\psi^\varepsilon_0\|_{L^2}).$$

If $\beta<1$, we choose $R=\varepsilon^{-\gamma}$, $N=1+d(\gamma+1)$ with $\gamma\geq\frac{1}{n_\beta}(1-\beta)$. This gives Theorem 1.18.

More precisely, for a general $\vec{V} = \pi_1(t_0)\vec{V} + \pi_2(t_0)\vec{V}$, we obtain

$$\begin{aligned}\mathcal{U}^\varepsilon_H(t,t_0)\psi^\varepsilon_0(x) = \mathcal{J}^{t,t_0}_{1,\mathrm{th}}\left(\widehat{\pi_1(t_0)\vec{V}}\,\phi^\varepsilon_0\right) + \mathcal{J}^{t,t_0}_{2,\mathrm{th}}\left(\widehat{\pi_2(t_0)\vec{V}}\,\phi^\varepsilon_0\right) + \sqrt{\varepsilon}\,\mathcal{J}^{t,t_0}_{1,2,\mathrm{th}}\left(\widehat{\pi_1(t_0)\vec{V}}\phi^\varepsilon_0\right)\\ + O\left(\varepsilon(C_\beta+\|\psi^\varepsilon_0\|_{L^2})\right).\end{aligned} \tag{3.2}$$

3.3. Frozen Gaussian approximations with transfers terms

It remains to pass from the thawed to the frozen approximation. As we have already mentioned, we use the argument developed in Lemma 3.2 and 3.4 of [**53**]. It is based on an evolution argument which crucially uses Corollary 2.21. We now explain that step.

End of the proof of Theorem 1.15. We start from the approximation given by the first part of Theorem 1.15: in $\Sigma^k_\varepsilon(\mathbb{R}^d)$, we have

$$\mathcal{U}^\varepsilon_H(t,t_0)\psi^\varepsilon_0(x) = \mathcal{J}^{t,t_0}_{1,\mathrm{th}}\left(\widehat{\pi_1(t_0)\vec{V}}\,\phi^\varepsilon_0\right) + O(\sqrt{\varepsilon}(C_\beta+\|\phi^\varepsilon_0\|_{L^2}))$$

and our aim is to prove that in $\Sigma^k_\varepsilon(\mathbb{R}^d)$

$$\mathcal{J}^{t,t_0}_{1,\mathrm{th}}\left(\widehat{\pi_1(t_0)\vec{V}}\,\phi^\varepsilon_0\right) = \mathcal{J}^{t,t_0}_{1,\mathrm{fr}}\left(\widehat{\pi_1(t_0)\vec{V}}\,\phi^\varepsilon_0\right) + O(\varepsilon).$$

Of course, a remainder of size $O(\sqrt{\varepsilon})$ would be enough for proving Theorem 1.15; however, it will be usefull to have it in order to prove Theorems 1.19 and 1.20.

The strategy dates back to [**53**]. We follow the presentation of [**21**]. We set for $s \in [0,1]$

$$\Theta(s,z) = (1-s)\Gamma_\ell(t,t_0,z) + is\mathbb{I}$$

where Γ_ℓ is given by (1.18). We consider the partially normalised Gaussian function

$$\widetilde{g}(t,s) = (\pi)^{-d/4} \mathrm{e}^{\frac{i}{2}\Theta(s,z)x\cdot x},\ x \in \mathbb{R}^d$$

and we set

$$\widetilde{g}^{\Theta(s),\varepsilon}_{\Phi_\ell^{t,t_0}(z)}(x) = \mathrm{WP}^\varepsilon_{\Phi_\ell^{t,t_0}(z)}\left(\widetilde{g}(t,s)\right),$$

The aim is to construct a map $s \mapsto a(s,z)$ such that for all $s \in [0,1]$ in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma^k_\varepsilon)$,

$$\frac{d}{ds}\mathcal{J}\left[a(s,z)\vec{V}_\ell(t,t_0,z)\widetilde{g}^{\Theta(s),\varepsilon}_{\Phi_\ell^{t,t_0}(z)}\right] = O(\varepsilon).$$

Choosing $a(0,z) = 1$, we have

$$\mathcal{J}^{t,t_0}_{\ell,\mathrm{th}} = \mathcal{J}\left[a(0,z)\vec{V}_\ell(t,t_0,z)\widetilde{g}^{\Theta(0),\varepsilon}_{\Phi_\ell^{t,t_0}(z)}\right],$$

and we will obtain that for any $f \in L^2(\mathbb{R}^d)$, we have in $\Sigma^k_\varepsilon(\mathbb{R}^d)$

$$\begin{aligned}\mathcal{J}^{t,t_0}_{\ell,\mathrm{th}}(\vec{V}f) &= \mathcal{J}\left[a(1,z)\vec{V}_\ell(t,t_0,z)\widetilde{g}^{\Theta(1),\varepsilon}_{\Phi_\ell^{t,t_0}(z)}\right](f) + O(\varepsilon)\\ &= \mathcal{J}^{t,t_0}_{\ell,\mathrm{fr}}(\vec{V}f) + O(\varepsilon)\end{aligned}$$

provided $a(1,z) = a_\ell(t,t_0,z)$ as defined in (1.24).

For constructing the map $s \mapsto a(s,z)$, we compute

$$\begin{aligned}\frac{d}{ds}\mathcal{J}\left[a(s,z)\vec{V}_\ell(t,t_0,z)\widetilde{g}^{\Theta(s),\varepsilon}_{\Phi_\ell^{t,t_0}(z)}\right] &= \mathcal{J}\left[\partial_s a(s,z)\vec{V}_\ell(t,t_0,z)\widetilde{g}^{\Theta(s),\varepsilon}_{\Phi_\ell^{t,t_0}(z)}\right]\\ &\quad + \frac{i}{2}\mathcal{J}\left[a(s,z)\vec{V}_\ell(t,t_0,z)\mathrm{WP}^\varepsilon_{\Phi_\ell^{t,t_0}(z)}\left(\partial_s\Theta(s)x\cdot x\widetilde{g}^{\Theta(s),\varepsilon}\right)\right].\end{aligned}$$

We use equation (2.20) of Corollary 2.21 to transform the second term of the right-hand side and obtain

$$\begin{aligned}&\mathcal{J}\left[a(s,z)\vec{V}_\ell(t,t_0,z)\mathrm{WP}^\varepsilon_{\Phi_\ell^{t,t_0}(z)}(\partial_s\Theta(s)x\cdot x g^{\,\Theta(s)})\right]\\ &\quad = \frac{1}{i}\mathcal{J}\left[a(s,z)\vec{V}_\ell(t,t_0,z)\mathrm{WP}^\varepsilon_{\Phi_\ell^{t,t_0}(z)}(\mathrm{Tr}(\Theta_1(s))g^{\,\Theta(s)})\right] + O(\varepsilon)\end{aligned}$$

in $\mathcal{L}(L^2(\mathbb{R}^d), \Sigma^k_\varepsilon)$ and with

$$\Theta_1(s) = \partial_s\Theta(s)\left[(A_\ell - iB_\ell)^{-1}(C_\ell - iD_\ell) - \Theta\right]^{-1}$$

where $M_\ell(s,z)$ is associated to $\Theta(s,z)$ according to (2.18). In particular, we have

$$\partial_s M(s) = -(A_\ell - iB_\ell)\partial_s\Theta(s).$$

We deduce

$$\Theta_1(s) = -(A_\ell - iB_\ell)^{-1}\partial_s M(s)M(s)^{-1}(A_\ell - iB_\ell)$$

and

$$\mathrm{Tr}(\Theta_1(s)) = -\mathrm{Tr}(\partial_s M(s)M(s)^{-1}) = -\mathrm{det}M(s)^{-1}\,\partial_s\left(\mathrm{det}M(s)\right).$$

Therefore, the condition

$$\partial_s a(s,z) - \frac{1}{2}\mathrm{Tr}(\partial_s M(s,z)M(s)^{-1})a(s,z) = 0$$

that we have to fulfilled, is realized by

$$a(s,z) = \frac{\det M(s)}{\det M(0)} a(0,z) = a_\ell(t,t_0,z).$$

□

Proof of Theorem 1.19. We now start from the result of Theorem 1.18, that is equation (3.2). In view of what has been done in the end proof of the proof of Theorem 1.15, we only have to prove

$$\mathcal{J}^{t,t_0}_{1,2,\mathrm{th}}\left(\widehat{\pi_1(t_0)\vec{V}}\phi_0^\varepsilon\right) = \mathcal{J}^{t,t_0}_{1,2,\mathrm{fr}}\left(\widehat{\pi_1(t_0)\vec{V}}\phi_0^\varepsilon\right) + O\left(\sqrt{\varepsilon}(C_\beta + \|\phi_0^\varepsilon\|_{L^2}\right).$$

As noticed in the introduction, when $t < t_{1,\min}(K)$, then $\tau_{1,2}(t,t_0,z) = 0$ for all $z \in K$ and when $t \in [t_{1,\max}(K), t_{2,\min}(K))$, $z \mapsto \tau_{1,2}(t,t_0,z)$ is smooth. Therefore, one can use the perturbative argument allowing to froze the covariances of the Gaussian terms as in the proof of Theorem 1.15 and one obtains the formula (1.35). □

Proof of Theorem 1.20. One now has to cope with the discontinuity of the transfer coefficient $\tau_{1,2}(t,t_0,z)$. We use Lemma 2.24. □

Part 2

Wave-packet propagation through smooth crossings

CHAPTER 4

Symbolic calculus and diagonalization of Hamiltonians with smooth crossings

In this section, we revisit the diagonalization of Hamiltonians in the case of the smooth crossings in which we are interested. We settle the algebraic setting that we will use in Section 5 for the propagation of wave packets.

We will use the *Moyal product* about which we recall some facts: if $A^\varepsilon, B^\varepsilon$ are semi-classical series, their Moyal product is the formal series

$$C^\varepsilon := A^\varepsilon \circledast B^\varepsilon \ \text{ where } \ C^\varepsilon = \sum_{j\geq 0} \varepsilon^j C_j$$

$$C_j(x,\xi) = \frac{1}{2^j} \sum_{|\alpha+\beta|=j} \frac{(-1)^{|\beta|}}{\alpha!\beta!} (D_x^\beta \partial_\xi^\alpha A).(D_x^\alpha \partial_\xi^\beta B)(x,\xi), \quad j \in \mathbb{N}. \tag{4.1}$$

We also introduce the *Moyal bracket*

$$\{A^\varepsilon, B^\varepsilon\}_\circledast := A^\varepsilon \circledast B^\varepsilon - B^\varepsilon \circledast A^\varepsilon.$$

Let us now consider a smooth matrix-valued symbol $H^\varepsilon = H_0 + \varepsilon H_1$, where the principal symbol $H_0 = h_1\pi_1 + h_2\pi_2$ has two smooth eigenvalues h_1 and h_2 with smooth eigenprojectors π_1 and π_2. We allow for a non-empty crossing set Υ as in Definition 1.2. By standard symbolic calculus with smooth symbols, we have for $\ell \in \{1,2\}$ the relations

$$\pi_\ell \circledast (i\varepsilon\partial_t - H^\varepsilon) = (i\varepsilon\partial_t - h_\ell) \circledast \pi_\ell = O(\varepsilon). \tag{4.2}$$

We are going to see two manners to replace the projector π_ℓ and the Hamiltonian h_ℓ by asymptotic series so that the relation above holds at a better order.

We call "rough" the first diagonalization process that we propose. It will hold everywhere, including Υ and is comparable the reduction performed in [**4**] for avoided crossings. It is the subject of Section 4.2.

The second one, more sophisticated, will require to work in a domain that does not meet Υ. Based on the use of superadiabatic projectors, as developed in [**5, 46, 55, 58**]. This strategy is implemented in Section 4.3. The new element comparatively to the references that we have mentioned, is that we keep a careful memory of the dependence of the constructed elements with respect to the distance of their support from Υ. For this reason, we will use a pseudodifferential setting that we precise in the next Section 4.1.

4.1. Formal asymptotic series

We consider formal semi-classical series

$$A^\varepsilon = \sum_{j\geq 0} \varepsilon^j A_j$$

where all the functions A_j are smooth (matrix-valued) in an open set $\mathcal{D} \subset \mathbb{R}\times\mathbb{R}^{2d}$, that is, $A_j \in \mathcal{C}^\infty(\mathcal{D}, \mathbb{C}^{m,m})$.

Notation. If $A^\varepsilon = \sum_{j\geq 0} \varepsilon^j A_j$ is a formal series and $N \in \mathbb{N}$, we denote by $A^{\varepsilon,N}$ the function

$$A^{\varepsilon,N} = \sum_{0\leq j\leq N} \varepsilon^j A_j. \tag{4.3}$$

The formal series that we will consider in Section 4.3 will present two small parameters: the semi-classical parameter $\varepsilon > 0$ and another parameter $\delta > 0$ that controls the growth of the symbol and of its derivatives. For our intended application, δ is related to the size of the gap between the eigenvalues of the Hamiltonian's symbol.

Definition 4.1 (Symbol spaces). Let $\mu \in \mathbb{R}$ and $\delta \in (0, 1]$.

(i) We denote by $\boldsymbol{S}^\mu_\delta(\mathcal{D})$ the set of smooth (matrix-valued) functions in $\mathcal{D}$ such

$$|\partial_z^\gamma A(t, z)| \leq C_\gamma \delta^{\mu-|\gamma|}, \ \ \forall (t, z) \in \mathcal{D}.$$

Notice that the set $\boldsymbol{S}_\delta(\mathcal{D}) := \boldsymbol{S}^0_\delta(\mathcal{D})$ has the algebraic structure of a ring.

(ii) We shall say that a formal series $A^\varepsilon = \sum_{j\geq 0} \varepsilon^j A_j$ is in $\boldsymbol{S}^\mu_{\varepsilon,\delta}(\mathcal{D})$ if $A_j \in \boldsymbol{S}^{\mu-2j}_\delta(\mathcal{D})$ for all $j \in \mathbb{N}$. We set $\boldsymbol{S}_{\varepsilon,\delta}(\mathcal{D}) := \boldsymbol{S}^0_{\varepsilon,\delta}(\mathcal{D})$.

Remark 4.2. (1) If $A \in \mathbf{S}^\mu_\delta$, $B \in \mathbf{S}^\mu_{\delta'}$ then $AB \in \mathbf{S}^{\mu+\mu'}_\delta$ while $\{A, B\} \in \mathbf{S}^{\mu+\mu'-2}_\delta$. Besides, if $A \in \boldsymbol{S}^\mu_\delta(\mathcal{D})$, then $\partial_z^\gamma A \in \boldsymbol{S}^{\mu-|\gamma|}_\delta(\mathcal{D})$.

(2) When $\delta = 1$, as in the next Section 4.2, then for all $\mu \in \mathbb{R}$, $S^\mu_1 = S^0_1$ coincides with the standard class of Calderón-Vaillancourt symbols, those smooth functions that are bounded together with their derivatives. Similarly, $S^\mu_{\varepsilon,1} = S^\mu_\varepsilon$ coincides with asymptotic series of symbols.

(3) The parameter δ can be understood as a loss that appears at each differentiation. However, in the asymptotic series, one loose δ^2 when passing from some j-th term of to the $(j+1)$-th. one. In Section 4.3, δ will monitor the size of the gap function f in the domain $\mathcal{D}$.

The Moyal bracket satisfies the property stated in the next lemma.

Lemma 4.3. *Let δ_A, $\delta_B \in]0, 1]$. If A^ε and B^ε are formal series of $\mathbf{S}_{\varepsilon,\delta_A}(\mathcal{D})$ and $\mathbf{S}_{\varepsilon,\delta_B}(\mathcal{D})$, respectively. then $A^\varepsilon \circledast B^\varepsilon$ is a formal series of $\mathbf{S}_{\varepsilon,\min(\delta_A,\delta_B)}(\mathcal{D})$. Besides, for $N \in \mathbb{N}$,*

$$A^{\varepsilon,N} \circledast B^{\varepsilon,N} = \sum_{0\leq j\leq N} \varepsilon^j C_j + \varepsilon^{N+1} R^{\varepsilon,N}_{A,B}$$

where for all $\gamma \in \mathbb{N}^{2d}$, there exists $C_{N,\gamma}$ independent on $\delta_{A,B}$ and ε such that

$$|\partial_z^\gamma R^{\varepsilon,N}_{A,B}(t, z)| \leq C_{N,\gamma} \left[\min(\delta_A, \delta_B)\right]^{-N-\kappa_0}, \ \forall \varepsilon \in]0, 1], \ \ \forall (t, z) \in \mathcal{D},$$

where κ_0 is a universal constant depending only on the dimension d.

PROOF. The estimate is a direct consequence of [**6**, Theorem A1]. In Appendix B, Theorem B.1 we give a detailed proof. □

When $\delta_A = 1$ and $\delta_B = \delta \in (0,1]$, $\min(\delta_A, \delta_B) = \delta$. This shows that

$$\mathbf{S}_{\varepsilon,1}(\mathcal{D}) \circledast \mathbf{S}_{\varepsilon,\delta}(\mathcal{D}) \subset \mathbf{S}_{\varepsilon,\delta}(\mathcal{D}).$$

Let us conclude this Section by comments on the quantization of symbols of the classes $\mathbf{S}^{\mu}_{\delta}$. The Calderón-Vaillancourt estimate for pseudodifferential operators (see [**14, 64**]) states that there exists a constant $C > 0$ such that for all $a \in \mathcal{C}^{\infty}(\mathbb{R}^{2d})$,

$$\|\mathrm{op}_{\varepsilon}(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq C \sup_{0\leq|\gamma|\leq d+1} \varepsilon^{\frac{|\gamma|}{2}} \sup_{z\in\mathbb{R}^d} |\partial_z^{\gamma} a(z)|.$$

Actually, the article [**9**] treats the case $\varepsilon = 1$ and the estimate in the semi-classical case comes from the observation that

$$\mathrm{op}_{\varepsilon}(a) = \Lambda_{\varepsilon}^{*} \mathrm{op}_1(a(\sqrt{\varepsilon}\cdot))\Lambda_{\varepsilon}$$

where Λ_{ε} is the L^2-unitary scaling operator defined on function $f \in \mathcal{S}(\mathbb{R}^d)$ by

$$\Lambda_{\varepsilon} f(x) = \varepsilon^{-\frac{d}{4}} f\left(\frac{x}{\sqrt{\varepsilon}}\right), \quad x \in \mathbb{R}^d.$$

One can derive an estimate in the sets Σ^k_{ε} by observing

$$\left(x^{\alpha}(\varepsilon\partial_x)^{\beta}\right) \circ \mathrm{op}_{\varepsilon}(a) = \sum_{|\gamma_1|+|\gamma_2|+|\gamma_3|\leq k} \varepsilon^{\frac{|\gamma_1|}{2}} c_{\gamma_1,\gamma_2,\gamma_3}(\varepsilon)\, \mathrm{op}_{\varepsilon}(\partial_z^{\gamma_1} a) \circ (x^{\gamma_2}(\varepsilon\partial_x)^{\gamma_3})$$

for some coefficients $c_{\gamma_1,\gamma_2,\gamma_3}(\varepsilon)$, uniformly bounded with respect to $\varepsilon \in [0,1]$. This implies the boundedness of $\mathrm{op}_{\varepsilon}(a)$ in weighted Sobolev spaces: for all $k \in \mathbb{N}$, there exists a constant $C_k > 0$ such that for all $a \in \mathcal{S}(\mathbb{R}^{2d})$,

$$\|\mathrm{op}_{\varepsilon}(a)\|_{\mathcal{L}(\Sigma^k_{\varepsilon})} \leq C_k \sum_{0\leq|\gamma|\leq d+k+1} \varepsilon^{\frac{|\gamma|}{2}} \sup_{z\in\mathbb{R}^d} |\partial_z^{\gamma} a(z)|. \tag{4.4}$$

PROPOSITION 4.4. Let $A \in \mathbf{S}^{\mu-2j}_{\delta}$ for $\mu \in \mathbb{R}$, $j \in \mathbb{N}$. Then, for $k \in \mathbb{N}$

$$\|\mathrm{op}_{\varepsilon}(A)\|_{\mathcal{L}(\Sigma^k_{\varepsilon})} \leq C_k \sup_{0\leq|\gamma|\leq d+1} \varepsilon^{\frac{|\gamma|}{2}} \delta^{\mu-2j-k-|\gamma|}$$

Therefore, if $\delta \geq \sqrt{\varepsilon}$

$$\|\mathrm{op}_{\varepsilon}(A)\|_{\mathcal{L}(\Sigma^k_{\varepsilon})} \leq C_k\, \delta^{\mu-k-2j}. \tag{4.5}$$

We will use such estimates. Questions related with symbolic calculus in the classes $\mathbf{S}^{\mu}_{\delta,\varepsilon}$ are discussed in Appendix B.2.

4.2. 'Rough' reduction

The next result gives a reduction of the Hamiltonian in a block diagonalized form. We will use this reduction on small interval of times.

THEOREM 4.5. *Assume $H^\varepsilon = H_0 + \varepsilon H_1$ with H_0 having smooth eigenprojectors and eigenvalues. There exist matrix-valued asymptotic series*

$$\pi_1^\varepsilon = \pi_1 + \sum_{j\geq 1} \varepsilon^j \pi_{1,j}, \quad h_\ell^\varepsilon = h_\ell \mathbb{I} + \sum_{j\geq 1} \varepsilon^j h_{\ell,j}, \quad W^\varepsilon = \sum_{j\geq 1} \varepsilon^j W_j, \quad \ell \in \{1,2\}$$

such that for all $N \in \mathbb{N}$, $\pi_1^{\varepsilon,N}$ and $\pi_2^{\varepsilon,N} = 1 - \pi_1^{\varepsilon,N}$ are approximate projectors

$$\pi_\ell^{\varepsilon,N} \circledast \pi_\ell^{\varepsilon,N} = \pi_\ell^{\varepsilon,N} + O(\varepsilon^{N+1}), \quad \ell \in \{1,2\} \tag{4.6}$$

and $H^\varepsilon = H_0 + \varepsilon H_1$ reduces according to

$$\pi_1^{\varepsilon,N} \circledast (i\varepsilon\partial_t - H^\varepsilon) = (i\varepsilon\partial_t - h_1^{\varepsilon,N}) \circledast \pi_1^{\varepsilon,N} + W^{\varepsilon,N} \circledast \pi_2^{\varepsilon,N} + O(\varepsilon^{N+1}), \tag{4.7}$$

$$\pi_2^{\varepsilon,N} \circledast (i\varepsilon\partial_t - H^\varepsilon) = (i\varepsilon\partial_t - h_2^{\varepsilon,N}) \circledast \pi_2^{\varepsilon,N} + (W^{\varepsilon,N})^* \circledast \pi_1^{\varepsilon,N} + O(\varepsilon^{N+1}). \tag{4.8}$$

Moreover, for all $\ell \in \{1,2\}$ and $j \geq 1$, the symbols $\pi_{\ell,j}$ and $h_{\ell,j}$ are self-adjoint, the matrices W_j are the off-diagonal (see equation (1.44) for the value of W_1) and

$$h_{\ell,1} = \pi_\ell H_1 \pi_\ell + (-1)^\ell \frac{i}{2}(h_1 - h_2)\pi_\ell\{\pi_1,\pi_1\}\pi_\ell. \tag{4.9}$$

If H^ε also satisfies Assumption 1.4 on the time interval I, then the 4×4 matrix-valued Hamiltonian

$$\underline{H}^\varepsilon := \begin{pmatrix} h_1^\varepsilon & W^\varepsilon \\ (W^\varepsilon)^* & h_2^\varepsilon \end{pmatrix}$$

is subquadratic according to Definition 1.1.

Note that in $\underline{H}^\varepsilon$, the off-diagonal blocks are of lower order than the diagonal ones since the asymptotic series W^ε has no term of order 0.

Theorem 4.5 allows to put the equation (1.1) in a reduced form by setting

$$\underline{\psi}^\varepsilon = {}^t(\underline{\psi}_1^\varepsilon, \underline{\psi}_2^\varepsilon) \text{ with } \underline{\psi}_\ell^\varepsilon = \widehat{\pi_\ell^\varepsilon}\psi^\varepsilon.$$

Indeed, we then have

$$i\varepsilon\partial_t \underline{\psi}^\varepsilon = \underline{\widehat{H}}^\varepsilon \underline{\psi}^\varepsilon + O(\varepsilon^\infty), \quad \underline{\psi}^\varepsilon_{|t=0} = {}^t\left(\widehat{\pi_1^\varepsilon}\,\psi_0^\varepsilon, \widehat{\pi_2^\varepsilon}\,\psi_0^\varepsilon\right). \tag{4.10}$$

We deduce the corollary.

COROLLARY 4.6. Formally, we have for $t \in I$,

$$\mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon = \underline{\psi_1^\varepsilon} + \underline{\psi_2^\varepsilon},$$

where $\underline{\psi}^\varepsilon$ solves (4.10).

PROOF. The proof relies on a recursive argument.

The case $N = 0$ is equivalent to (4.2)

The case $N = 1$ has been proved in Lemma B.2 in [**20**]. However, we revisit the proof in order to compute W_1. We first compute $\pi_{\ell,\ell}$ by requiring $\pi^{\varepsilon,(\ell)} \circledast \pi^{\varepsilon,(\ell)} = \pi^{\varepsilon,(\ell)} + O(\varepsilon^2)$, which admits the solution

$$\pi_{1,1} = -\pi_{2,1} = -\frac{1}{2i}\pi_1\{\pi_1,\pi_1\}\pi_1 + \frac{1}{2i}\pi_2\{\pi_1,\pi_1\}\pi_2.$$

We recall that $\{\pi_1, \pi_1\}$ is diagonal and skew-symmetric (see Lemma B.1 in [**20**]). Then, we observe

$$\pi_\ell \circledast (i\varepsilon\partial_t - H^\varepsilon) = (i\varepsilon\partial_t - h_\ell) \circledast \pi_\ell + \varepsilon\Theta_\ell + O(\varepsilon^2)$$

with

$$\Theta_\ell = -\frac{1}{2i}\{\pi_\ell, H_0\} - \pi_\ell H_1 - i\partial_t\pi_\ell + \frac{1}{2i}\{h_\ell, \pi_\ell\}$$

or, equivalently

$$\begin{aligned}
\Theta_1 &= \frac{1}{2i}(h_2 - h_1)\{\pi_1, \pi_1\} - i\partial_t\pi_1 - \pi_1 H_1 + \frac{1}{i}\{h_1, \pi_1\}\pi_1 + \frac{1}{2i}\{h_1 + h_2, \pi_1\}\pi_2,\\
\Theta_2 &= \frac{1}{2i}(h_1 - h_2)\{\pi_2, \pi_2\} - i\partial_t\pi_2 - \pi_2 H_1 + \frac{1}{i}\{h_2, \pi_2\}\pi_2 + \frac{1}{2i}\{h_1 + h_2, \pi_2\}\pi_1\\
&= -\frac{1}{2i}(h_2 - h_1)\{\pi_1, \pi_1\} + i\partial_t\pi_1 - \pi_2 H_1 - \frac{1}{i}\{h_2, \pi_1\}\pi_2 - \frac{1}{2i}\{h_1 + h_2, \pi_2\}\pi_1
\end{aligned}$$

We observe

$$\Theta_2^* = -\frac{1}{2i}(h_2 - h_1)\{\pi_1, \pi_1\} - i\partial_t\pi_1 - H_1\pi_2 + \frac{1}{i}\pi_2\{h_2, \pi_1\} + \frac{1}{2i}\pi_1\{h_1 + h_2, \pi_2\}$$

and

$$\pi_1\Theta_2^*\pi_2 = \pi_1\Theta_1\pi_2. \tag{4.11}$$

Thus, we have to solve

$$\begin{aligned}
-\pi_{1,1}H_0 &= -h_{1,1}\pi_1 - h_1\pi_{1,1} + i\partial_t\pi_1 + \Theta_1 + W_1\pi_2,\\
-\pi_{2,1}H_0 &= -h_{2,1}\pi_2 - h_2\pi_{2,1} + i\partial_t\pi_2 + \Theta_2 + W_1^*\pi_1.
\end{aligned}$$

Multiplying on the right the first equation by π_1 and the second by π_2, we obtain that $h_{1,1}$ and $h_{2,1}$ have to solve

$$h_{1,1}\pi_1 = i\partial_t\pi_1\pi_1 + \Theta_1\pi_1 \text{ and } h_{2,1}\pi_2 = i\partial_t\pi_2\pi_2 + \Theta_2\pi_2$$

which is solved by taking the self-adjoint matrices

$$\begin{aligned}
h_{1,1} &= i\partial_t\pi_1\pi_1 + \Theta_1\pi_1 - i\pi_1\partial_t\pi_1\pi_2 + \pi_1\Theta_1^*\pi_2,\\
h_{2,1} &= i\partial_t\pi_2\pi_2 + \Theta_2\pi_2 - i\pi_2\partial_t\pi_2\pi_1 + \pi_2\Theta_2^*\pi_1.
\end{aligned}$$

Multiplying on the right the first equation by π_2 and the second by π_1, we obtain that W_1 has to solve

$$W_1\pi_2 = -(h_2 - h_1)\pi_{1,1}\pi_2 - \Theta_1\pi_2 \text{ and } W_1^*\pi_1 = (h_2 - h_1)\pi_{2,1}\pi_1 - \Theta_2\pi_1.$$

Using the relations $\pi_{1,1}^* = \pi_{1,1} = -\pi_{2,1}$, $\pi_1\partial_{t,z}\pi_1 = \partial_{t,z}\pi_1\pi_2$ and (4.11), we obtain

$$W_1\pi_2 = \pi_1 W_1 = \pi_1\left(H_1 + i\partial_t\pi_1 + \frac{1}{2}\{h_1 + h_2, \pi_1\}\right)\pi_2,$$

whence (1.44).

One can now perform the recursive argument. Assume that we have obtained (4.6), (4.7) and (4.8) for some $N \geq 1$ and let us look for $\pi_{1,N+1}$, $h_{1,N+1}$, $h_{2,N+1}$ and W_{N+1} such that the relations for $N+1$ too.

We start with $\pi_{1,N+1}$. We write

$$\pi_1^{\varepsilon,N} \circledast \pi_1^{\varepsilon,N} = \pi_1^{\varepsilon,N} + \varepsilon^{N+1}R^\varepsilon,$$

where R^ε is an asymptotic series with first term R_N. We first observe that R_N is diagonal. Indeed, we have

$$(1-\pi_1^{\varepsilon,N})\circledast\pi_1^{\varepsilon,N}\circledast\pi_1^{\varepsilon,N}=\pi_1^{\varepsilon,N}\circledast\pi_1^{\varepsilon,N}\circledast(1-\pi_1^{\varepsilon,N})$$

and

$$(1-\pi_1^{\varepsilon,N})\circledast\pi_1^{\varepsilon,N}\circledast\pi_1^{\varepsilon,N}=-\varepsilon^{N+1}R^\varepsilon\circledast\pi_1^{\varepsilon,N},\ \ \pi_1^{\varepsilon,N}\circledast\pi_1^{\varepsilon,N}\circledast(1-\pi_1^{\varepsilon,N})=-\varepsilon^{N+1}\pi_1^{\varepsilon,N}\circledast R^\varepsilon.$$

This yields $\pi_1^{\varepsilon,N}\circledast R^\varepsilon=R^\varepsilon\circledast\pi_1^{\varepsilon,N}$ and imply $\pi_1R_N=R_N\pi_1$. We now look to $\pi_{1,N+1}$ that must satisfy

$$\pi_{1,N+1}=R_N+\pi_{1,N+1}\pi_1+\pi_1\pi_{1,N+1}.$$

This relation fixes the diagonal part of $\pi_{1,N+1}$ according to

$$\pi_1\pi_{1,N+1}\pi_1=-\pi_1R_N\pi_1\ \text{ and }\ \pi_2\pi_{1,N+1}\pi_2=\pi_2R_N\pi_2,$$

We will see later that we do not need to prescribe off-diagonal components to $\pi_{1,N+1}$.

Let us now focus on $h_{1,N+1}$, $h_{2,N+1}$ and W_{N+1}. We write

$$\pi_1^{\varepsilon,N}\circledast(i\varepsilon\partial_t-H^\varepsilon)=(i\varepsilon\partial_t-h_1^{\varepsilon,N})\circledast\pi_1^{\varepsilon,N}+W^{\varepsilon,N}\circledast\pi_2^{\varepsilon,N}+\varepsilon^{N+1}\Theta_1^\varepsilon$$

where Θ_1^ε is an asymptotic series of first term $\Theta_{1,N}$. For obtaining information about $\Theta_{1,N}$, we compute

$$\pi_\ell^{\varepsilon,N}\circledast(i\varepsilon\partial_t-H^\varepsilon)\circledast\pi_{\ell'}^{\varepsilon,N}$$

for different choices of $\ell,\ell'\in\{1,2\}$.

- Taking $\ell\neq\ell'$ gives two relations

$$\begin{aligned}&\pi_1^{\varepsilon,N}\circledast(i\varepsilon\partial_t-H^\varepsilon)\circledast\pi_2^{\varepsilon,N}\\&\qquad=\pi_1^{\varepsilon,N}\circledast W^{\varepsilon,N}\circledast\pi_2^{\varepsilon,N}+\varepsilon^{N+1}\pi_1^{\varepsilon,N}\circledast\Theta_1^\varepsilon\circledast\pi_2^{\varepsilon,N}+O(\varepsilon^{N+2})\\&\pi_2^{\varepsilon,N}\circledast(i\varepsilon\partial_t-H^\varepsilon)\circledast\pi_1^{\varepsilon,N}\\&\qquad=\pi_2^{\varepsilon,N}\circledast(W^{\varepsilon,N})^*\circledast\pi_1^{\varepsilon,N}+\varepsilon^{N+1}\pi_2^{\varepsilon,N}\circledast\Theta_2^\varepsilon\circledast\pi_1^{\varepsilon,N}+O(\varepsilon^{N+2}),\end{aligned}$$

  from which we deduce $\pi_2\Theta_{2,N}\pi_1=(\pi_1\Theta_{1,N}\pi_2)^*$.
- Taking $\ell=\ell'$ gives the relations

$$\begin{aligned}&\pi_\ell^{\varepsilon,N}\circledast(i\varepsilon\partial_t-H^\varepsilon)\circledast\pi_\ell^{\varepsilon,N}\\&\qquad=\pi_\ell^{\varepsilon,N}\circledast(i\varepsilon\partial_t-h_\ell^{\varepsilon,N})\circledast\pi_\ell^{\varepsilon,N}+\varepsilon^{N+1}\pi_\ell^{\varepsilon,N}\circledast\Theta_\ell^\varepsilon\circledast\pi_\ell^{\varepsilon,N}+O(\varepsilon^{N+2}),\end{aligned}$$

  whence the self-adjointness of the diagonal part of Θ_ℓ^ε.

We now enter into the construction of $h_{1,N+1}$, $h_{2,N+1}$ and W_{N+1}. We write the asymptotic series

$$\begin{aligned}&\pi_1^{\varepsilon,N+1}\circledast(i\varepsilon\partial_t-H^\varepsilon)=\pi_1^{\varepsilon,N}\circledast(i\varepsilon\partial_t-H^\varepsilon)-\varepsilon^{N+1}\pi_{1,N+1}H_0+O(\varepsilon^{N+2}),\\&(i\varepsilon\partial_t-h_1^{\varepsilon,N+1})\circledast\pi_1^{\varepsilon,N+1}+W^{\varepsilon,N+1}\circledast\pi_2^{\varepsilon,N+1}=(i\varepsilon\partial_t-h_1^{\varepsilon,N})\circledast\pi_1^{\varepsilon,N}+W^{\varepsilon,N}\circledast\pi_2^{\varepsilon,N}\\&\qquad+\varepsilon^{N+1}\left(i\partial_t\pi_{1,N}-h_{1,N+1}\pi_1-h_1\pi_{1,N+1}+W_{N+1}\pi_2\right)+O(\varepsilon^{N+2}).\end{aligned}$$

Therefore, we look for $h_{1,N+1}$ and W_{N+1} such that

$$-\pi_{1,N+1}H_0=i\partial_t\pi_{1,N}-h_{1,N+1}\pi_1-h_1\pi_{1,N+1}+W_{N+1}\pi_2+\Theta_{1,N}$$

or equivalently

$$0=i\partial_t\pi_{1,N}-h_{1,N+1}\pi_1+(h_2-h_1)\pi_{1,N+1}\pi_2+W_{N+1}\pi_2+\Theta_{1,N}.$$

By multiplying on the right by $\pi_1 2$ and π_2, we are left with the two equations

$$h_{1,N+1}\pi_1 = \Theta_{1,N}\pi_1 + i\partial_t\pi_{1,N}\pi_1 \text{ and } W_{N+1}\pi_2 = \Theta_{1,N}\pi_2 + (h_2-h_1)\pi_{1,N+1}\pi_2 + i\partial_t\pi_{1,N}\pi_2. \tag{4.12}$$

Considering similarly the conditions for the mode h_2, we obtain that $h_{2,N+1}$ and W^*_{N+1} have to satisfy

$$h_{2,N+1}\pi_2 = \Theta_{2,N}\pi_2 + i\partial_t\pi_{2,N}\pi_2 \text{ and } W^*_{N+1}\pi_1 = \Theta_{2,N}\pi_1 - (h_2-h_1)\pi_{2,N+1}\pi_1 + i\partial_t\pi_{2,N}\pi_1.$$

Since $\pi_{2,N} = -\pi_{1,N}$ for $N \geq 1$, we are left with the relation

$$h_{2,N+1}\pi_2 = \Theta_{2,N}\pi_2 - i\partial_t\pi_{1,N}\pi_2 \text{ and } W^*_{N+1}\pi_1 = \Theta_{2,N}\pi_1 + (h_2-h_1)\pi_{1,N+1}\pi_1 - i\partial_t\pi_{1,N}\pi_1. \tag{4.13}$$

We set

$$\begin{aligned} h_{1,N+1} &= \Theta_{1,N}\pi_1 + i\partial_t\pi_{1,N}\pi_1 + \pi_1\Theta^*_{1,N}\pi_2 - i\pi_1\partial_t\pi_{1,N}\pi_2, \\ h_{2,N+1} &= \Theta_{2,N}\pi_2 + i\partial_t\pi_{2,N}\pi_2 + \pi_2\Theta^*_{2,N}\pi_1 - i\pi_2\partial_t\pi_{2,N}\pi_1. \end{aligned}$$

Then, $h_{1,N+1}$ and $h_{2,N+1}$ are self-adjoint and satisfy the first part of (4.12) and (4.13) respectively.

The construction of W_{N+1} requires to be more careful because there is a compatibility condition between (4.12) and (4.13). We look for W_{N+1} of the form

$$W_{N+1} = \Theta_{1,N}\pi_2 + (h_2-h_1)\pi_{1,N+1}\pi_2 + i\partial_t\pi_{1,N}\pi_2 + U_{N+1}\pi_1,$$

which guarantees (4.12). Then, one has

$$W^*_{N+1} = \pi_2\Theta^*_{1,N} + (h_2-h_1)\pi_2\pi_{1,N+1} - i\pi_2\partial_t\pi_{1,N} + \pi_1 U^*_{N+1}$$

and

$$\begin{aligned} W^*_{N+1}\pi_1 &= \pi_2\Theta^*_{1,N}\pi_1 - i\pi_2\partial_t\pi_{1,N}\pi_1 + \pi_1 U^*_{N+1}\pi_1 \\ &= \pi_2\Theta_{2,N}\pi_1 - i\pi_2\partial_t\pi_{1,N}\pi_1 + \pi_1 U^*_{N+1}\pi_1 \end{aligned}$$

where we have used the first property of the matrices $\Theta_{1,N}$ and $\Theta_{2,N}$ that we have exhibited, together with the fact that $\pi_{1,N+1}$ is diagonal. It is then enough to choose

$$U_{N+1} = \pi_1\left(\Theta^*_{2,N} + (h_2-h_1)\pi_{1,N+1} + i\partial_t\pi_{1,N}\right)\pi_1$$

since it implies

$$\begin{aligned} W^*_{N+1}\pi_1 &= \pi_2\Theta_{2,N}\pi_1 - i\pi_2\partial_t\pi_{1,N}\pi_1 \\ &\quad + \pi_1(\Theta_{2,N} + i\partial_t\pi_{1,N} + (h_2-h_1)\pi_{1,N+1})\pi_1 \\ &= \Theta_{2,N}\pi_1 + (h_2-h_1)\pi_{1,N+1}\pi_1 - i\pi_2\partial_t\pi_{1,N}\pi_1, \end{aligned}$$

where we have used $\pi_{1,N+1}\pi_1 = \pi_1\pi_{1,N+1}\pi_1$. As a consequence, the second part of (4.13) is satisfied. This concludes the recursive argument and the proof of the Theorem 4.5 since the growth properties of the matrices that we have constructed come with the recursive equations. □

4.3. Superadiabatic projectors and diagonalization

One now wants to get rid of the off-diagonal elements $\widehat{W^\varepsilon}$, which is possible outside Υ. We are going to take into account how far from the crossing set we are by introducing a gap assumption.

ASSUMPTION 4.7 (Gap assumption). Let $t_0 < t_1$, I an open interval of $\mathbb{R}$ containing $[t_0, t_1]$ and Ω an open subset of $\mathbb{R}^{2d}$. We say that the eigenvalue h has a gap larger than $\delta \in (0, 1]$ in $\mathcal{D} := I \times \Omega$ if one has

$$(NC_\delta) \qquad d\left(h(t,z), \mathrm{Sp}(H_0(t,z))\right) \geq \delta, \ \ \forall (t,z) \in \mathcal{D}.$$

The construction of superadiabatic projectors dates to [**5**] which was inspired by the paper [**17**]. It has then been carefully developed in [**46**] and [**55**] (see also the book [**58**]). We revisit here the construction of superadiabatic projectors, in order to control their norms with respect to the parameter δ.

We follow the construction of the Section 14.4 of the latest edition of [**13**] (2021), that we adapt to our context. One proceeds in two steps: first by defining the formal series for the projectors and then for the Hamiltonians. In order to simplify the notations in the construction, we just consider an eigenvalue h and we will then apply the result to the eigenvalues h_1 and h_2.

4.3.1. Formal superadiabatic projectors.

THEOREM 4.8 (semiclassical projector evolution). *Assume the eigenvalue h of the Hamiltonian H_0 satisfies Assumption 4.7 in $\mathcal{D}$. Then, there exists a unique formal series $\sum_{j\geq 1} \varepsilon^{j-1}\Pi_j$ in $\boldsymbol{S}^{-1}_{\varepsilon,\delta}(\mathcal{D})$ such that setting $\Pi_0(t,z) = \pi(t,z)$, the formal series*

$$\Pi^\varepsilon(t,z) = \sum_{j\geq 0} \varepsilon^j \Pi_j(t,z)$$

is a formal projection and

$$i\varepsilon\partial_t \Pi^\varepsilon(t) = [H^\varepsilon(t), \Pi^\varepsilon(t)]_\circledast. \tag{4.14}$$

Moreover the sub-principal term $\Pi_1(t)$ is an Hermitian matrix given by the following formulas:

$$\begin{aligned} \pi(t)\Pi_1(t)\pi(t) &= -\frac{1}{2i}\pi(t)\{\pi(t), \pi(t)\}\pi(t), \\ \pi(t)^\perp \Pi_1(t)\pi(t)^\perp &= \frac{1}{2i}\pi(t)^\perp\{\pi(t), \pi(t)\}\pi(t)^\perp, \\ \pi(t)^\perp \Pi_1(t)\pi(t) &= \pi(t)^\perp (H_0(t) - h(t))^{-1}\pi(t)^\perp R_1(t)\pi(t), \end{aligned} \tag{4.15}$$

where

$$R_1(t) = i\partial_t\pi(t) - \frac{1}{2i}\left(\{H_0(t), \pi(t)\} - \{\pi(t), H_0(t)\}\right) - [H_1(t), \pi(t)].$$

PROOF. With Notations 4.3,

$$\Pi^{\varepsilon,N} \circledast \Pi^{\varepsilon,N} - \Pi^{\varepsilon,N} = \varepsilon^{N+1} S_{N+1} + O(\varepsilon^{N+2}), \tag{4.16}$$

$$i\varepsilon\partial_t \Pi^{\varepsilon,N} - \left[H_0 + \varepsilon H_1, \Pi^{\varepsilon,N}\right]_\circledast = \varepsilon^{N+1} R_{N+1} + O(\varepsilon^{N+2}). \tag{4.17}$$

Step $N = 1$. We start with $N = 0$. We have $\Pi^{(0)} = \pi \in \boldsymbol{S}^0_\delta(\mathcal{D})$. Since $\pi^2 = \pi$ and $[H_0, \pi] = 0$, we obtain

$$S_1 = \tfrac{1}{2i}\{\pi, \pi\} \text{ and } R_1 = i\partial_t\pi - \tfrac{1}{2i}(\{H_0, \pi\} - \{\pi, H_0\}) - [H_1, \pi],$$

and we have $R_1, S_1 \in \boldsymbol{S}^0_\delta(\mathcal{D})$. Two structural observations are in order:

(1) The matrix S_1 is symmetric and satisfies $\pi S_1 \pi^\perp = \pi^\perp S_1 \pi = 0$.
(2) The matrix R_1 is skew-symmetric. It satisfies

$$\pi R_1 \pi = 0 \quad \text{and} \quad \pi^\perp R_1 \pi^\perp = [H_0, \pi^\perp S_1 \pi^\perp].$$

If H_0 has only two eigenvalues, H_0 expresses only in terms of π and the expression of R_1 given above shows that R_1 is off-diagonal. The situation is more complicated if H_0 has strictly more than two distinct eigenvalues. For verifying (2) in that case, one uses the Poisson bracket rule $\{A, BC\} - \{AB, C\} = \{A, B\}C - A\{B, C\}$ two times. We obtain

$$\begin{aligned}\{H_0, \pi\} - \{\pi, H_0\} &= \{H_0, \pi^2\} - \{\pi^2, H_0\} \\ &= \{h\pi, \pi\} + \{H_0, \pi\}\pi - H_0\{\pi, \pi\} - \{\pi, h\pi\} + \{\pi, \pi\}H_0 - \pi\{\pi, H_0\} \\ &= \pi\{h, \pi\} - \{\pi, h\}\pi + [\{\pi, \pi\}, H_0] + \{H_0, \pi\}\pi - \pi\{\pi, H_0\},\end{aligned}$$

which implies

$$\pi^\perp(\{H_0, \pi\} - \{\pi, H_0\})\pi^\perp = \pi^\perp[\{\pi, \pi\}, H_0]\pi^\perp.$$

For determining the π-diagonal component, we choose $A = \pi$, $B = H_0\pi^\perp$, and $C = \pi$ to obtain

$$\begin{aligned}0 &= \{\pi, H_0\pi^\perp\}\pi - \pi\{H_0\pi^\perp, \pi\} \\ &= \{\pi, H_0\}\pi - \{\pi, h\pi\}\pi - \pi\{H_0, \pi\} + \pi\{h\pi, \pi\} \\ &= \{\pi, H_0\}\pi - \{\pi, h\}\pi - \pi\{H_0, \pi\} + \pi\{h, \pi\}.\end{aligned}$$

This relation implies

$$\pi(\{H_0, \pi\} - \{\pi, H_0\})\pi = 0.$$

For constructing the matrix Π_1 that defines $\Pi^{(1)} = \pi + \varepsilon\Pi_1$, we need to satisfy

$$\pi\Pi_1 + \Pi_1\pi - \Pi_1 = -S_1 \quad \text{and} \quad -[H_0, \Pi_1] = -R_1.$$

The first of these two equations uniquely determines the diagonal blocks of Π_1, while the second equation uniquely determines the off-diagonal blocks. We obtain

$$\begin{aligned}&\pi\Pi_1\pi = -\pi S_1\pi \ \text{ and } \ \pi^\perp\Pi_1\pi^\perp = \pi^\perp S_1\pi^\perp, \\ &\pi\Pi_1\pi^\perp = -\pi R_1\pi^\perp(H_0 - h)^{-1} \ \text{ and } \ \pi^\perp\Pi_1\pi = (H_0 - h)^{-1}\pi^\perp R_1\pi.\end{aligned}$$

For concluding this first step, we deduce from $R_1, S_1 \in \boldsymbol{S}^0_\delta(\mathcal{D})$ that $\Pi_1 \in \boldsymbol{S}^{-1}_\delta(\mathcal{D})$.

Step $N \geq 1$. Next we proceed by induction and assume that we have constructed the matrices $\Pi_j(t) \in \boldsymbol{S}^{1-2j}_\delta(\mathcal{D})$ for $1 \leq j \leq N$ such that (4.16) and (4.17) hold. Note that by Lemma 4.3, this implies

$$R_{N+1}(t) \in \boldsymbol{S}^{-2N}_\delta(\mathcal{D}) \ \text{ and } \ S_{N+1}(t) \in \boldsymbol{S}^{-2N}_\delta(\mathcal{D}).$$

Indeed, $i\varepsilon\partial_t\Pi^{\varepsilon,N} - \big[H_0 + \varepsilon H_1, \Pi^{\varepsilon,N}\big]_\circledast$ is a formal series of $\varepsilon\,\boldsymbol{S}^{-2}_{\varepsilon,\delta}(\mathcal{D})$ while $\Pi^N \circledast \Pi^{\varepsilon,N} - \Pi^{\varepsilon,N}$ is a formal series of $\varepsilon\boldsymbol{S}^{-1}_{\varepsilon,\delta}(\mathcal{D})$. In order to go one step further, we see that Π_{N+1} has to satisfy

$$\pi\Pi_{N+1} + \Pi_{N+1}\pi - \Pi_{N+1} = -S_{N+2} \quad \text{and} \quad -[H_0, \Pi_{N+1}] = -R_{N+2}.$$

For solving these equations, and achieving the recursive process, we need to verify that at each step

(1) The matrix S_N is symmetric and satisfies $\pi S_N \pi^\perp = \pi^\perp S_N \pi = 0$.
(2) The matrix R_N is skew-symmetric and off-diagonal. It satisfies

$$\pi R_N \pi = 0 \quad \text{and} \quad \pi^\perp R_N \pi^\perp = [H_0, \pi^\perp S_N \pi^\perp].$$

Then, we will be able to construct $\Pi_{N+1}(t) \in \boldsymbol{S}_\delta^{-2N-1)}(\mathcal{D})$ and we will have as a by product $R_{N+2}(t) \in \boldsymbol{S}_\delta^{-2N-2}(\mathcal{D})$, $S_{N+2}(t) \in \boldsymbol{S}_\delta^{-2N-2}(\mathcal{D})$ because of equations (4.16), (4.17) and Lemma 4.3.

For proving (1), we take advantage of the fact that

$$Z := \Pi^{\varepsilon,N} \circledast \left((\Pi^{\varepsilon,N})^{2\circledast} - \Pi^{\varepsilon,N}\right) \circledast (\mathbb{I} - \Pi^{\varepsilon,N}) = \varepsilon^{N+1}\pi S_{N+1}\pi^\perp + O(\varepsilon^{N+2}),$$

while one also has by construction

$$Z = \left((\Pi^{\varepsilon,N})^{2\circledast} - \Pi^{\varepsilon,N}\right) \circledast \left(\Pi^{\varepsilon,N} - (\Pi^{\varepsilon,N})^{2\circledast}\right) = \mathcal{O}(\varepsilon^{2N+2}).$$

This implies that $\pi S_{N+1}\pi^\perp = 0$ and, using that S_{N+1} is hermitian, we deduce that it is diagonal.

For proving (2), we argue similarly with

$$Z' := \Pi^{\varepsilon,N} \circledast \left(i\varepsilon\partial_t\Pi^{\varepsilon,N} - \left[H_0 + \varepsilon H_1, \Pi^{\varepsilon,N}\right]_\circledast\right) \circledast \Pi^{\varepsilon,N} = \varepsilon^{N+1}\pi R_{N+1}\pi + O(\varepsilon^{N+2}),$$

which also satisfies

$$Z' = \left((\Pi^{\varepsilon,N})^{2\circledast} - \Pi^{\varepsilon,N}\right) \circledast (H_0 + \varepsilon H_1)\Pi^{\varepsilon,N} - \Pi^{\varepsilon,N}(H_0 + \varepsilon H_1)\left((\Pi^{\varepsilon,N})^{2\circledast} - \Pi^{\varepsilon,N}\right) = O(\varepsilon^{2N+2}).$$

This implies $\pi R_{N+1}\pi = 0$ and one can argue similarly with $1 - \Pi^{\varepsilon,N}$ for obtaining the other relation $\pi^\perp R_{N+1}\pi^\perp = 0$. □

4.3.2. Formal adiabatic decoupling. The second (and decisive) part of the analysis is a formal adiabatic decoupling using the superadiabatic projectors introduced before.

THEOREM 4.9 (formal adiabatic decoupling). *Assume the eigenvalue h of the Hamiltonian H_0 satisfies Assumption 4.7 in $\mathcal{D}$. There exists a formal time dependent Hermitian Hamiltonian in $\mathcal{D}$,*

$$H^{\mathrm{adia},\varepsilon} = \sum_{j\geq 0} \varepsilon^j H_j^{\mathrm{adia}}$$

such that

$$\Pi^\varepsilon \circledast (i\varepsilon\partial_t - H^\varepsilon) = (i\varepsilon\partial_t - H^{\mathrm{adia},\varepsilon}) \circledast \Pi^\varepsilon \tag{4.18}$$

with the following properties:

1. *The principal symbol is $H_0^{\mathrm{adia}} = h\,\mathbb{I}_{\mathbb{C}^m}$.*
2. *The subprincipal term H_1^{adia} is a Hermitian matrix satisfying*

$$\pi^\perp H_1^{\mathrm{adia}}\pi = \pi^\perp\left(i\partial_t\pi + i\{h,\pi\}\right)\pi \quad \textit{and} \quad \pi H_1^{\mathrm{adia}}\pi = \pi H_1\pi + \frac{1}{2i}\pi\{H_0,\pi\}\pi$$

   (see (1.19)) and we can choose $\pi^\perp H_1^{\mathrm{adia},\varepsilon}\pi^\perp = 0$.
3. *We have*

$$\varepsilon^{-2}\left(H^{\mathrm{adia},\varepsilon} - h\mathbb{I}_{m,m} - \varepsilon H_1^{\mathrm{adia}}\right) \in \mathbf{S}_{\varepsilon,\delta}^{-1}(\mathcal{D}).$$

4. *Finally, $\pi(t)$ satisfies a transport equation along the classical flow for $h(t)$.*

$$\partial_t\pi + \{h,\pi\} = \frac{1}{i}[H_1^{\mathrm{adia}},\pi]. \tag{4.19}$$

REMARK 4.10. Note that equations (1.19) implies that $H_1^{\mathrm{adia}}(t,z)$ is smooth everywhere, including on the crossing set, if any.

The above construction applied to the Hamiltonian H^ε with two smooth eigenvalues (h_1,h_2) and two smooth eigenprojectors (π_1,π_2) imply the construction of two pairs of formal series

$$\Pi_\ell^\varepsilon = \sum_{j\geq 0}\varepsilon^j\Pi_{\ell,j} \quad \text{and} \quad H_\ell^{\mathrm{adia},\varepsilon} = \sum_{j\geq 0}\varepsilon^j H_{\ell,j}^{\mathrm{adia}}. \tag{4.20}$$

COROLLARY 4.11. At the level of the evolution operator, the result implies

$$\mathcal{U}_H^\varepsilon(t,t_0) = \widehat{\Pi_1^\varepsilon}(t)\mathcal{U}_1^{\mathrm{adia},\varepsilon}(t,t_0)\widehat{\Pi_1^\varepsilon}(t_0) + \widehat{\Pi_2^\varepsilon}(t)\mathcal{U}_2^{\mathrm{adia},\varepsilon}(t,t_0)\widehat{\Pi_2^\varepsilon}(t_0)$$

where for $\ell \in \{1,2\}$, $\mathcal{U}_\ell^{\mathrm{adia},\varepsilon}(t,t_0)$ are the evolution operators associated with the Hamiltonian $H_\ell^{\mathrm{adia},\varepsilon}$

PROOF. This result is Theorem 80 of Chapter 14 in [**13**] combined with Lemma 4.3. We first observe that equation (4.18) reduces to proving

$$\Pi^\varepsilon \circledast (i\varepsilon\partial_t - H^\varepsilon) = (i\varepsilon\partial_t - H^{\mathrm{adia},\varepsilon}) \circledast \Pi^\varepsilon. \tag{4.21}$$

For proving the latter relation, one first observes that if $H_0^{\mathrm{adia}} = h$, then we have

$$(H^{\mathrm{adia},\varepsilon} - H_0 - \varepsilon H_1) \circledast \Pi^\varepsilon = \varepsilon\left((h-H_0)\Pi_1 + (H_1^{\mathrm{adia}} - H_1)\pi + \frac{1}{2i}\{h - H_0, \pi\}\right) + i\partial_t\pi + \mathcal{O}(\varepsilon^2).$$

Therefore, H_1 has to be chosen so that

$$(H_1^{\mathrm{adia}} - H_1)\pi = (H_0 - h)\Pi_1 + \frac{1}{2i}\{H_0 - h, \pi\} + i\partial_t\pi.$$

In view of (4.15), this requires

$$\pi(H_1^{\mathrm{adia}} - H_1)\pi = \frac{1}{2i}\pi\{H_0,\pi\}\pi,$$

which is given by the second relation of (1.19), and, using again (4.15)

$$\pi^\perp(H_1^{\mathrm{adia}} - H_1)\pi = \pi^\perp(R_1 + \frac{1}{2i}\{H_0 - h, \pi\} + i\partial_t\pi)\pi = \pi^\perp(i\partial_t\pi + \frac{1}{2i}\{\pi, H_0\} - \frac{1}{2i}\{h,\pi\} - H_1)\pi$$

which is also given by the first relation of (1.19) in view of the observation that

$$\pi^\perp\{\pi, H_0, \pi\}\pi = -\pi^\perp\{h,\pi\}\pi.$$

For proving this relation, one uses the Poisson bracket rule

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

several times. First, one gets

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

Then, taking $A = \pi^\perp$, $B = \pi$, $C = H_0$, one gets

$$\{\pi^\perp, h\pi\} - 0 = \{\pi^\perp, \pi\}H_0 - \pi^\perp\{\pi, H_0\},$$

whence $-\pi^\perp\{\pi,h\}\pi = -\pi^\perp\{\pi,H_0\}\pi$. Finally, for concluding the construction of H_1^{adia}, It remains to check that

$$\left((H_0 - h)\Pi_1 + \frac{1}{2i}\{H_0 - h, \pi\} + i\partial_t\pi\right)\pi^\perp = 0$$

which comes from the latter observation about $\{H_0, \pi\}$.

Now that H_0^{adia} and H_1^{adia} are constructed, one uses a recursive argument: assume that one has constructed H_j^{adia} for $0 \le j \le N$ with $H_j^{\mathrm{adia}} \in \boldsymbol{S}_\delta^{-2j}$ for $j \in \{2, \cdots, N\}$ and such that has (4.21) holds up to $\mathcal{O}(\varepsilon^{N+1})$. Let us construct H_{N+1}^{adia}. Setting as in Notation 4.3

$$H^{\mathrm{adia},\varepsilon,N} = \sum_{j=1}^N \varepsilon^j H_j^{\mathrm{adia}}$$

we write

$$(H^{\mathrm{adia},\varepsilon,N} - H_0 - \varepsilon H_1) \circledast \Pi^{\varepsilon,N} = \varepsilon^{N+1} T_N + O(\varepsilon^{N+2})$$

with $T_N \in \boldsymbol{S}_\delta^{-2N-3}$ and we look for H_{N+1}^{adia} such that $\pi H_{N+1}^{\mathrm{adia}} = T_N$. This is doable as long as $\pi^\perp T_N = 0$, which comes form the observation that

$$(H_0 + \varepsilon H_1 - H^{\mathrm{adia},\varepsilon,N}) \circledast \Pi^{\varepsilon,N} \circledast (1 - \Pi^{\varepsilon,N}) = \varepsilon^{N+1} \pi^\perp T_N + \mathcal{O}(\varepsilon^{N+1}) = \mathcal{O}(\varepsilon^{N+1})$$

by the properties of superadiabatic projectors. Besides, $H_{N+1}^{\mathrm{adia}} \in \boldsymbol{S}_\delta^{-2N-3}$, which fits with (ii) of Definition 4.1

(3) comes from Lemma 4.3.

(4) comes from (1.19). □

CHAPTER 5

Propagation of wave packets through smooth crossings

In this section, we prove Theorem 1.21. We consider a subquadratic Hamiltonian $H^\varepsilon = H_0 + \varepsilon H_1$ satisfying Assumptions 1.2 in $I \times \Omega$, $\Omega \subset \mathbb{R}^{2d}$, and we are interested in the description of the solution to equation (1.1) for initial data that is a wave packet as in (1.8).

The proof consists in three steps: one first propagates the wave packet from time t_0 to some time $t^\flat - \delta$, $\delta > 0$ in a zone that is at a distance of Υ of size larger than $c\delta$ for some constant $c > 0$. In this zone, we use the superadiabatic projectors. Then, we propagate the wave packet from time $t^\flat - \delta$ to $t^\flat + \delta$, using the rough diagonalization in the crossing region. Finally, between times $t^\flat + \delta$ and t_1, we are again at distance larger than $c\delta$ to Υ and the analysis with superadiabatic projectors apply. The parameter δ will be taken afterwards as $\delta \approx \varepsilon^\alpha$; the analysis of Section 5.2 will ask for $\alpha < \frac{1}{2}$ (see Theorem 5.9).

In order to explain carefully each step of the proof, we start by proving the propagation faraway from the crossing area in Section 5.1. That allows us to settle the arguments, before doing it precisely close to Υ in Section 5.2. Then, Section 5.3 is devoted to the calculus of the transitions in the crossing region.

All along Section 5, we will use Assumption 4.7 and the following dynamical Assumption 5.1.

Assumption 5.1 (Dynamical assumption). We say that Ω_1 and t_1 satisfy the dynamical assumption (DA) for the mode h_ℓ if we have

(DA) $\Phi_\ell^{t,t_0}(\Omega_1) \subset \Omega$ for all $t \in [t_0, t_1]$.

5.1. Propagation faraway from the crossing area

In this section, we analyze the propagation of wave packets in a region where the gap is bounded from below. It gives the opportunity to introduce the method that we shall use in the next section for a small gap region. So, we fix $\delta = \delta_0$, $\delta_0 > 0$ small but independent on ε and we work in the open set

$$\Omega := \{z \in \mathbb{R}^{2d},\ |h_2(t,z) - h_1(t,z)| > \delta_0,\ \ \forall t \in [t_0, t_1]\},\ \ \mathcal{D} = I \times \Omega$$

where I is an open interval of $\mathbb{R}$ containing $[t_0, t_1]$ and where the gap condition is also satisfied. We associate with H^ε the formal series of Theorems 4.9 and 4.8 for each of the modes:

$$\Pi_\ell^\varepsilon = \sum_{j \geq 0} \varepsilon^j \Pi_{\ell,j} \ \text{ and } \ H_\ell^{\mathrm{adia},\varepsilon} = \sum_{j \geq 0} \varepsilon^j H_{\ell,j}^{\mathrm{adia}}$$

and we will use the notation introduced in (4.3).

With $z_0 \in \Omega$, we associate the open sets Ω_0, Ω_1, Ω_2 and Ω_3 such that

$$z_0 \in \Omega_0 \Subset \Omega_2 \Subset \Omega_1 \Subset \Omega_3 \Subset \Omega$$

where Ω_0 and Ω_2 are constructed so that for any initial data $z \in \Omega_0$ the flows are staying in Ω_2:

$$\Phi_{h_\ell}^{t,t_0}(z) \in \Omega_2, \ \ \forall t \in [t_0, t_1], \ \ \forall z \in \Omega_0, \ \ \forall \ell \in \{1,2\}.$$

We associate cut-offs to these subsets. We take $\chi_0 \in C_0^\infty(\Omega_0)$ with $\chi_0 = 1$ near z_0. Then, we choose K_0 a compact neighborhood of z_0 in Ω_0, which implies that Ω_2 is a neighborhood of

$$\widetilde{K}_{\ell,0} := \{\Phi_{h_\ell}^{t,t_0}(K_0), \ t_0 \leq t \leq t_1\}, \ \ \ell \in \{1,2\}.$$

So we can choose $\chi_2 \in C_0^\infty(\Omega)$ with $\chi_2 = 1$ on $\widetilde{K}_0 = \widetilde{K}_{1,0} \cup \widetilde{K}_{2,0}$. Finally, we take $\chi_1, \chi_3 \in C_0^\infty(\Omega)$ with $\chi_1 = 1$ on $\mathrm{supp}(\chi_2)$ and $\chi_3 = 1$ on $\mathrm{supp}(\chi_1)$.

For $\ell \in \{1,2\}$, we set

$$\widetilde{H}_\ell^{\mathrm{adia},\varepsilon,N}(t) = \chi_3 \, H_\ell^{\mathrm{adia},\varepsilon,N}(t),$$

which is a smooth subquadratic Hamitonian, and we consider $\mathcal{U}_\ell^{\mathrm{adia},\varepsilon,N}(t,s)$ the propagator associated with the Hamiltonian $\chi_1 \, H_\ell^{\mathrm{adia},\varepsilon,N}(t)$.

The next result is the usual adiabatic decoupling that results from the preceding analysis.

PROPOSITION 5.2 (adiabatic decoupling - I). Let $k \in \mathbb{N}$.

(i) For any $\ell \in \{1,2\}$, we have in $\mathcal{L}(\Sigma_\varepsilon^k)$,

$$\begin{aligned} \Big(i\varepsilon\partial_t - \widehat{H}^\varepsilon(t)\Big) \, \mathrm{op}_\varepsilon\Big(\chi_1 \Pi_\ell^{N,\varepsilon}(t)\Big) \, \mathrm{op}_\varepsilon(\chi_2) = \\ \mathrm{op}_\varepsilon\Big(\chi_1 \Pi_\ell^{N,\varepsilon}(t)\Big) \, \Big(i\varepsilon\partial_t - \mathrm{op}_\varepsilon\Big(\chi_3 H_\ell^{\mathrm{adia},N,\varepsilon}(t)\Big)\Big) \, \mathrm{op}_\varepsilon(\chi_2) + \mathcal{O}(\varepsilon^{N+1}). \end{aligned} \tag{5.1}$$

(ii) Let $\psi_0^\varepsilon \in \Sigma_\varepsilon^k$ such that $\widehat{\chi}_0 \psi_0^\varepsilon = \psi_0^\varepsilon + \mathcal{O}(\varepsilon^\infty)$. Set

$$\psi_\ell^{\varepsilon,N}(t) = \mathrm{op}_\varepsilon\Big(\chi_1 \Pi_\ell^{N,\varepsilon}(t)\Big) \, \mathcal{U}_\ell^{\mathrm{adia},N,\varepsilon}(t,t_0) \, \mathrm{op}_\varepsilon\Big(\chi_0 \Pi_\ell^{N,\varepsilon}(t_0)\Big) \, \psi_0^\varepsilon, \ \ \ell \in \{1,2\}.$$

Then we have in Σ_ε^k,

$$\mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon = \psi_1^{\varepsilon,N}(t) + \psi_2^{\varepsilon,N}(t) + \mathcal{O}(\varepsilon^{N+1}), \ \forall t \in [t_0,t_1]. \tag{5.2}$$

REMARK 5.3. (1) The assumption satisfied by $(\psi_0^\varepsilon)_{\varepsilon>0}$ in (ii) of Proposition 5.2 is sometimes referred in the literature as having a compact semi-classical wave front set.

(2) In the proof below, the reader will notice that we do not need to assume that $H^\varepsilon(t)$ is sub-quadratic, we only need to know that $\widehat{H}^\varepsilon(t)$ defines a unitary Schrödinger propagator in $L^2(\mathbb{R}^d, \mathbb{C}^m)$. However, we use the boundedness of the derivatives of the projectors.

PROOF. (i) We fix $\ell \in \{1,2\}$. Using Theorem 4.9, we obtain

$$\begin{aligned} (i\varepsilon\partial_t - H^\varepsilon(t)) \circledast (\chi_1 \Pi_\ell^{\varepsilon,N}(t)\Big) &= \chi_1 (i\varepsilon\partial_t - H^\varepsilon(t)) \circledast \Big(\chi_1 \Pi_\ell^{\varepsilon,N}(t)\Big) + \varepsilon^{N+1} R_N^\varepsilon \\ &= \chi_1 \Big(\Pi_\ell^{\varepsilon,N}(t)\Big) \circledast \Big(i\varepsilon\partial_t - H_\ell^{\mathrm{adia},\varepsilon,N}(t)\Big) + \varepsilon^{N+1} R_N^\varepsilon \\ &= \Big(\chi_1 \Pi_\ell^{\varepsilon,N}(t)\Big) \circledast \Big(i\varepsilon\partial_t - \widetilde{H}_\ell^{\mathrm{adia},\varepsilon,N}(t)\Big) + \varepsilon^{N+1} R_N^\varepsilon \end{aligned}$$

where the R_N^εs are rest terms that may change from one line to the other one and all satisfy $\chi_2 R_N^\varepsilon = 0$ and where we have used that $\chi_3 \chi_1 = \chi_1$. The relation on operators follows from Theorem B.1 and Corollary B.2 (with $\delta = 1$).

(ii) Let $K_0 = \mathrm{supp}(\chi_0)$. We apply (5.1) and we use that χ_2 is identically equal to 1 on the compact set $\widetilde{K}_0$. Hence, using Egorov Theorem of Appendix C.1, we have for $\ell \in \{1,2\}$

$$\begin{aligned}\widehat{\chi}_1\,\mathcal{U}_\ell^{\mathrm{adia},N,\varepsilon}(t,t_0)\,\widehat{\chi}_0 &= \widehat{\chi}_1\,\mathcal{U}_\ell^{\mathrm{adia},N,\varepsilon}(t,t_0)\,\widehat{\chi}_0\,\mathcal{U}_\ell^{\mathrm{adia},N,\varepsilon}(t,t_0)^{-1}\,\mathcal{U}_\ell^{\mathrm{adia},N,\varepsilon}(t,t_0)\\ &= \mathcal{U}_\ell^{\mathrm{adia},N,\varepsilon}(t,t_0)\,\widehat{\chi}_0 + \mathcal{O}(\varepsilon^{N+1}).\end{aligned}$$

Hence we deduce (5.2) from (5.1) using again the Egorov Theorem and that

$$\mathrm{op}_\varepsilon\left(\chi_1\Pi_1^{N,\varepsilon} + \chi_1\Pi_2^{N,\varepsilon}\right)\widehat{\chi}_0 = \widehat{\chi}_0 + \mathcal{O}(\varepsilon^{N+1}).$$

□

The adiabatic decoupling of Proposition 5.2 and Egorov Theorem (see Proposition C.1) allows to give an explicit description at any order of the solution of equation (1.1) for initial data that are focalized wave packets.

Indeed, by the technics of Appendix C that are classic when $\delta = 1$ (see for example the recent edition of [**13**]), one constructs two maps $\mathcal{R}_1(t,t_0,z)$ and $\mathcal{R}_2(t,t_0,z)$ introduced in (1.20)) and one has the following result (see Proposition C.5).

THEOREM 5.4. *Assume that ψ_0^ε a polarized wave packet:*

$$\psi_0^\varepsilon = \vec{V}_0\mathrm{WP}_{z_0}^\varepsilon(f_0), \quad \textit{with} \ \ f_0 \in \mathcal{S}(\mathbb{R}^d) \ \ \textit{and} \ \ \vec{V}_0 \in \mathbb{C}^m.$$

Let $N \geq 1$ and $k \geq 0$. Then, there exists a constant $C_{N,k} > 0$ such that the solution $\psi^\varepsilon(t)$ of (1.1) satisfies for all $t \in [t_0,t_1]$,

$$\left\|\psi^\varepsilon(t) - \left(\psi_1^{\varepsilon,N}(t) + \psi_2^{\varepsilon,N}(t)\right)\right\|_{\Sigma_\varepsilon^k} \leq C_{N,k}\,\varepsilon^N,$$

with for $\ell \in \{1,2\}$ and for all $M \geq 0$,

$$\psi_\ell^{\varepsilon,N}(t) = \mathrm{e}^{\frac{i}{\varepsilon}S_\ell(t,t_0,z_0)}\,\mathrm{WP}_{z_\ell(t)}^\varepsilon\left(\mathcal{R}_\ell(t,t_0,z_0)\mathcal{M}[F_\ell(t,t_0)]\sum_{0\leq j\leq M}\varepsilon^{j/2}\vec{B}_{\ell,j}(t)f_0\right) + \mathcal{O}(\varepsilon^{M/2}),$$

where $\vec{B}_{\ell,j}(t)$ are differential operators of degree $\leq 3j$ with vector-valued time-dependent coefficients satisfying (1.40) and (1.41).

5.2. Propagation close to the crossing area

Our goal in this section is to extend the result of Theorem 5.4 up a the time $t^\flat - c\delta$ for some $c > 0$ and $\delta \ll 1$. We follow the same strategy as in the preceding section and checks carefully the dependence in δ of the estimates.

More precisely, the situation is the following: we consider a wave packet at initial time t_0 that is focalized along the mode h_1 at some point z_0. We let it evolve along that mode according to Theorem 5.4, up to (t_1,z_1) conveniently chosen and we consider $\psi^\varepsilon(t_1)$ as a new initial data, knowing that it is a wave-packet, modulo $\mathcal{O}(\varepsilon^\infty)$. The point (t_1,z_1) is chosen close enough to $(t^\flat,\zeta^\flat)$ such that $|t_1 - t^\flat| + |z_1 - \zeta^\flat| \leq \eta_0$ where η_0 is defined in the next Lemma.

LEMMA 5.5. *Assume $(t^\flat,\zeta^\flat)$ is a generic smooth crossing point as in Definition 1.2 and consider $\delta \in (0,1]$.*

(1) *There exist $\eta_0 > 0$ and $c_0 > 0$ such that we have*

$$|f(t,\Phi_{h_1}^{t,t_1}(z))| \geq c_0|t - t^\flat| \ \ \textit{if} \ \ |t - t^\flat| + |z - \zeta^\flat| \leq \eta_0.$$

(2) *There exists $c, M > 0$ such that for all (t, z) satisfying $\left|z - \Phi_{h_1}^{t,t_1}(z_1)\right| \leq c\delta$, we have*

$$|f(t,z)| \geq c_0\delta - Mc\delta \geq \frac{c_0}{2}\delta.$$

PROOF. The result comes readily from the transversality of the curve $t \mapsto \Phi_{h_1}^{t,t_1}(z)$ to the set $\Upsilon = \{f = 0\}$. Recall that this transversality is due to Point (b) of Assumption 1.2. □

Our goal is to prove accurate estimates for the evolution of the solution $\psi^\varepsilon(t)$ of the Schrödinger equation with the initial data $\psi^\varepsilon(t_1)$, for $t \in [t_1, t^\flat - c\delta]$. We thus have to improve in this precise setting the accuracy of the estimates obtained before for fixed $\delta = \delta_0$.

We use the control in the small parameter δ of the Moyal product rule for ε-Weyl quantization as stated in Lemma 4.3 and the estimates in the Egorov Theorem for symbols in the classes $\mathbf{S}_{\varepsilon,\delta}$. Finally, the construction of the cut-off functions relies on the fact that due to Point (b) of Assumption 1.2, we can apply a straightening theorem for vector fields.

In several place we need to replace δ by $c\delta$, for a finite number of $0 < c = c_0, c_1, \cdots, c_L$ ($L \in \mathbb{N}$). We will not mention that point each time.

5.2.1. Localization up to the crossing region. We construct the cut-off functions by using thin tubes along the classical trajectories. We use a straightening theorem for non singular vector fields. We set $D(z_1, \rho_1) = \{|z - z_1| \leq \rho_1\}$ and consider a branch of trajectory

$$\mathcal{T}_1 := \{\Phi_h^{t,t_1}(z_1),\ t \in [t_1, t_1^+]\},\ \ t_1^+ > t^\flat.$$

LEMMA 5.6. [**2**] *Let be P_1 a transverse hyperplane to the curve $\mathcal{T}_1$ in z_1. There exist $\rho_1 > 0$ and $t_1^- < t_1 < t^\flat < t_1^+$ such that the map*

$$(t, z) \mapsto \Phi_h^{t,t_1}(z)$$

is a diffeomorphism from $]t_1^-, t_1^+[\times D(z_1, \rho_1)$ onto a neighborhood $\mathcal{W}_1$ of $\mathcal{T}_1$ in P_1.

Hence for any z in the tube $\mathcal{W}_1$, we have

$$z = \Phi_h^{\tau(z),t_1}(Y(z))$$

where τ and Y are smooth functions of z, $\tau(z) \in [t_1, t_1^+]$, $Y(z) \in D(z_1, \rho_1)$.

We then define the cut-off functions as follows: consider

- $\zeta \in C_0^\infty(]-2, 2[)$ equal to 1 in $[-1, 1]$,
- $\theta \in C^\infty(\mathbb{R})$ with $\theta(t) = 0$ if $t \leq -1$ and $\theta(t) = 1$ if $t \geq 1$,

we set for $\delta > 0$,

$$\chi^\delta(z) = \theta\left(\frac{\tau(z) - t_1^-}{\eta}\right)(1 - \zeta)\left(\frac{\tau(z) - t^\flat}{c\delta}\right)\zeta\left(\frac{|z - \Phi_h^{\tau(z),t_1}(z_1)|^2}{(C\delta)^2}\right),$$

where $c > 0, C > 0$ and $\eta > 0$ is a small enough constant.

By adapting the constants c and C conveniently, we construct some functions

$$\chi_j^\delta \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}, [0, 1]),\ \ j \in \{1, 2, 3\},$$

such that

(1) $\chi_j^\delta = 1$ on $\bigcup_{t_0 \leq t \leq t_1} B\left(\Phi_h^{t_0,t}(z_0), c_j\delta\right)$ and χ_j^δ is supported in $\bigcup_{t_0 \leq t \leq t_1} B\left(\Phi_h^{t_0,t}(z_0), 2c_j\delta\right)$,

(2) for all $\gamma \in \mathbb{N}^{2d}$, there exists C_γ such that for all $z \in \mathbb{R}^{2d}$

$$|\partial_z^\gamma \chi_j^\delta(z)| \leq C_\gamma\, \delta^{-|\gamma|},$$

(3) $\chi_3^\delta = 1$ on $\mathrm{supp}\chi_1^\delta$ and $\chi_1^\delta = 1$ on $\mathrm{supp}\chi_2^\delta$.

Finally, with $\chi_0 \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}, [0,1])$ satisfying $\chi_0 = 1$ on $B(0,1)$ and $\chi_0(z) = 0$ for $|z| \geq 2$, we associate

$$\chi_0^\delta(z) = \chi_0\left(\frac{z_1 - z}{\delta}\right).$$

And we consider χ_4 a smooth fixed cut-off (δ-independent).

5.2.2. Adiabatic decoupling close to the gap. Omitting the mode index, we set

$$\widetilde{H}^{\mathrm{adia},N,\varepsilon}(t) = \chi_4\left(h(t) + \varepsilon H_1^{\mathrm{adia}}(t)\right) + \chi_3^\delta\left(\sum_{2\leq j\leq N} \varepsilon^j H_j^{\mathrm{adia}}(t)\right). \tag{5.3}$$

Notice that, because the crossing is smooth, the eigenavalues h_ℓ, π_ℓ and the first adiabatic correctors $H_{\ell,1}^{\mathrm{adia}}$ are smooth, even in a neighborhood of $(t^\flat, \zeta^\flat)$.

Let $\mathcal{U}^{\mathrm{adia},N,\varepsilon}(t,s)$ be the quantum propagator associated with the Hamiltonian $\widetilde{H}^{\mathrm{adia},N,\varepsilon}(t)$ (omitting once again the index $\ell = 1$). The following result is a consequence of the sharp estimates given in [**6**] concerning propagation of quantum observables (see (ii) of the Egorov Theorem C.1).

Proposition 5.7. Consider the cut-off functions χ_0^δ and χ_2^δ defined above and set for $t \in [t_1, t^\flat - c\delta]$

$$\mathrm{op}_\varepsilon(\chi_0^\delta(t,t_1)) := \mathcal{U}^{\mathrm{adia},\varepsilon,N}(t,t_1)\,\mathrm{op}_\varepsilon(\chi_0^\delta)\,\mathcal{U}^{\mathrm{adia},\varepsilon,N}(t_1,t).$$

Then, for any $M \geq 1$, $z \in \mathbb{R}^{2d}$ and $t \in [t_1, t^\flat - c\delta]$, we have:

$$(1 - \chi_2^\delta) \circledast \chi_0^\delta(t,t_0,z) = \left(\frac{\varepsilon}{\delta^2}\right)^M \zeta_M(t) \ \text{ with } \ \zeta_M(t,z) \in \boldsymbol{S}_{\delta^2}(\mathcal{D}).$$

Revisiting the proof of Proposition 5.2, using Lemma 4.3 for the formal series $\Pi_\ell^\varepsilon \in \boldsymbol{S}_{\delta^2}^0(\mathcal{D})$ and using (3) of Theorem 4.9 about $H_\ell^{\varepsilon,\mathrm{adia}}$, we obtain the following result.

Proposition 5.8 (adiabatic decoupling - II). With the previous notations, we have the following properties.

(ii) For $t_1 \leq t \leq t^\flat - \delta$, we have

$$\begin{aligned}\Big(i\varepsilon\partial_t - \widehat{H}^\varepsilon(t)\Big)\ \mathrm{op}_\varepsilon\left(\chi_1^\delta\,\Pi^{N,\varepsilon}(t)\right)\ \mathrm{op}_\varepsilon(\chi_2^\delta)& \\ = \mathrm{op}_\varepsilon\left(\chi_1^\delta\,\Pi^{N,\varepsilon}(t)\right)\Big(i\varepsilon\partial_t - \mathrm{op}_\varepsilon(\widetilde{H}^{\mathrm{adia},N,\varepsilon}(t))\Big)\ \mathrm{op}_\varepsilon(\chi_2^\delta) + \mathcal{O}\left(\left(\frac{\varepsilon}{\delta^2}\right)^{N+1}\delta^{-\kappa_0}\right)&\end{aligned} \tag{5.4}$$

where $\kappa_0 \in \mathbb{N}$ is N-independent.

(ii) Set for $\ell = 1$,

$$\psi_\ell^{\varepsilon,N}(t) = \mathrm{op}_\varepsilon\left(\chi_1^\delta \Pi_\ell^{N,\varepsilon}(t)\right)\mathcal{U}_\ell^{\mathrm{adia},N,\varepsilon}(t,t_1)\,\mathrm{op}_\varepsilon\left(\chi_0^\delta \Pi_\ell^{N,\varepsilon}(t_1)\right)\psi^\varepsilon(t_1)$$

where $\psi^\varepsilon(t_1) = \mathcal{U}_H^\varepsilon(t_1,t_0)\psi^\varepsilon(t_0)$. Then we have, for $N \geq 2$ and for all $t \in [t_1, t^\flat - \delta]$,

$$\mathcal{U}_H^\varepsilon(t,t_0)\psi_0^\varepsilon = \psi_1^{\varepsilon,N}(t) + \psi_2^{\varepsilon,N}(t) + \mathcal{O}\left(\left(\frac{\varepsilon}{\delta^2}\right)^{N+1}\delta^{-\kappa_0}\right).$$

where $\mathcal{U}_\ell^{\mathrm{adia},N,\varepsilon}$ is the propagator associated with the Hamiltonian $\widetilde{H}^{\mathrm{adia},N,\varepsilon}(t)$.

The Remark 5.3 is valid also for this Proposition, furthermore here the coefficients of the expansion of $\psi_j^{\varepsilon,N}(t)$ in $\sqrt{\varepsilon}$ are δ-dependent for the order $\varepsilon^{k/2}$ for $k \geq 2$.

Note that the integer κ_0 stems from the symbolic calculus estimates of Theorem B.1.

5.2.3. Application to wave packets. As in Theorem 5.4, the previous results have consequences for wave packets propagation and give an asymptotic expansion mod $\mathcal{O}(\varepsilon^\infty)$ for any $\alpha < 1/2$ if $\delta \approx \varepsilon^\alpha$. In other words the super-adiabatic approximation is valid for times t such that $|t - t^\flat| \geq \varepsilon^{1/2-\eta}$, for any $\eta > 0$. The results of Appendix C give the following result.

THEOREM 5.9. *Consider*

$$\psi_1^\varepsilon := \psi^\varepsilon(t_1) = \mathrm{WP}^\varepsilon_{z_1}(\varphi_1^\varepsilon), \;\; \varphi_1^\varepsilon \in \mathcal{S}(\mathbb{R}^d) \;\; \textit{modulo } \mathcal{O}(\varepsilon^\infty).$$

There exist $N_0 \in \mathbb{N}$ and two families of differential operators $\left(\vec{B}_{\ell,j}(t)\right)_{j\in\mathbb{N}}$, $\ell \in \{1,2\}$ such that setting for $t \in [t_1, t^\flat - \delta]$

$$\psi_\ell^{\varepsilon,N}(t) = \mathrm{e}^{\frac{i}{\varepsilon}S_\ell(t,t_0,z_0)}\mathrm{WP}^\varepsilon_{z_\ell(t)}\left(\mathcal{R}_\ell(t,t_0)\,\mathcal{M}[F_\ell(t,t_0)]\sum_{0\leq j\leq 2N}\varepsilon^{j/2}\vec{B}_{\ell,j}(t)\varphi_0\right), \tag{5.5}$$

one has the following property: for all $k \in \mathbb{N}$, $N \in \mathbb{N}$, there exists $C_{N,k} > 0$ such that the solution $\psi^\varepsilon(t)$ of (1.1) satisfies for all $t \in [t_1, t^\flat - \delta]$.

$$\left\|\psi^\varepsilon(t) - \left(\psi_1^{\varepsilon,N}(t) + \psi_2^{\varepsilon,N}(t)\right)\right\|_{\Sigma^k_\varepsilon} \leq C_{N,k}\left(\frac{\varepsilon}{\delta^2}\right)^{N+1}\delta^{-\kappa_0}.$$

Moreover the operators $B_{\ell,j}(t)$ are differential operators of degree $\leq 3j$ with time dependent smooth vector-valued coefficients and satisfy (1.40) and (1.41).

5.3. Propagation through the crossing set

We now use the rough reduction of section 4.2 to treat the zone around the crossing. We fix the point $(t^\flat, \zeta^\flat) \in \Upsilon$ and consider trajectories $z_1(t)$ and $z_2(t)$ arriving simultaneously at time $t^\flat$ in the point $\zeta^\flat$. We consider $N \in \mathbb{N}$ and we set

$$\underline{\psi}_\ell^{\varepsilon,N}(t) = \widehat{\pi_\ell^{\varepsilon,N}(t)}\psi^\varepsilon(t), \;\; \ell \in \{1,2\}.$$

By Theorem 4.5, if $k \in \mathbb{N}$, the solution $\psi^\varepsilon(t)$ of the Schrödinger equation (1.1) satisfies in Σ^k_ε,

$$\psi^\varepsilon(t) = \underline{\psi}_1^{\varepsilon,N}(t) + \underline{\psi}_2^{\varepsilon,N}(t) + O(\varepsilon^{N+1}). \tag{5.6}$$

Our aim in this section is to determine $\psi^\varepsilon(t^\flat + \delta)$ in terms of $\psi^\varepsilon(t^\flat - \delta)$ by using the description (5.6) of $\psi^\varepsilon(t)$.

The family $\underline{\psi}^{\varepsilon,N} = {}^t(\underline{\psi}_1^{\varepsilon,N}, \underline{\psi}_2^{\varepsilon,N})$ satisfies

$$i\varepsilon\partial_t\underline{\psi}^{\varepsilon,N} = \widehat{\underline{H}^{\varepsilon,N}}(t)\underline{\psi}^{\varepsilon,N} \tag{5.7}$$

with

$$\underline{H}^{\varepsilon,N}(t) := \begin{pmatrix} h_1^{\varepsilon,N}(t,z) & 0 \\ 0 & h_2^{\varepsilon,N}(t,z)\end{pmatrix} + \begin{pmatrix} 0 & W^{\varepsilon,N}(t) \\ W^{\varepsilon,N}(t)^* & 0\end{pmatrix}.$$

According to Theorem 4.5, the Hamiltonian $\underline{H}^\varepsilon$ is subquadratic (see Definition 1.1), thus for $k, N \in \mathbb{N}$ there exists $C_{k,N} > 0$ such that for all $\varepsilon > 0$ and $t \in I$,

$$\|\widehat{W}^{\varepsilon,N}(t)\|_{\mathcal{L}(\Sigma^{k+1}_\varepsilon, \Sigma^k_\varepsilon)} \leq C_{k,N}\varepsilon. \tag{5.8}$$

We have used here the fact that the asymptotic series $W^{\varepsilon,}$ starts with the term of order ε and we recall that the value of W_1 is given in (1.44).

Let us summarize the information about the data that comes from the preceding section. Let $\delta > 0$, for all $s \in (t^\flat - \delta, t^\flat - \frac{\delta}{2})$,

$$\underline{\psi}^{\varepsilon,N}(s) = {}^t\left(\mathrm{WP}^{\varepsilon}_{z_1(s)}(\varphi_1^{\varepsilon,N}(s)), \mathrm{WP}^{\varepsilon}_{z_2(s)}(\varphi_2^{\varepsilon,N}(s))\right), \tag{5.9}$$

with for $\ell = 1, 2$,

$$\varphi_\ell^{\varepsilon,N} = \sum_{j=0}^{N} \varepsilon^{\frac{j}{2}} \varphi_{j,\ell}, \quad \varphi_{j,\ell} \in \mathcal{S}(\mathbb{R}^d).$$

Our aim is to prove that the description of $\underline{\psi}^{\varepsilon,N}(s)$ given in Equation (5.9) extends to $s = t^\flat + \delta$ and to derive precise formula for $\varphi_{j,\ell}(t^\flat + \delta)$ when $j = \{0, 1\}$ and $\ell \in \{1, 2\}$.

We consider the Hamiltonians

$$H^{\varepsilon,N}_{\mathrm{diag}}(t,z) = \begin{pmatrix} h_1^{\varepsilon,N}(t,z) & 0 \\ 0 & h_2^{\varepsilon,N}(t,z) \end{pmatrix}$$

and

$$\varepsilon H^{\varepsilon,N}_{\mathrm{adiag}}(t,z) = \begin{pmatrix} 0 & W^{\varepsilon,N}(t) \\ W^{\varepsilon,N}(t)^* & 0 \end{pmatrix}.$$

so that $\underline{H}^{\varepsilon,N} = H^{\varepsilon,N}_{\mathrm{diag}} + \varepsilon H^{\varepsilon,N}_{\mathrm{adiag}}$. We fix N large enough and, for simplifying the notations, we drop the mentions of N in the following. We use the notations

$$\mathcal{U}^{\varepsilon}_{\underline{H}}(t,s) \text{ and } \mathcal{U}^{\varepsilon}_{H_{\mathrm{diag}}}(t,s)$$

for the propagators associated to the truncated Hamiltonians $H^{\varepsilon,\delta,N}(t)$ and $H^{\varepsilon,N}_{\mathrm{diag}}(t)$ respectively, omitting the mention of δ in $\mathcal{U}^{\varepsilon}_{\underline{H}}(t,s)$. The action of $\mathcal{U}^{\varepsilon}_{\underline{H}}(t,s)$ on wave packets is described by the next Theorem on which we focus now. It gives a precise description of the action of $\mathcal{U}^{\varepsilon}_{\underline{H}}(t^\flat + \delta, t^\flat - \delta)$ on a wave packet and describes the propagation of a wave packet through the crossing set, in particular the exchange of modes at the crossing points.

THEOREM 5.10. *Let $k, N, M \in \mathbb{N}$ with $M \leq N$. Let $\delta > 0$ such that $\delta^2 \geq \sqrt{\varepsilon}$. Then, there exists $C > 0$ and an operator $\Theta^{\varepsilon,\delta}_M$ such that for all $\varepsilon \in (0,1)$,*

$$\mathcal{U}^{\varepsilon}_{\underline{H}}(t^\flat + \delta, t^\flat - \delta) = \mathcal{U}^{\varepsilon}_{\mathrm{diag}}(t^\flat + \delta, t^\flat)\, \Theta^{\varepsilon,\delta}_M\, \mathcal{U}^{\varepsilon}_{\mathrm{diag}}(t^\flat, t^\flat - \delta) + R^{\varepsilon,\delta}_M \tag{5.10}$$

with $\|R^{\varepsilon,\delta}_M\|_{\mathcal{L}(\Sigma^{k+M+1}_\varepsilon, \Sigma^k)} \leq C\delta^{M+1}$ and

$$\Theta^{\varepsilon,\delta}_M(t^\flat) = \mathbb{I} + \sum_{1 \leq m \leq M} \Theta^{\varepsilon,\delta}_{m,M}(t^\flat).$$

Moreover, there exists $\varepsilon_0 > 0$, and a family of operators $(\mathcal{T}^{\varepsilon,\delta}_{m,M})_{m \geq 1}$ such that for all $\vec{\varphi} \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^2)$, $m \geq 1$, $\varepsilon \in (0, \varepsilon_0)$,

$$\Theta^{\varepsilon,\delta}_{m,M} \mathrm{WP}_{\zeta^\flat}(\varphi) = \mathrm{WP}^{\varepsilon}_{\zeta^\flat}(\mathcal{T}^{\varepsilon,\delta}_{m,M}\vec{\varphi}) + O(\sqrt{\varepsilon}\|\varphi\|_{\Sigma^{k+2m+2}}) \tag{5.11}$$

with

$$\|\mathcal{T}^{\varepsilon,\delta}_{m,M}\vec{\varphi}\|_{\Sigma^k} \leq c_{k,m,M}\, \varepsilon^{\frac{m}{2}} |\log\varepsilon|^{\max(0,m-1)}\, \|\vec{\varphi}\|_{\Sigma^{k+2m+1}} \tag{5.12}$$

for some constants $c_{k,m} > 0$. Besides, with the notation (1.43)

$$\mathcal{T}^{\varepsilon,\delta}_{1,M} = \begin{pmatrix} 0 & W_1(t^\flat,\zeta^\flat)\mathcal{T}^\flat_{2\to 1} \\ W_1(t^\flat,\zeta^\flat)^*\mathcal{T}^\flat_{1\to 2} & 0 \end{pmatrix}. \tag{5.13}$$

We point out that some additional action effects will appear when applying $\mathcal{U}^\varepsilon_{\underline{H}}(t^\flat+\delta,t^\flat-\delta)$ to a wave packet via the operators $\mathcal{U}^\varepsilon_{\mathrm{diag}}(t^\flat+\delta,t^\flat)$ and $\mathcal{U}^\varepsilon_{\mathrm{diag}}(t^\flat,t^\flat-\delta)$. When applied to a Gaussian wave packets, i.e. when $\varphi_{\ell,1} = g^\Gamma_\ell$ in (5.9), the leading order correction term at time $t^\flat+\delta$ due to the crossing is

$$\sqrt{\varepsilon}\begin{pmatrix} \mathrm{e}^{\frac{i}{\varepsilon}S_1(t^\flat+\delta,t^\flat,\zeta^\flat)+\frac{i}{\varepsilon}S_2(t^\flat,t_0,z_0)}\mathrm{WP}^\varepsilon_{z_1(t^\flat+\delta)}(\varphi_1) \\ \mathrm{e}^{\frac{i}{\varepsilon}S_2(t^\flat+\delta,t^\flat,\zeta^\flat)+\frac{i}{\varepsilon}S_1(t^\flat,t_0,z_0)}\mathrm{WP}^\varepsilon_{z_2(t^\flat+\delta)}(\varphi_2) \end{pmatrix}$$

with

$$\begin{aligned}\varphi_1 &= \mathcal{M}[F_1(t^\flat+\delta,t^\flat,\zeta^\flat)]W_1(t^\flat,\zeta^\flat)\mathcal{T}^\flat_{2\to 1}\mathcal{M}[F_2(t^\flat,t_0,z_0)]g^\Gamma_2,\\ \varphi_2 &= \mathcal{M}[F_2(t^\flat+\delta,t^\flat,\zeta^\flat)]W_1(t^\flat,\zeta^\flat)^*\mathcal{T}^\flat_{1\to 2}\mathcal{M}[F_1(t^\flat,t_0,z_0)]g^\Gamma_1.\end{aligned}$$

Recall that W_1 is the off-diagonal matrix described in (1.44).

The remainder of this section is devoted to the proof of Theorem 5.10. The use of Dyson series allows to obtain the decomposition (5.10) (see Section 5.3.1). Then, the analysis of each terms of the series is made in Sections 5.3.2 and 5.3.3. Finally, we recall how to compute explicitly the quantities $\mathcal{T}^{\varepsilon,\delta}_{m,M}$ and $S^\flat_{1,m}$ in Section 5.3.5, which was already done in [**20**].

Before starting the proof, we introduce a cut-off $\chi_\delta(t) = \chi\left(\frac{t-t^\flat}{\delta}\right)$, $\chi_0 \in C^\infty_0]-1,1[$, $\chi_0(t)=1$ if $|t|\le 1/2$. We set

$$\underline{H}^{\varepsilon,\delta,N}(t) = H^{\varepsilon,N}_{\mathrm{diag}}(t) + \varepsilon\chi_\delta(t-t^\flat)H^{\varepsilon,N}_{\mathrm{adiag}}(t)$$

and we consider the propagator $\mathcal{U}^\varepsilon_{\underline{H}_\delta}(t,s)$ associated with $\underline{H}^{\varepsilon,\delta,N}$. We claim that if Theorem 5.10 holds for $\mathcal{U}^\varepsilon_{\underline{H}_\delta}(t,s)$, then it also holds for $\mathcal{U}^\varepsilon_{\underline{H}}(t,s)$.

Indeed, we have for $t\in[t^\flat+\delta,t^\flat+\frac{\delta}{2}]$,

$$\mathcal{U}^\varepsilon_{\underline{H}}(t,t^\flat-\delta) = \mathcal{U}^\varepsilon_{\underline{H}_\delta}(t^\flat+\delta,t^\flat-\delta)\underline{\psi}^{\varepsilon,N}(t^\flat-\delta) + i\int_{t^\flat-\delta}^t \mathcal{U}^\varepsilon_{\underline{H}_\delta}(t,s)(1-\chi_\delta)(s-t^\flat)\widehat{\underline{H}^{\varepsilon,N}_{\mathrm{adiag}}}(s)\mathcal{U}^\varepsilon_{\underline{H}}(s,t^\flat-\delta)ds.$$

This formula allows to obtain (5.10) for $\mathcal{U}^\varepsilon_{\underline{H}}(t,t^\flat-\delta)$. It remains to consider the action of $\mathcal{U}^\varepsilon_{\underline{H}}(t,t^\flat-\delta)$ on asymptotic sum of wave packets We observe that in the support of the integral, $|t^\flat-s|>\frac{\delta}{2}$ and $-\delta\le s-t^\flat\le\frac{\delta}{2}$. Therefore, $s\in[t^\flat-\delta,t^\flat-\frac{\delta}{2}]$ on the support of the integral. where we know that $\mathcal{U}^\varepsilon_{\underline{H}}(s,t^\flat-\delta)$ propagates wave packets, whence the expansion in wave packets To conclude, we observe that since $|t^\flat-s|>\frac{\delta}{2}$ on the support of the integral term, we have

$$\mathcal{U}^\varepsilon_{\underline{H}}(t^\flat+\delta,t^\flat-\delta) = \mathcal{U}^\varepsilon_{\underline{H}_\delta}(t^\flat+\delta,t^\flat-\delta) + O(\delta^2) = \mathcal{U}^\varepsilon_{\underline{H}_\delta}(t^\flat+\delta,t^\flat-\delta) + o(\sqrt{\varepsilon})$$

so the formula for the first two terms of the asymptotic assumptions are the same.

In view of these considerations, we focus in the next sections in proving Theorem 5.10 for the Hamiltonian $\underline{H}^{\varepsilon,\delta,N}(t)$.

5.3.1. Dyson expansion. We perform a Dyson expansion via the Duhamel formula. A first use of Duhamel formula gives for $t_1, t_2 \in \mathbb{R}$,

$$\mathcal{U}^\varepsilon_{\underline{H}}(t_2,t_1) = \mathcal{U}^\varepsilon_{H_{\rm diag}}(t_2,t_1) + i^{-1}\int_{t_1}^{t_2} \mathcal{U}^\varepsilon_{\underline{H}}(t_2,s_1)\widehat{H^\varepsilon_{\rm adiag}}(s_1)\mathcal{U}^\varepsilon_{H_{\rm diag}}(s_1,t_1)ds_1. \tag{5.14}$$

With one iteration of the Duhamel formula, we obtain

$$\begin{aligned}\mathcal{U}^\varepsilon_{\underline{H}}(t_2,t_1) = \mathcal{U}^\varepsilon_{H_{\rm diag}}(t_2,t_1) &+ i^{-1}\int_{t_1}^{t_2} \mathcal{U}^\varepsilon_{H_{\rm diag}}(t_2,s_1)\widehat{H^\varepsilon_{\rm adiag}}(s_1)\mathcal{U}^\varepsilon_{H_{\rm diag}}(s_1,t_1)ds_1\\ &- \int_{t_1}^{t_2}\int_{s_1}^{t_2} \mathcal{U}^\varepsilon_{\underline{H}}(t_2,s_2)\widehat{H^\varepsilon_{\rm adiag}}(s_2)\mathcal{U}^\varepsilon_{H_{\rm diag}}(s_2,s_1)\widehat{H^\varepsilon_{\rm adiag}}(s_1)\mathcal{U}^\varepsilon_{H_{\rm diag}}(s_1,t_1)ds_1ds_2.\end{aligned}$$

With two iterations, we have

$$\begin{aligned}\mathcal{U}^\varepsilon_{\underline{H}}(t_2,t_1) = \mathcal{U}^\varepsilon_{H_{\rm diag}}(t_2,t_1) &+ i^{-1}\int_{t_1}^{t_2} \mathcal{U}^\varepsilon_{H_{\rm diag}}(t_2,s_1)\widehat{H^\varepsilon_{\rm adiag}}(s_1)\mathcal{U}^\varepsilon_{H_{\rm diag}}(s_1,t_1)ds_1\\ &- \int_{t_1}^{t_2}\int_{s_1}^{t_2} \mathcal{U}^\varepsilon_{\rm diag}(t_2,s_2)\widehat{H^\varepsilon_{\rm adiag}}(s_2)\mathcal{U}^\varepsilon_{H_{\rm diag}}(s_2,s_1)\widehat{H^\varepsilon_{\rm adiag}}(s_1)\mathcal{U}^\varepsilon_{H_{\rm diag}}(s_1,t_1)ds_1ds_2\\ &- \frac{1}{i}\int_{t_1}^{t_2}\int_{s_2}^{t_2}\int_{s_1}^{t_2} \mathcal{U}^\varepsilon_{H_{\rm diag}}(t_2,s_3)\widehat{H^\varepsilon_{\rm adiag}}(s_3)\mathcal{U}^\varepsilon_{\rm diag}(s_3,s_2)\widehat{H^\varepsilon_{\rm adiag}}(s_2)\\ &\qquad\qquad \times \mathcal{U}^\varepsilon_{H_{\rm diag}}(s_2,s_1)\widehat{H^\varepsilon_{\rm adiag}}(s_1)\mathcal{U}^\varepsilon_{H_{\rm diag}}(s_1,t_1)ds_1ds_2\end{aligned}$$

After M iterations, $M \in \mathbb{N}$, we have the Dyson formula

$$\begin{aligned}\mathcal{U}^\varepsilon_{\underline{H}}(t_2,t_1) = \mathcal{U}^\varepsilon_{H_{\rm diag}}(t_2,t_1)\Bigg(\mathbb{I} &+\\ \sum_{1\le m\le M}(i)^{-m}\int_{\mathcal{P}(t_2,t_1)} &F^\varepsilon(s_1,\cdots,s_m,t_1)ds_m\cdots ds_1\Bigg) + R^\varepsilon_M(t_2,t_1)\end{aligned}$$

with

$$F^\varepsilon(s_1,\cdots,s_m,t_1) = E(s_m,t_1)E(s_{m-1},t_1)\cdots E(s_2,t_1)E(s_1,t_1), \tag{5.15}$$

where the operators $E(s,t_1)$ are given by

$$E(s,t_1) = \mathcal{U}^\varepsilon_{H_{\rm diag}}(t_1,s)\widehat{H^\varepsilon_{\rm adiag}}(s)\mathcal{U}^\varepsilon_{H_{\rm diag}}(s,t_1), \tag{5.16}$$

and the set of integration $\mathcal{P}(t_2,t_1) \subset \mathbb{R}^M$ satisfies

$$\mathcal{P}(t_2,t_1) = \{t_1 \le s_M \le \cdots \le s_2 \le s_1 \le t_2\}.$$

Besides, by (5.8) there exists a constant $C > 0$ such that

$$\|R^\varepsilon_M(t_2,t_1)\|_{\mathcal{L}(\Sigma^{k+M+1}_\varepsilon,\Sigma^k_\varepsilon)} \le C|t_2-t_1|^{M+1}.$$

We apply this formula to $t_1 = t^\flat$, $t_2 = t^\flat + \delta$,

$$\mathcal{U}^\varepsilon_{\underline{H}}(t^\flat+\delta, t^\flat-\delta) = \mathcal{U}^\varepsilon_{H_{\rm diag}}(t^\flat+\delta, t^\flat)\Big(\mathbb{I} + \sum_{1\le m\le M}(i)^{-m}\int_{s_M\in\mathbb{R}}\int_{-\infty}^{s_M}\cdots\int_{-\infty}^{s_2} F^\varepsilon(s_1,\cdots,s_M,t^\flat)ds_M\cdots ds_1\Big)\mathcal{U}^\varepsilon_{H_{\rm diag}}(t^\flat, t^\flat-\delta) + R^\varepsilon_M(t^\flat+\delta,t^\flat)\mathcal{U}^\varepsilon_{H_{\rm diag}}(t^\flat,t^\flat-\delta)$$

which gives equation (5.10) with

$$\Theta^{\varepsilon,\delta}_{m,M} = (i)^{-m}\int_{s_M\in\mathbb{R}}\int_{-\infty}^{s_M}\cdots\int_{-\infty}^{s_2} F^\varepsilon(s_1,\cdots,s_M,t^\flat)ds_M\cdots ds_1$$

and $R^{\varepsilon,\delta}_M = R^\varepsilon_M(t^\flat+\delta,t^\flat-\delta)\mathcal{U}^\varepsilon_{H_{\rm diag}}(t^\flat,t^\flat-\delta)$ satisfies

$$\|R^{\varepsilon,\delta}_M\|_{\mathcal{L}(\Sigma^{k+M+1}_\varepsilon,\Sigma^k)} \le C\delta^{M+1}.$$

The operators $\Theta^{\varepsilon,\delta}_{m,M}$ contain all the information about the interactions between the modes h_1 and h_2 modulo $O(\delta^\infty)$ when M goes to $+\infty$.

In the next sections, we focus in understanding the action of $\Theta^{\varepsilon,\delta}_{m,M}$ on wave packets of the form

$$\mathrm{WP}^\varepsilon_{\zeta^\flat}(\vec{\varphi}) = \begin{pmatrix}\mathrm{WP}^\varepsilon_{\zeta^\flat}(\varphi_1)\\ \mathrm{WP}^\varepsilon_{\zeta^\flat}(\varphi_2)\end{pmatrix}$$

and in proving equations (5.11), (5.12) and (5.13).

5.3.2. Analysis of the matrices $E(s,t^\flat)$. We have

$$E(s,t^\flat) = \begin{pmatrix}0 & \mathcal{I}(s,t^\flat)\\ \mathcal{I}^*(s,t^\flat) & 0\end{pmatrix},\quad s\in[t^\flat-\delta, t^\flat+\delta]$$

with

$$\mathcal{I}(s,t^\flat) = \mathcal{U}^\varepsilon_{h_1^{\varepsilon,N}}(t^\flat,s)\chi_\delta(s-t^\flat)W^{\varepsilon,N}(s)\,\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(s,t^\flat). \tag{5.17}$$

This operator combines conjugation of the pseudodifferential operator $\chi_\delta(s-t^\flat)W^{\varepsilon,N}(s)$ by the propagator $\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(s,t^\flat)$ and composition by two different propagators $\mathcal{U}^\varepsilon_{h_1^{\varepsilon,N}}(t^\flat,s)$ and $\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(t^\flat,s)$. Indeed, we can write

$$\mathcal{I}(s,t^\flat) = \Big(\mathcal{U}^\varepsilon_{h_1^{\varepsilon,N}}(t^\flat,s)W^{\varepsilon,N}(s)\,\mathcal{U}^\varepsilon_{h_1^{\varepsilon,N}}(s,t^\flat)\Big)\circ\Big(\mathcal{U}^\varepsilon_{h_1^{\varepsilon,N}}(t^\flat,s)\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(s,t^\flat)\Big).$$

The conjugation of a pseudo by a propagator is perfectly understood and is described in our setting by the Egorov Theorem of Appendix C (with $\delta=1$). The operator $\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(t^\flat,s)W^{\varepsilon,N}(s)\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(s,t^\flat)$ has an asymptotic expansion.

$$\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(t^\flat,s)W^{\varepsilon,N}(s)\,\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(s,t^\flat) = \sum_{j\ge1}\varepsilon^j\underline{W}_j(s).$$

Similarly, for $\mathcal{I}^*(s,t^\flat)$, one writes

$$\mathcal{I}^*(s,t^\flat) = \Big(\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(t^\flat,s)W^{\varepsilon,N}(s)^*\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(s,t^\flat)\Big)\circ\Big(\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(t^\flat,s)\mathcal{U}^\varepsilon_{h_1^{\varepsilon,N}}(s,t^\flat)\Big).$$

Note that the actions of these two operators are perfectly adapted to the geometric context: $\mathcal{I}(s,t^\flat)$ picks the contribution of the second component (the lower one), which lives on the mode 2, transforms it into something related with the mode 1 (the upper one), via the operator $\mathcal{U}^\varepsilon_{h_1^{\varepsilon,N}}(t^\flat,s)\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(s,t^\flat)$, and then, an operator related to the first mode acts on what is now a component living on this precise mode. And conversely for $\mathcal{I}^*(s,t^\flat)$.

The action on wave packets of two different propagators acting one backwards and the other one forwards has been studied in [**20**] (see Section 5.2). Using Egorov theorem, the action of scalar propagators on wave packets, and the precise computation of the operator $\mathcal{U}^\varepsilon_{h_1^{\varepsilon,N}}(t^\flat,s)\,\mathcal{U}^\varepsilon_{h_2^{\varepsilon,N}}(s,t^\flat)$ performed therein (which involves the canonical transformation of the phase space $z\mapsto \Phi_1^{t^\flat,s}\circ\Phi_2^{s,t^\flat}(z)$), one obtains the analogue of Lemma 5.3 of [**20**], which writes in our context as follows.

LEMMA 5.11. *Let $k\in\mathbb{N}$. There exist*

- *A smooth real-valued map $s\mapsto\Lambda(s)$ with $\Lambda(0)=0$, $\dot\Lambda(0)=0$, $\ddot\Lambda(0)=2\mu^\flat+\alpha^\flat\cdot\beta^\flat$,*
- *A smooth vector-valued map $s\mapsto z(s)=(q(s),p(s))$ with $z(0)=0$, $\dot z(0)=(\alpha^\flat,\beta^\flat)$,*
- *A smooth map $\sigma\mapsto\mathcal{Q}^\varepsilon(s)$ of pseudodifferential operators, that maps Schwartz functions to Schwartz functions, with $\mathcal{Q}^\varepsilon(s)=\sum_{j=0}^M\varepsilon^j\mathcal{Q}_j(s)+\mathcal{Q}^\varepsilon_{M+1}$,*

$$\mathcal{Q}_0(0)=W_1(t^\flat,\zeta^\flat)^*$$

such that for all $\varphi\in\mathcal{S}(\mathbb{R}^d)$,

$$I(s,t^\flat)^*\mathrm{WP}^\varepsilon(\varphi)(y)=\mathrm{WP}^\varepsilon\left(\mathrm{e}^{\frac{i}{\varepsilon}\Lambda(s-t^\flat)}\mathcal{Q}^\varepsilon(s-t^\flat)\mathrm{e}^{ip_\varepsilon(s-t^\flat)\cdot(y-q_\varepsilon(s-t^\flat))}\varphi(y-q_\varepsilon(s-t^\flat))+R^\varepsilon\varphi\right)$$

with, for some $c_M>0$

$$\begin{aligned}&\|\mathcal{Q}_j(s)\varphi\|_{\Sigma^k}\le c_M\|\varphi\|_{\Sigma^{k+1}},\ \ \forall j\in\{1,\cdots,M\},\\&\|\mathcal{Q}_{M+1}(s)\varphi\|_{\Sigma^k}\le c_M\|\varphi\|_{\Sigma^{k+1+\kappa_0}},\\&\|R^\varepsilon\varphi\|_{\Sigma^k}\le c_M\,\|\varphi\|_{\Sigma^{k+1+\kappa_0}},\end{aligned}$$

where we have used the scaling notation $z_\varepsilon(s)=z(s)/\sqrt{\varepsilon}$ and where κ_0 is the universal constant of Theorem B.1.

A similar result holds for $I(s,t^\flat)$ by replacing $W_1(t^\flat,\zeta^\flat)^*$ by $W_1(t^\flat,\zeta^\flat)$ and exchanging the roles of the modes h_1 and h_2.

5.3.3. Uniform estimates for the elements of the Dyson series. We now focus on the operators $\Theta^{\varepsilon,\delta}_{m,M}$. For $s\in[t^\flat-\delta,t^\flat+\delta]$, we define recursively the quantities $J_m(s)$ for $m\in\{1,\cdots M\}$ by

$$J_1(s)=-i\int_{-\infty}^s E(s_1,t^\flat)ds_1$$

and for $m\ge2$,

$$J_m(s)=-i\int_{-\infty}^s E(s_m,t^\flat)J_{m-1}(s_m)ds_m.$$

We recall that $E_1(s,t^\flat)$ is supported on $|t^\flat-s|\le\delta$ due to the cut-off function $\chi_\delta(s-t^\flat)$ that appears in (5.17). With these notations,

$$\Theta^{\varepsilon,\delta}_{m,M}=J_m(t^\flat+\delta).$$

We are reduced to proving the existence of operators $s \mapsto \mathcal{T}_m^{\varepsilon,\delta}(s)$ such that for all $s \in [t^\flat - \delta, t^\flat + \delta]$ and $\vec{\varphi} \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^2)$,

$$J_m(s)\mathrm{WP}^\varepsilon_{\zeta^\flat}(\vec{\varphi}) = \mathrm{WP}^\varepsilon_{\zeta^\flat}(\mathcal{T}_m^{\varepsilon,\delta}(s)\vec{\varphi}), \tag{5.18}$$

with for all $k \in \mathbb{N}$, the estimate 5.12. Note that we are omitting the index M of the notations of Theorem 5.10.

If the functions $\mathcal{T}_m^{\varepsilon,\delta}$ exist, they satisfy for $s' \in [t^\flat - \delta, t^\flat + \delta]$ the recursive equations

$$\mathrm{WP}^\varepsilon_{\zeta^\flat}\left(T_{m+1}^{\varepsilon,\delta}(s)\vec{\varphi}\right)_2 = -i\int_{-\infty}^{s'} I(s,t^\flat)^*\mathrm{WP}^\varepsilon_{\zeta^\flat}\left(T_m^{\varepsilon,\delta}(s)\vec{\varphi}\right)_1 ds$$

and

$$\mathrm{WP}^\varepsilon_{\zeta^\flat}\left(T_{m+1}^{\varepsilon,\delta}(s)\vec{\varphi}\right)_1 = -i\int_{-\infty}^{s'} I(s,t^\flat)\mathrm{WP}^\varepsilon_{\zeta^\flat}\left(T_m^{\varepsilon,\delta}(s)\vec{\varphi}\right)_2 ds.$$

Therefore, by Lemma 5.11, if the functions $\mathcal{T}_m^{\varepsilon,\delta}$ exist, they satisfy for $s' \in [t^\flat - \delta, t^\flat + \delta]$ the recursive equations

$$\left(\mathcal{T}_{m+1}^{\varepsilon,\delta}(s)\vec{\varphi}\right)_2 = \int_{-\infty}^{s'} \mathrm{e}^{\frac{i}{\varepsilon}\Lambda(s-t^\flat)}\mathcal{Q}^\varepsilon(s-t^\flat)\mathrm{e}^{ip_\varepsilon(s-t^\flat)\cdot(y-q_\varepsilon(s-t^\flat))}(\mathcal{T}_m^{\varepsilon,\delta}(s)\vec{\varphi})_1(y-q_\varepsilon(s-t^\flat))ds$$

and some analogue equation for the other components.

At the stage of the proof, the operators $\mathcal{T}_m^{\varepsilon,\delta}$ are defined by a recursive process that we are going to study for proving (5.12). Therefore, we focus on the analysis for scalar valued functions φ of

$$I_\varphi^m := \int_{-\infty}^{s'} \mathrm{e}^{\frac{i}{\varepsilon}\Lambda(s-t^\flat)}\mathcal{Q}^\varepsilon(s-t^\flat)\mathrm{e}^{ip_\varepsilon(s-t^\flat)\cdot(y-q_\varepsilon(s-t^\flat))}(T_m^{\varepsilon,\delta}(s)\varphi)(y-q_\varepsilon(s-t^\flat))ds.$$

In the following sections, we prove (5.18) recursively:

(1) In Section 5.3.4, we prove that if $m > 1$ and if (5.18) holds for $m' = 1, 2, \cdots, m-1$, then it also holds for $m' = m$.
(2) In Section 5.3.5, we prove (5.18) when $m = 1$.

5.3.4. Proof of Lemma 5.12: the recursive argument. We use Lemma 5.11 to perform a recursive argument on the structure of $J_m(s)$.

LEMMA 5.12. *Assume there exists $m \in \{1, 2, \cdots, M-1\}$ such that for all $k \in \mathbb{N}$, we have* (5.18) *with the inequality* (5.12) *for m and for the integers between 1 and m. Then, for all $k \in \mathbb{N}$, there exists a constant $C_{k,m+1}$ such that for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we have*

$$\|I_\varphi\|_{\Sigma^k} \leq C_{k,m+1}\varepsilon^{\frac{m+1}{2}}|\log\varepsilon|^{\max(0,m)}\|\varphi\|_{\Sigma^{k+2(m+1)+1}}.$$

This lemma, together with the precise computation of $J_1(t^\flat + \delta)$ (see [**20**] and Section 5.3.5 below) concludes the proof of Theorem 5.10.

Note that at each step of the recursion one loose 2 degrees of regularity. One degree is lost because the operator $\mathcal{Q}^\varepsilon$ that may has linear growth, and another loss is due to an integration by parts that will involve the term $y \cdot p_\varepsilon$ in the phase and the argument q_ε inside the function φ. The initial loss of regularity when $m = 1$ comes from similar reasons: one step is due to the presence of the operator $\mathcal{Q}^\varepsilon$ and the two other ones by integration by parts.

Let us start by exhibiting basic properties of I_φ. After the change of variables $s = t^\flat + \sigma\sqrt{\varepsilon}$ and letting appear a cut-off $\widetilde{\chi}$ such that $\chi\tilde{\chi} = \chi$, we write

$$I_\varphi = \sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}} \mathrm{e}^{\frac{i}{\varepsilon}\Lambda(\sigma\sqrt{\varepsilon})}\chi(\sigma/\lambda)\mathcal{Q}^\varepsilon(\sigma\sqrt{\varepsilon})\mathrm{e}^{ip_\varepsilon(\sigma\sqrt{\varepsilon})\cdot(y-q_\varepsilon(\sigma\sqrt{\varepsilon}))} \times (T_m^{\varepsilon,\delta}(t^\flat+\sigma\sqrt{\varepsilon})\varphi)(y-q_\varepsilon(\sigma\sqrt{\varepsilon}))d\sigma$$

with

$$\lambda = \frac{\delta}{\sqrt{\varepsilon}}.$$

One sees that the change of variable has exhibited a power $\sqrt{\varepsilon}$, which is exactly what one wants to earn for the recursive process. However, even though the integrand is bounded, the size of the support of the integral is large: it is of size $\lambda = \frac{\delta}{\sqrt{\varepsilon}}$, which spoils that gain of $\sqrt{\varepsilon}$. This integral will turn out to be smaller than what gives this rough estimate because of the oscillations of the phase. The proof then consists in integration by parts. For this reason, we are interested in derivatives and we observe that the recursive assumption yields

$$\|\partial_s T_m^{\varepsilon,\delta}(s)\vec{\varphi}\|_{\Sigma^k} \leq C_{k,m}\varepsilon^{\frac{m-1}{2}}|\log\varepsilon|^{\max(0,m-2)}\|\vec{\varphi}\|_{\Sigma^{k+2(m-1)+1}} \tag{5.19}$$

and similarly for the integers between 2 and m.

Analysis of the phase. We know analyze the phase of the integral I_φ. We set

$$\phi^\varepsilon(\sigma) = \Lambda(\sigma\sqrt{\varepsilon}) - \frac{1}{2}p_\varepsilon(\sigma\sqrt{\varepsilon})\cdot(y-q_\varepsilon(\sigma\sqrt{\varepsilon})) \text{ and } L = \beta^\flat\cdot y - \alpha^\flat\cdot D_y.$$

We will use that e^{isL} maps Σ^k into itself continuously for all $s\in\mathbb{R}$ and $k\in\mathbb{N}$. Besides, for $\delta\leq\delta_0$, $\delta_0>0$ small enough, we have

$$\left|\frac{d}{ds}\phi^\varepsilon(s)\right| \geq c_0|s|,\ \forall|s|\leq\lambda$$

and

$$\mathrm{e}^{i\phi^\varepsilon(s)} = \frac{1}{s}b^\varepsilon(s)\partial_s\mathrm{e}^{i\phi^\varepsilon(s)} \text{ with } b^\varepsilon(s) := \frac{s}{i\partial_s\phi^\varepsilon(s)}.$$

The function $b^\varepsilon(s)$ is uniformly bounded, as well as its derivatives, for $|s|\geq 1/2$. Then, following [**20**], we have

$$I_\varphi^m = \sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}} \mathrm{e}^{i\phi^\varepsilon(\sigma)}\mathcal{Q}^\varepsilon(\sigma\sqrt{\varepsilon})\chi(\sigma/\lambda)\mathrm{e}^{iL\sigma}T_m^{\varepsilon,\delta}(t^\flat+\sigma\sqrt{\varepsilon})\varphi d\sigma$$

and there exists a smooth function f such that

$$\phi^\varepsilon(\sigma) = \mu^\flat\sigma^2 + \sqrt{\varepsilon}\,\sigma^3\,f(\sigma\sqrt{\varepsilon}).$$

At the stage of the proof, all the elements have been collected to perform the recursive argument.

Because of the considerations we have made on the support of the integral and because the phase $\phi^\varepsilon(s)$ is oscillating for s far away from 0, we use the cut-off function χ to write

$$I_\varphi^m = I_\varphi^{m,1} + I_\varphi^{m,2}$$

with

$$I_\varphi^{m,1} = \sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}} \mathrm{e}^{i\phi^\varepsilon(\sigma)}\chi(\sigma)\chi(\sigma/\lambda)\mathcal{Q}^\varepsilon(\sigma\sqrt{\varepsilon})\mathrm{e}^{iL\sigma}\mathcal{T}_m^{\varepsilon,\delta}(t^\flat+\sigma\sqrt{\varepsilon})\varphi d\sigma$$

The compactly supported term. The term $I_\varphi^{m,1}$ is the easiest to deal with since it has compact support, independently of ε and δ. Therefore,

$$\begin{aligned}\|I_\varphi^{m,1}\|_{\Sigma^k} &\leq C\sqrt{\varepsilon}\sup_{s\in[t^\flat-\delta,t^\flat+\delta]}\|\mathcal{T}_m^{\varepsilon,\delta}(s)\varphi\|_{\Sigma^{k+1}}\\ &\leq C\varepsilon^{\frac{m+1}{2}}|\log\varepsilon|^{\max(0,m-1)}\,\|\varphi\|_{\Sigma^{k+2m+2}}.\end{aligned}$$

Note that the presence of $\mathcal{Q}^\varepsilon$ induces a loss of regularity of 1.

The oscillating term. For dealing with the term $I_\varphi^{m,2}$, we take advantage of the oscillating phase for compensating the fact that the support is large and we perform integration by parts. We write

$$\begin{aligned}I_\varphi^{m,2} &= \sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}}\partial_\sigma\left(\mathrm{e}^{i\phi^\varepsilon(\sigma)}\right)\frac{1}{\sigma}b^\varepsilon(\sigma)(1-\chi)(\sigma)\chi(\sigma/\lambda)\mathcal{Q}^\varepsilon(\sigma\sqrt{\varepsilon})\\ &\qquad\times\mathrm{e}^{iL\sigma}(\mathcal{T}_m^{\varepsilon,\delta}(t^\flat+\sigma\sqrt{\varepsilon})\varphi)d\sigma\\ &= -\sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}}\mathrm{e}^{i\phi^\varepsilon(\sigma)}\partial_\sigma\left(\frac{1}{\sigma}b_1^\varepsilon(\sigma)\mathrm{e}^{iL\sigma}\mathcal{T}_m^{\varepsilon,\delta}(t^\flat+\sigma\sqrt{\varepsilon})\varphi\right)d\sigma\\ &\qquad+\sqrt{\varepsilon}\left(\mathrm{e}^{i\phi^\varepsilon(\sigma)}\frac{1}{\sigma}b_1^\varepsilon(\sigma)\mathrm{e}^{iL\sigma}\right)\Big|_{\sigma=\frac{s'-t^\flat}{\sqrt{\varepsilon}}}\mathcal{T}_m^{\varepsilon,\delta}(s')\varphi\end{aligned}$$

with

$$b_1^\varepsilon(\sigma)=(1-\chi)(\sigma)\chi(\sigma/\lambda)\mathcal{Q}^\varepsilon(\sigma\sqrt{\varepsilon}).$$

Note that the operator-valued functions $\sigma\mapsto b_1^\varepsilon(\sigma)$ and $\sigma\mapsto\frac{1}{\sigma}b_1^\varepsilon(\sigma)$ are bounded form Σ_ε^{k+1} to Σ_ε^k (with a loss due to the presence of the operator $\mathcal{Q}^\varepsilon$), and similarly for its derivatives. We write

$$\begin{aligned}I_\varphi^{m,2} &= -\sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}}\mathrm{e}^{i\phi^\varepsilon(\sigma)}\partial_\sigma\left(\frac{1}{\sigma}b_1^\varepsilon(\sigma)\right)\mathrm{e}^{iL\sigma}(\mathcal{T}_m^{\varepsilon,\delta}(t^\flat+\sigma\sqrt{\varepsilon})\varphi)d\sigma\\ &\quad-\sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}}\mathrm{e}^{i\phi^\varepsilon(\sigma)}\frac{1}{\sigma}b_1^\varepsilon(\sigma)\mathrm{e}^{iL\sigma}(iL\mathcal{T}_m^{\varepsilon,\delta}(t^\flat+\sigma\sqrt{\varepsilon})\varphi+\sqrt{\varepsilon}\partial_sT_m^{\varepsilon,\delta}(t^\flat+\sigma\sqrt{\varepsilon})\varphi)d\sigma\\ &\quad+\sqrt{\varepsilon}\left(\mathrm{e}^{i\phi^\varepsilon(\sigma)}\frac{1}{\sigma}b_1^\varepsilon(\sigma)\mathrm{e}^{iL\sigma}\right)\Big|_{\sigma=\frac{s'-t^\flat}{\sqrt{\varepsilon}}}\mathcal{T}_m^{\varepsilon,\delta}(s')\varphi\end{aligned}$$

and we check

$$\begin{aligned}&\left\|I_\varphi^{m,2}\right\|_{\Sigma^k}\leq C\sqrt{\varepsilon}\\ &\times\sup_{s\in[t^\flat-\delta,t^\flat+\delta]}\left(\|\mathcal{T}_m^{\varepsilon,\delta}(s)\varphi\|_{\Sigma^{k+1}}+(\|L\mathcal{T}_m^{\varepsilon,\delta}(s)\varphi\|_{\Sigma^{k+1}}+\sqrt{\varepsilon}\|\partial_s\mathcal{T}_m^{\varepsilon,\delta}(s)\varphi\|_{\Sigma^{k+1}})\int_{\frac12\leq|s|\leq\frac{\delta}{\sqrt{\varepsilon}}}\frac{d\sigma}{\sigma}\right)\\ &\qquad\leq C\left(\sqrt{\varepsilon}\,\varepsilon^{\frac{m}{2}}|\log\varepsilon|^{\max(0,m-1)}\,\|\varphi\|_{\Sigma^{k+2m+3}}+\varepsilon|\log\varepsilon|\varepsilon^{\frac{m-1}{2}}|\log\varepsilon|^{\max(0,m-1)}\|\varphi\|_{\Sigma^{k+2m}}\right)\\ &\qquad\leq C\varepsilon^{\frac{m+1}{2}}|\log\varepsilon|^{\max(0,m)}\,\|\varphi\|_{\Sigma^{k+2(m+1)+1}}.\end{aligned}$$

We point out that it is at that very last stage that we loose some $\log\varepsilon$ coefficient. Note also that the loss of regularity in the recursive process is covered by the $m\to m+1$ process. It will appear in the initialization process ($m=1$) in which we will get rid of the logarithmic loss $|\log\varepsilon|$ by trading it as a loss of regularity.

5.3.5. Proof of Lemma 5.12: the initialization of the recursion. For initializing the recursive process, we have to study $J_1(s)$, i.e. the integral I_φ^m replacing the transfer operator of the integrand by $\mathbb{I}$, the identity operator. We obtain

$$I_\varphi^{m=1} = \sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}} \mathrm{e}^{i\phi^\varepsilon(\sigma)}\mathcal{Q}^\varepsilon(\sigma\sqrt{\varepsilon})\chi(\sigma/\lambda)\mathrm{e}^{iL\sigma}\varphi\, d\sigma.$$

Besides the estimate of the norm of $I_\varphi^{m=1}$, we also want to calculate the leading order term when $s = t^\flat + \delta$. The main difference with the preceding analysis is that we can push the integration by parts at any order because the integrand is simpler.

LEMMA 5.13. *Let $k \in \mathbb{N}$. Then, there exists a constant $C_{k,1}$ such that for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$*

$$\|I_\varphi^{m=1}\|_{\Sigma^k} \leq C_{k,1}\sqrt{\varepsilon}\,\|\varphi\|_{k+3}.$$

Moreover, there exists an operator $\Theta^{\varepsilon,\delta} = \Theta_1^{\varepsilon,\delta} + \sqrt{\varepsilon}\Theta_2^{\varepsilon,\delta}$ and a constant $c_{k,M}$ such that for all $M \in \mathbb{N}$,

$$\|\ I_\varphi^{m=1}\big|_{s'=t^\flat+\delta} - \sqrt{\varepsilon}W_1(t^\flat,\zeta^\flat)^*\mathcal{T}_{1\to 2}^\flat\varphi - \varepsilon\,\Theta^{\varepsilon,\delta}\varphi\|_{\Sigma^k} \leq C_{k,M}\sqrt{\varepsilon}\left(\frac{\sqrt{\varepsilon}}{\delta}\right)^{M+1}\|\varphi\|_{\Sigma^{k+M+3}}$$

with for $\ell = 1, 2$, $\|\Theta_\ell^{\varepsilon,\delta}\varphi\|_{\Sigma_k} \leq c_{k,M}\|\varphi\|_{\Sigma^{k+3}}$.

We recall that $\mathcal{T}_{1\to 2}^\flat$ is the transfer operator defined in (1.43). In [**20**], this Lemma has already be proved with $M = 1$. We ameliorate here this result. This terminates the proof of Theorem 5.10 with $(\mathcal{T}_{1,M}^{\varepsilon,\delta})_2 = W_1(t^\flat,\zeta^\flat)^*\mathcal{T}_{1\to 2}^\flat$.

PROOF. Following the same lines of proofs than above, we write $I_\varphi^{m=1} = I_\varphi^{1,1} + I_\varphi^{1,2}$ with

$$I_\varphi^{1,1} = \sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}} \mathrm{e}^{i\phi^\varepsilon(\sigma)}\chi(\sigma)\chi(\sigma/\lambda)\mathcal{Q}^\varepsilon(\sigma\sqrt{\varepsilon})\mathrm{e}^{iL\sigma}\varphi d\sigma.$$

We point out that we use here the same notation than in the preceding section for a simpler integrand. Like before, this term satisfies the estimate

$$\|I_\varphi^1\|_{\Sigma^k} \ \leq C\,\sqrt{\varepsilon}\,\|\varphi\|_{\Sigma^{k+1}}.$$

We proceed to integration by parts in I_φ^2. We obtain

$$\begin{aligned} I_\varphi^{1,2} = &-\sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}} \mathrm{e}^{i\phi^\varepsilon(\sigma)}\partial_\sigma\left(\frac{1}{\sigma}b_1^\varepsilon(\sigma)\right)\mathrm{e}^{iL\sigma}\varphi d\sigma \\ &- i\sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}} \mathrm{e}^{i\phi^\varepsilon(\sigma)}\frac{1}{\sigma}b_1^\varepsilon(\sigma)\mathrm{e}^{iL\sigma}\,L\,\varphi d\sigma + \sqrt{\varepsilon}\left(\mathrm{e}^{i\phi^\varepsilon(\sigma)}\frac{1}{\sigma}b_1^\varepsilon(\sigma)\mathrm{e}^{iL\sigma}\right)\Big|_{\sigma=\frac{s'-t^\flat}{\sqrt{\varepsilon}}}\varphi. \end{aligned}$$

We write

$$\partial_\sigma\left(\frac{1}{\sigma}b_1^\varepsilon(\sigma)\right) = b_2^\varepsilon(\sigma) + \frac{1}{\sigma}b_3^\varepsilon(\sigma) \text{ with } b_3^\varepsilon(\sigma) = \partial_\sigma b_1^\varepsilon(\sigma) + \sqrt{\varepsilon}(1-\chi)(\sigma)\chi(\sigma/\lambda)\partial_s\mathcal{Q}^\varepsilon(\sqrt{\varepsilon}\sigma).$$

where the maps $\sigma \mapsto b_2^\varepsilon(\sigma)$, $\sigma \mapsto b_3^\varepsilon(\sigma)$ and $\sigma \mapsto \frac{1}{\sigma}b_3^\varepsilon(\sigma)$ are bounded from Σ_ε^{k+1} to Σ_ε^k (with a loss of regularity because of the presence of $\mathcal{Q}^\varepsilon(s)$) with the additional property

$$\int_{\mathbb{R}} \|b_2^\varepsilon(\sigma)\|_{\mathcal{L}(\Sigma_\varepsilon^{k+1},\,\Sigma_\varepsilon^k)}d\sigma < c_0 < +\infty$$

for some constant c_0 independent of ε and δ. Therefore, in Σ^k,

$$I_\varphi^{1,2} = -\sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}} \mathrm{e}^{i\phi^\varepsilon(\sigma)}\frac{1}{\sigma}(b_3^\varepsilon(\sigma)+ib_1^\varepsilon(\sigma)L)\mathrm{e}^{iL\sigma}\varphi d\sigma + O(\sqrt{\varepsilon}\|\varphi\|_{\Sigma^{k+1}}).$$

Another integration by parts gives

$$\begin{aligned} I_\varphi^{1,2} &= \sqrt{\varepsilon}\int_{-\infty}^{(s'-t^\flat)/\sqrt{\varepsilon}} \mathrm{e}^{i\phi^\varepsilon(\sigma)}\partial_\sigma\left(\frac{1}{\sigma^2}b^\varepsilon(\sigma)(b_3^\varepsilon(\sigma)+ib_1^\varepsilon(\sigma)L)\right)\mathrm{e}^{iL\sigma}\varphi d\sigma \\ &\quad - \sqrt{\varepsilon}\left(\mathrm{e}^{i\phi^\varepsilon(\sigma)}\frac{1}{\sigma^2}b^\varepsilon(\sigma)(b_3^\varepsilon(\sigma)+ib_1^\varepsilon(\sigma)L)\mathrm{e}^{iL\sigma}\varphi\right)\Big|_{\sigma=\frac{s'-t^\flat}{\sqrt{\varepsilon}}} + O(\sqrt{\varepsilon}\|\varphi\|_{\Sigma^{k+1}}) \\ &= O(\sqrt{\varepsilon}\|\varphi\|_{\Sigma^{k+3}}), \end{aligned}$$

since the integrand has gained integrability. Note that it is at that very place that we have a loss of 3 momenta and derivatives in the estimate. We have obtained the first inequality that allows to initiate the recursive process of the preceding section. It remains to focus on the case $s' = t^\flat + \delta$.

We now consider the operator

$$\mathfrak{I}_\varphi = \frac{1}{\sqrt{\varepsilon}}\, I_\varphi^{m=1}\big|_{s'=t^\flat+\delta} - W_1(t^\flat,\zeta^\flat)\mathcal{T}_{1\to 2}^\flat.$$

Note first that by the construction of the function χ,

$$I_\varphi^{m=1}\big|_{s'=t^\flat+\delta} = \sqrt{\varepsilon}\int_{\mathbb{R}} \mathrm{e}^{i\phi^\varepsilon(\sigma)}\chi(\sigma/\lambda)\mathcal{Q}^\varepsilon(\sigma\sqrt{\varepsilon})\mathrm{e}^{iL\sigma}\varphi d\sigma$$

Following [**20**] Section 5.3, we first transform the expression $I_\varphi^{m=1}\big|_{s'=t^\flat+\delta}$ by performing the change of variable

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

and observe that $\sigma = z(1+\sqrt{\varepsilon}zg_1(z\sqrt{\varepsilon}))$ and $\partial_\sigma z = 1+\sqrt{\varepsilon}zg_2(z\sqrt{\varepsilon})$ for some smooth bounded functions g_1 and g_2 with bounded derivatives. Note that we have used that $\sigma\sqrt{\varepsilon}$ is of order δ, thus small, in the domain of the integral. Besides, there exists a family of operator $\widetilde{\mathcal{Q}}^\varepsilon(z)$ such that $\mathcal{Q}^\varepsilon(\sigma\sqrt{\varepsilon}) = \widetilde{\mathcal{Q}}^\varepsilon(z\sqrt{\varepsilon})$ with $\widetilde{\mathcal{Q}}^\varepsilon(0) = \mathcal{Q}^\varepsilon(0)$ and $\mathcal{Q}_0(0) = W_1(t^\flat,\zeta^\flat)$ and a compactly supported function $\tilde{\chi}$, such that

$$I_\varphi^{m=1}\big|_{s'=t^\flat+\delta} = \sqrt{\varepsilon}\int_{\mathbb{R}} \mathrm{e}^{i\mu^\flat z^2}\tilde{\chi}(z/\lambda)\widetilde{\mathcal{Q}}^\varepsilon(z\sqrt{\varepsilon})\mathrm{e}^{iz(1+\sqrt{\varepsilon}zg_1(z\sqrt{\varepsilon}))\,L}\varphi\frac{dz}{1+\sqrt{\varepsilon}zg_2(z\sqrt{\varepsilon})}.$$

A Taylor expansion allows to write

$$\widetilde{\mathcal{Q}}^\varepsilon(z\sqrt{\varepsilon})\mathrm{e}^{i\sqrt{\varepsilon}z^2g_1(z\sqrt{\varepsilon}))\,L}\frac{1}{1+\sqrt{\varepsilon}zg_2(z\sqrt{\varepsilon})} = \mathcal{Q}_0(0) + \sqrt{\varepsilon}z(\widetilde{\mathcal{Q}}_1^\varepsilon(z\sqrt{\varepsilon}) + z\widetilde{\mathcal{Q}}_2^\varepsilon(z\sqrt{\varepsilon}))$$

for some smooth operator-valued maps $z\mapsto\widetilde{\mathcal{Q}}_j^\varepsilon(z\sqrt{\varepsilon})$ mapping $\mathcal{S}(\mathbb{R}^d)$ into itself, such that for all $\varphi\in\mathcal{S}(\mathbb{R}^d)$ the family $\|\widetilde{\mathcal{Q}}_j^\varepsilon(z\sqrt{\varepsilon})\varphi\|_{\Sigma^k}\le c_j\|\varphi\|_{\Sigma^{k+2}}$ (because of the loss of regularity involved by L and $\mathcal{Q}^\varepsilon$) We obtain

$$\mathfrak{I}_\varphi = \mathfrak{I}_\varphi^1 + \mathfrak{I}_\varphi^2$$

with

$$\mathfrak{I}^1_\varphi = \sqrt{\varepsilon}\int_{\mathbb{R}} z\,\mathrm{e}^{i\mu^\flat z^2}\tilde\chi(z/\lambda)(\widetilde{\mathcal{Q}}^\varepsilon_1(z\sqrt{\varepsilon})+z\widetilde{\mathcal{Q}}^\varepsilon_2(z\sqrt{\varepsilon}))\mathrm{e}^{izL}\,\varphi dz,$$
$$\mathfrak{I}^2_\varphi = \mathcal{Q}_0(0)\int_{\mathbb{R}} \mathrm{e}^{i\mu^\flat z^2}(1-\tilde\chi)(z/\lambda)\,\mathrm{e}^{izL}\,\varphi dz.$$

Let us study $\mathfrak{I}^1_\varphi$. Arguing by integration by parts as previously, we obtain

$$\begin{aligned}\mathfrak{I}^1_\varphi =& -\frac{\sqrt{\varepsilon}}{2i\mu^\flat}\int_{\mathbb{R}}\mathrm{e}^{i\mu^\flat z^2}\frac{d}{dz}\left(\tilde\chi(z/\lambda)(\widetilde{\mathcal{Q}}^\varepsilon_1(z\sqrt{\varepsilon})+z\widetilde{\mathcal{Q}}^\varepsilon_2(z\sqrt{\varepsilon})\mathrm{e}^{izL}\right)dz\\ =& -\frac{\varepsilon}{2i\mu^\flat}\int_{\mathbb{R}}\mathrm{e}^{i\mu^\flat z^2}\tilde\chi(z/\lambda)\partial_z\widetilde{\mathcal{Q}}^\varepsilon_1(z\sqrt{\varepsilon})\mathrm{e}^{izL}\,dz\\ &-\frac{\sqrt{\varepsilon}}{2i\mu^\flat}\int_{\mathbb{R}}\tilde\chi(z/\lambda)(\,\mathrm{e}^{i\mu^\flat z^2}\partial_z\left(\widetilde{\mathcal{Q}}^\varepsilon_2(z\sqrt{\varepsilon})+\sqrt{\varepsilon}z\partial_z\widetilde{\mathcal{Q}}^\varepsilon_2(z\sqrt{\varepsilon})\mathrm{e}^{izL}\right)dz\\ &-\frac{\sqrt{\varepsilon}}{2i\mu^\flat}\int_{\mathbb{R}}\mathrm{e}^{i\mu^\flat z^2}\tilde\chi'(z/\lambda)\left(\lambda^{-1}\mathcal{Q}^\varepsilon_1(z\sqrt{\varepsilon})+\frac{z}{\lambda}\widetilde{\mathcal{Q}}^\varepsilon_2(z\sqrt{\varepsilon})\right)\mathrm{e}^{izL}\,dz.\end{aligned}$$

One then performs $M+2$ integration by parts in the last term of the right-hand side that is supported in $|z|>\frac{\lambda}{2}$ and we obtain

$$\begin{aligned}\mathfrak{I}^1_\varphi =& -\frac{\varepsilon}{2i\mu^\flat}\int_{\mathbb{R}}\mathrm{e}^{i\mu^\flat z^2}\tilde\chi(z/\lambda)(\partial_z\widetilde{\mathcal{Q}}^\varepsilon_1(z\sqrt{\varepsilon})+2\partial_z\widetilde{\mathcal{Q}}^\varepsilon_2(z\sqrt{\varepsilon}))\mathrm{e}^{izL}\,dz\\ &-\frac{\varepsilon}{2i\mu^\flat}\int_{\mathbb{R}}\tilde\chi(z/\lambda)\,\mathrm{e}^{i\mu^\flat z^2}z\partial_z^2\widetilde{\mathcal{Q}}^\varepsilon_2(z\sqrt{\varepsilon})\mathrm{e}^{izL}\,dz+O\left(\sqrt{\varepsilon}\left(\frac{\varepsilon}{\delta}\right)^{M+1}\|\varphi\|_{\Sigma^{k+M+3}}\right)\\ =&\sqrt{\varepsilon}\,\Theta^{\varepsilon,\delta}_1\varphi+O\left(\left(\frac{\varepsilon}{\delta}\right)^M\|\varphi\|_{\Sigma^{k+M+3}}\right)+\frac{\varepsilon}{(2i\mu^\flat)^2}\int_{\mathbb{R}}\mathrm{e}^{i\mu^\flat z^2}\partial_z\left(\tilde\chi(z/\lambda)\partial_z^2\widetilde{\mathcal{Q}}^\varepsilon_2(z\sqrt{\varepsilon})\mathrm{e}^{izL}\right)dz\\ =&\sqrt{\varepsilon}\,\Theta^{\varepsilon,\delta}_1\varphi+\varepsilon\,\Theta^{\varepsilon,\delta}_2\varphi+O\left(\left(\frac{\varepsilon}{\delta}\right)^M\|\varphi\|_{\Sigma^{k+M+3}}\right)\end{aligned}$$

with

$$\|\Theta^{\varepsilon,\delta}_1\|_{\Sigma^k}\le c\,\delta\|\varphi\|_{\Sigma^{k+3}}.$$

It remains to observe that the term $\mathfrak{I}^2_\varphi$ satisfies after $M+1$ integration by parts

$$\|\mathfrak{I}^2_\varphi\|_{\Sigma^k}\le C\left(\frac{\sqrt{\varepsilon}}{\delta}\right)^{M+1}\|\varphi\|_{\Sigma^{k+M+3}}.$$

□

5.4. Propagation of wave packets - Proof of Theorem 1.21

Let $k\in\mathbb{N}$ and let be ψ^ε_0 a polarized wave packet as in (1.39):

$$\psi^\varepsilon_0=\vec V_0\mathrm{WP}^\varepsilon_{z_0}(f_0)\ \text{ with }\ f_0\in\mathcal{S}(\mathbb{R}^d)\ \text{ and }\ \vec V_0\in\mathbb{C}^m.$$

Let $\delta>0$. By Theorem 5.9, for $t\in[t_0,t^\flat-\delta]$, and in Σ^k_ε, $\psi^\varepsilon(t)$ is an asymptotic sum of wave packets and writes

$$\psi^\varepsilon(t)=\psi^{\varepsilon,N}_1(t)+\psi^{\varepsilon,N}_2(t)+\mathcal{O}\left(\left(\frac{\varepsilon}{\delta^2}\right)^N\delta^{-\kappa_0}\right).$$

with $\psi^{\varepsilon,N}_\ell(t)$ given by (5.5).

We now take the vector

$$\underline{\psi}^{\varepsilon,N}(t^\flat-\delta)={}^t\left(\underline{\psi}_1^{\varepsilon,N}(t^\flat-\delta),\underline{\psi}_2^{\varepsilon,N}(t^\flat-\delta)\right),\ \ \underline{\psi}_\ell^{\varepsilon,N}(t^\flat-\delta)=\psi_\ell^{\varepsilon,N}(t^\flat-\delta),\ \ell=1,2,$$

as initial data in the system (5.7). It is a sum of N wave packets. By construction, in particular because of the linearity of the equation, we have for all $t\in[t^\flat-\delta,t^\flat+\delta]$,

$$\psi^\varepsilon(t)=\underline{\psi}_1^{\varepsilon,N}(t)+\underline{\psi}_2^{\varepsilon,N}(t)+\mathcal{O}\left(\left(\frac{\varepsilon}{\delta^2}\right)^N\delta^{-\kappa_0}\right)$$

in Σ_ε^k. When $t=t^\flat+\delta$, we deduce from Theorem 5.10 that in Σ_ε^k,

$$\underline{\psi}^{\varepsilon,N}(t^\flat+\delta)=\mathcal{U}_{\rm diag}^\varepsilon(t^\flat+\delta,t^\flat)\left(\mathbb{I}+\sum_{1\leq m\leq M}\Theta_{m,M}^{\varepsilon,\delta}\right)\mathcal{U}_{\rm diag}^\varepsilon(t^\flat,t^\flat-\delta)\underline{\psi}^{\varepsilon,N}(t^\flat-\delta)+O(\delta^M).$$

By Proposition C.5 of the Appendix, $\underline{\psi}_\ell^{\varepsilon,N}(t^\flat+\delta)$ is a sum of wave packets

$$\underline{\psi}_\ell^{\varepsilon,N}(t^\flat+\delta)=\sum_{0\leq m\leq M}\varepsilon^{\frac{m}{2}}\underline{\psi}_\ell^{\varepsilon,m,M,N}(t^\flat+\delta)$$

where each term $\underline{\psi}_\ell^{\varepsilon,m,M,N}(t^\flat+\delta)$ involves a term of action. When $m=0$ and $m=1$, these terms have been computed precisely:

- If $m=0$, for $\ell=1,2$,

$$\underline{\psi}_\ell^{\varepsilon,0,M,N}(t^\flat+\delta)=\mathrm{e}^{\frac{i}{\varepsilon}S_\ell(t^\flat+\delta,t^\flat-\delta,\zeta^\flat)}\mathrm{WP}^\varepsilon_{\Phi^{t^\flat+\delta,t_0}(z_0)}\left(\mathcal{M}[F_\ell(t^\flat+\delta,t_0,z_0)]\pi_\ell(t_0,z_0)\vec{V}_0f_0\right)$$

  where we have used the property of the scalar propagation of wave packets.
- If $m=1$, only the term with $\ell=2$ contributes and

$$\underline{\psi}_2^{\varepsilon,1,M,N}(t^\flat+\delta)=\mathrm{e}^{\frac{i}{\varepsilon}S_2(t^\flat+\delta,t^\flat,\zeta^\flat)+\frac{i}{\varepsilon}S_1(t^\flat,t_0,z_0)}\mathrm{WP}^\varepsilon_{\Phi_2^{t^\flat+\delta,t^\flat}(\zeta^\flat)}(\varphi_2)$$

  with

$$\varphi_2=\mathcal{M}[F_2(t^\flat+\delta,t^\flat,\zeta^\flat)]W_1(t^\flat,\zeta^\flat)^*\mathcal{T}^\flat_{1\to2}\mathcal{M}[F_1(t^\flat,t_0,z_0)]\pi_1(t_0,z_0)\vec{V}_0f_0,$$

  where W_1 is the off-diagonal matrix computed in (1.44).

At that stage of the proof, we have obtained that $\psi^\varepsilon(t^\flat+\delta)$ is a sum of wave packet in Σ_ε^k up to $\mathcal{O}\left(\left(\frac{\varepsilon}{\delta^2}\right)^N\delta^{-\kappa_0}+\delta^{M+1}\right)$ and we know precisely the terms of order ε^0 and $\varepsilon^{\frac12}$.

For concluding, we take the vector

$$\psi^\varepsilon_{\rm app}(t^\flat+\delta):=\underline{\psi}_1^{\varepsilon,N}(t^\flat+\delta)+\underline{\psi}_2^{\varepsilon,N}(t^\flat+\delta)$$

as initial data at time $t=t^\flat+\delta$ in the equation (1.1). The function $\psi^\varepsilon_{\rm app}(t^\flat+\delta)$ is an approximation of $\psi^\varepsilon(t^\flat+\delta)$ at order $\mathcal{O}\left(\left(\frac{\varepsilon}{\delta^2}\right)^N\delta^{-\kappa_0}+\delta^{M+1}\right)$ in Σ_ε^k. By construction and because of the linearity of the equation, for all times $t\in[t^\flat+\delta,t_0+T]$,

$$\psi^\varepsilon(t)=\mathcal{U}_H(t,t^\flat+\delta)\psi^\varepsilon_{\rm app}(t^\flat+\delta)+\mathcal{O}\left(\left(\frac{\varepsilon}{\delta^2}\right)^N\delta^{-\kappa_0}+\delta^{M+1}\right).$$

We then applies Theorem 5.9 between times $t^\flat+\delta$ and t. Indeed, the classical trajectories involved in the construction do not meet Υ again and we are in an adiabatic regime, as in theorem 5.9. This concludes the proof of Theorem 1.21.

APPENDIX A

Matrix-valued Hamiltonians

We explain here the set-up and the technical assumptions that we make on the Hamiltonian H^ε. It is the occasion of motivating the set of Assumptions 1.4 and deriving their consequences. The objectives of these assumptions are first to ensure the existence of the propagators associated with the full matrix-valued Hamiltonian and with its eigenvalues, and secondly to guarantee adequate properties of growth at infinity which are used in our analysis.

In this section, we work with $m \times m$ ($m \in \mathbb{N}$) matrix-valued Hamiltonians H that are sub-quadratic:

$$\forall \beta \in \mathbb{N}^d,\ \exists C_\beta > 0,\ \forall (t,z) \in I \times \mathbb{R}^d,\ |\partial^\beta H(t,z)|_{\mathbb{C}^{m,m}} \leq C_\beta \langle z \rangle^{(2-|\beta|)+}. \tag{A.1}$$

LEMMA A.1. *Assume that the matrix-valued function $H \in \mathcal{C}^\infty(I \times \mathbb{R}^d, \mathbb{C}^{m,m})$ satisfies* (A.1). *Assume that for all $(t,z) \in I \times \mathbb{R}^{2d}$, $H(t,z)$ has a smooth eigenvalue h with a smooth eigenprojector $\pi(t,z)$ of constant rank for $|z| > m$, > 0. Then, there exists a constant $C > 0$ such that for all $(t,z) \in I \times \mathbb{R}^{2d}$ with $|z| > m$,*

$$|h(t,z)| \leq C\langle z \rangle^2,\ \ |\nabla h(t,z)| \leq C\langle z \rangle.$$

PROOF. The relation $H\pi = h\pi$ implies $|h(t,z)| \leq C\langle z \rangle^2$. Moreover, writing

$$H = h\pi + H(1-\pi) = h\pi + (1-\pi)H$$

and differentiating these two relations, we obtain for all $j \in \{1, \cdots 2d\}$, denoting ∂_{z_j} by ∂_j

$$\partial_j H = \partial_j h\, \pi + h\partial_j \pi + \partial_j H(1-\pi) - H\partial_j \pi = \partial_j h\, \pi + h\partial_j \pi + (1-\pi)\partial_j H - \partial_j \pi H. \tag{A.2}$$

Multiplying from the left and the right with π and using that $\partial\pi$ is off-diagonal, we obtain the relation $\pi\partial_j H\pi = \partial_j h\pi$, whence with $c = \mathrm{Rank}(\pi) = cte$,

$$\partial_j h = c\,\mathrm{Tr}(\pi\partial_j H\pi).$$

This implies $|\partial_j h(t,z)| \leq C\langle z \rangle$. □

This proof shows that the study of higher derivatives of the eigenvalues requires a control on the derivatives of the eigenprojectors. The following example shows that the situation may become very intricate and one can have smooth subquadratic eigenvalues while the derivatives of the projectors are unbounded.

EXAMPLE A.2. Assume $d = 1$. Let $\rho, \theta \in \mathcal{C}^\infty(\mathbb{R})$ such that ρ has with bounded derivatives and with

$$\rho(x) = \frac{1}{x^3} \ \text{ and } \ \theta(x) = x\ln(x) - x \ \text{ for } \ |x| > 1.$$

Define

$$H(x) = \rho(x) \begin{pmatrix} \cos(\theta(x)) & \sin(\theta(x)) \\ \sin(\theta(x)) & -\cos(\theta(x)) \end{pmatrix}.$$

The eigenvalues of H are $\pm\rho$ and the eigenprojector associated with the eigenvalue ρ is

$$\pi(x) = \frac{1}{2}\left(1 + \begin{pmatrix} \cos(\theta(x)) & \sin(\theta(x)) \\ \sin(\theta(x)) & -\cos(\theta(x)) \end{pmatrix}\right).$$

Its derivative

$$\pi'(x) = \frac{1}{2}\theta'(x)\begin{pmatrix} -\sin(\theta(x)) & \cos(\theta(x)) \\ \cos(\theta(x)) & \sin(\theta(x)) \end{pmatrix}$$

is not bounded. On the other side, ρ and H are sub-quadratic. Indeed, for $|x| > 1$, the derivatives of the coefficient of H are of the form

$$\frac{1}{x^3}\left(p_1\left(\frac{1}{x}, \ln x\right)\cos\theta(x) + p_2\left(\frac{1}{x}, \ln x\right)\sin\theta(x)\right)$$

for p_1 and p_2 two polynomial functions of two variables and thus bounded.

A manner of controlling the growth of the potential consists in requiring a lower bound on the gap function f at infinity.

LEMMA A.3. *Let $\ell \in \{1, 2\}$. Assume that the matrix-valued function $H \in \mathcal{C}^\infty(I \times \mathbb{R}^d, \mathbb{C}^{m,m})$ satisfies* (A.1). *Assume that for all $(t, z) \in I \times \mathbb{R}^{2d}$, $H(t, z)$ has a smooth eigenvalue h with smooth associated eigenprojectors $\pi(t, z)$ of constant rank for $|z| > m$. Assume there exists $C, n_0 > 0$ such that for $(t, z) \in I \times \mathbb{R}^d$ with $|z| > m$,*

$$\operatorname{dist}\left(h(t, z), \operatorname{Sp}(H(t, z)) \setminus \{h(t, z)\}\right) \geq C\langle z\rangle^{-n_0}.$$

Then, for all $\gamma \in \mathbb{N}^{2d}$ with $|\gamma| \geq 2$, there exists a constant $C_\gamma > 0$ such that

$$\forall (t, z) \in I \times \mathbb{R}^{2d}, \ \ |\partial_z^\gamma \pi(t, z)| \leq C_\gamma \langle z\rangle^{|\gamma| n_0 + \ell - 1} \text{ and } |\partial_z^\gamma h(t, z)| \leq C_\gamma \langle z\rangle^{(|\gamma|-1)n_0 + 2(\ell-1)}.$$

PROOF. We work for $|z| > m$ and fix $j \in \{1, 2\}$. The relation (A.2) also implies

$$\partial_j \pi (H - h) = (H - h)\partial_j \pi = \partial_j (H - h)$$

where we keep the notation $\partial_j := \partial_{z_j}$ for $j \in \{1, \cdots, 2d\}$. Using that $\partial_j \pi$ is off diagonal and $(H - h)$ invertible on $\operatorname{Range}(1 - \pi)$, we deduce

$$\partial_j \pi = (1 - \pi)\partial_j \pi \, \pi + \pi \, \partial_j \pi (1 - \pi)$$

with

$$(1 - \pi)\partial_j \pi \, \pi = (H - h)^{-1}(1 - \pi)\partial_j (H - h)$$

and

$$\pi \, \partial_j \pi (1 - \pi) = \pi \, \partial_j (H - h)(1 - \pi)(H - h)^{-1} = \pi \partial_j (H - h)(H - h)^{-1}(1 - \pi).$$

On the range of π, the resolvent $(H - h)^{-1}$ is invertible, more precisely, there exists $c > 0$ such that

$$\|(H - h)^{-1}(1 - \pi)\|_{\mathcal{L}(\operatorname{Ran}(1-\pi))} \leq c \operatorname{dist}\left(h, \operatorname{Sp}(H) \setminus \{h\}\right)^{-1} \leq c\, C\langle z\rangle^{n_0 + \ell - 1},$$

whence $|\partial_j \pi(t, z)| \leq C\langle z\rangle^{n_0}$.

For analyzing the derivatives of π, one observes that the relation $\pi = \pi^2$ implies

$$\partial^\gamma \pi = \pi \partial^\gamma \pi + \partial^\gamma \pi \, \pi + \sum_{1 < |\alpha|, |\beta| < |\gamma|} c_{\alpha,\beta} \partial^\alpha \pi \partial^\beta \pi$$

for some coefficients $c_{\alpha,\beta}$. A recursive argument then gives the estimate on the growth of the eigenprojectors.

Let us now consider the eigenvalue h. The relation $H\pi = \pi H = h\pi$ gives

$$\partial h \pi = \partial H \pi - \partial \pi (H - h) = \pi \partial H - (H - h)\partial \pi.$$

Multiplying on both side by π, using $(H-h)\pi = 0$ and taking the matricial trace, we obtain

$$\partial h \,\mathrm{Tr}_{\mathbb{C}^{m,m}}(\pi) = \mathrm{Tr}_{\mathbb{C}^{m,m}}(\pi \partial H).$$

This implies $|\partial h| \leq C\langle z\rangle^{\ell-1}$.

To get the relation on higher derivatives, we differentiate this relation, which gives for $i,j \in \mathbb{N}^{2d}$,

$$\partial^2_{ij} h \,\mathrm{Tr}_{\mathbb{C}^{m,m}}(\pi) = \partial_i \left(\mathrm{Tr}_{\mathbb{C}^{m,m}}(\pi \partial_j H)\right) - \partial_j h \mathrm{Tr}_{\mathbb{C}^{m,m}}(\partial_i \pi).$$

Since $\mathrm{Tr}_{\mathbb{C}^{m,m}}(\partial_i \pi) = 0$, we are left with

$$\partial^2_{ij} h \,\mathrm{Tr}_{\mathbb{C}^{m,m}}(\pi) = \mathrm{Tr}_{\mathbb{C}^{m,m}}(\partial_i \pi \partial_j H) + \mathrm{Tr}_{\mathbb{C}^{m,m}}(\pi \partial_{ij} H).$$

We obtain a control of the form $\langle z\rangle^{n_0+2(\ell-1)}$. Besides, it allows to perform a recursive argument by writing for $\gamma \in \mathbb{N}^{2d}$,

$$\begin{aligned}
\partial^\gamma \partial^2_{ij} h \,\mathrm{Tr}_{\mathbb{C}^{m,m}}(\pi) &= \partial^\gamma \left(\mathrm{Tr}_{\mathbb{C}^{m,m}}(\partial_i \pi \partial_j H) + \mathrm{Tr}_{\mathbb{C}^{m,m}}(\pi \partial_{ij} H)\right) \\
&\qquad - \sum_{2\leq|\alpha|,\alpha\leq\gamma} c_\alpha \partial^{\gamma-\alpha} \partial^2_{ij} h \,\mathrm{Tr}_{\mathbb{C}^{m,m}}(\partial^\alpha \pi) \\
&= \sum_{\alpha\leq\gamma} c_\alpha \left(\mathrm{Tr}_{\mathbb{C}^{m,m}}(\partial^{\gamma-\alpha}\partial_i \pi\, \partial^\alpha \partial_j H) + \mathrm{Tr}_{\mathbb{C}^{m,m}}(\partial^{\gamma-\alpha}\pi \partial^\alpha \partial_{ij} H)\right) \\
&\qquad - \sum_{2\leq|\alpha|,\alpha\leq\gamma} c_\alpha \partial^{\gamma-\alpha} \partial^2_{ij} h \,\mathrm{Tr}_{\mathbb{C}^{m,m}}(\partial^\alpha \pi)
\end{aligned}$$

for some coefficients c_α. One can then conclude recursively to $|\partial^\gamma \partial^2_{ij} h| \leq c'_\gamma \langle z\rangle^{(|\gamma|+1)n_0+2(\ell-1)}$. □

These two Lemmata allow to derive the consequences of Assumptions 1.4 for a Hamiltonian $H^\varepsilon = H_0 + \varepsilon H_1$. We now fix $m = 2$.

Proposition A.4. Assume that $H^\varepsilon = H_0 + \varepsilon H_1$ satisfies the Assumptions 1.4. Then, for $j \in \{1,2\}$ we have the following properties:

(1) For all $\gamma \in \mathbb{N}^{2d}$ with $|\gamma| \geq 2$, there exists a constant $C_\gamma > 0$ such that

$$\forall (t,z) \in I \times \mathbb{R}^{2d},\ \ |\partial^\gamma_z \pi_j(t,z)| \leq C_\gamma \langle z\rangle^{|\gamma| n_0} \text{ and } |\partial^\gamma_z h_j(t,z)| \leq C_\gamma \langle z\rangle^{(|\gamma|-1)n_0}.$$

(2) If moreover $n_0 = 0$ in (1.6), then the maps $z \mapsto \partial^\gamma \pi_j(t,z)$ and $z \mapsto \partial^\gamma_z h_j(t,z)$ for $|\gamma| \geq 2$ are bounded. As a consequence, the Hamiltonian trajectories $\Phi_h^{t_0,t}(z)$ are globally defined for all $z \in \mathbb{R}$. Besides, there exists $C' > 0$ such that

$$|\Phi_{h_j}^{t_0,t}(z)| \leq C|z|\mathrm{e}^{C|t-t_0|}$$

and the Jacobian matrices $F_j(t,z) = \partial_z \Phi_{h_j}^{t,t_0}(z)$ (see (1.12)) satisfy

$$\|F_j(t,z)\|_{\mathbb{C}^{2d,2d}} \leq C\mathrm{e}^{C|t-t_0|}.$$

Remark A.5. Note that under the assumptions of Proposition A.4, for all $j \in \{1,\cdots,2d\}$, the matrices

$$f\partial_{z_j}\pi_1 = -f\partial_{z_j}\pi_2 = \frac{1}{2}\left(\partial_{z_j}(H-v) - \partial_{z_j} f(\pi_2 - \pi_1)\right)$$

are bounded. This comes from the differentiation of the relation $H = v\mathbb{I} + f(\pi_2 - \pi_1)$.

PROOF. Note first that Point 2 is a consequence of Point 1. We thus focus on Point 1. We use that π_2 is the projector of the matrix $H_0 - v\mathbb{I}$ for the eigenvalue f. And the matrix $H_0 - v\mathbb{I}$ satisfies the assumptions of Lemma A.3 with $\ell = 1$. Therefore, we have for $(t, z) \in I \times \mathbb{R}^d$ with $|z| \geq 1$ and for $\gamma \in \mathbb{N}^d$.

$$|\partial_z^\gamma \pi_j(t, z)| \leq C_\gamma \langle z \rangle^{|\gamma| n_0} \text{ and } |\partial_z^\gamma f(t, z)| \leq C_\gamma \langle z \rangle^{(|\gamma|-1) n_0}.$$

One concludes by observing that the function $v = 2\mathrm{Tr}(H)$ is subquadratic, whence the property of $h_2 = v + f$. One argues similarly for h_1. □

We close this Section with the proof of Lemma 1.10

PROOF OF LEMMA 1.10. The map $t \mapsto \mathcal{R}_\ell(t, t_0, z)$ is valued in the set of unitary maps because the matrix $H^{\mathrm{adia}}_{\ell,1}$ is self adjoint. Besides, the map

$$(t, z) \mapsto Z_\ell(t, z) = \pi_\ell(\Phi_\ell^{t,t_0}(z) \mathcal{R}_\ell(t, t_0, z) \pi_\ell^\perp(z)$$

satisfies the ODE

$$i\partial_t Z_\ell = -i \left(\pi_\ell(\partial_t \pi_\ell + \{h, \pi_\ell\})\right) \circ \Phi_\ell^{t,t_0} Z_\ell, \quad Z_\ell(t_0, z) = 0,$$

and thus coincides with the solution $Z_\ell(t) = 0$. □

APPENDIX B

Elements of symbolic calculus : the Moyal product

In this section, we revisit results about the remainder estimate for the Moyal product, aiming at their extension to the setting of the sets $\boldsymbol{S}^{\mu}_{\delta}(\mathcal{D})$ that we have introduced in Definition 4.1.

B.1. Formal expansion

We first recall the formal product rule for quantum observables with Weyl quantization. Let $A, B \in \mathcal{S}(\mathbb{R}^{2d}, \mathbb{C}^{m,m})$. The Moyal product $C := A \circledast B$ is the semi-classical observable C such that $\widehat{A} \circ \widehat{B} = \widehat{C}$. Some computations with the Fourier transform give the following well known formula [**34**, Theorems 18.1.8]

$$C(x,\xi) = \exp\left(\frac{i\varepsilon}{2}\sigma(D_q, D_p; D_{q'}, D_{p'})\right) A(q,p)B(q',p')|_{(q,p)=(q',p')=(x,\xi)}, \tag{B.1}$$

where σ is the symplectic bilinear form $\sigma((q,p),(q',p')) = p\cdot q' - p'\cdot q$ and $D = i^{-1}\nabla$. By expanding the exponential term, we obtain

$$C(x,\xi) = \sum_{j\geq 0} \frac{\varepsilon^j}{j!}\left(\frac{i}{2}\sigma(D_q, D_p; D_{q'}, D_{p'})\right)^j A(q,p)B(q',p')|_{(q,p)=(q',p')=(x,\xi)}. \tag{B.2}$$

So that $C = \sum_{j\geq 0}\varepsilon^j C_j$ is a formal power series in ε with coefficients given by (4.1).

B.2. Symbols with derivative bounds

For $\mu \geq 0$ denote by $\mathbf{P}(\mu)$ the linear space of matrix-valued $\mathcal{C}^\infty$ symbols $A : \mathbb{R}^{2d} \to \mathbb{C}^{m,m}$ such that for any $\gamma \in \mathbb{N}^{2d}$ with $|\gamma| \geq \mu$, there exists $C_\gamma > 0$ such that

$$|\partial_z^\gamma A(z)| \leq C_\gamma \ \ \forall z \in \mathbb{R}^{2d}.$$

Assuming that $A \in \mathbf{P}(\mu_A)$, $B \in \mathbf{P}(\mu_B)$ it is known that, for ε fixed, $A \circledast B = C$ where $C \in \mathbf{P}(\mu_C)$ with $\mu_C \geq \max\{\mu_A, \mu_B\}$ (see e.g. the proof [**34**, Theorem 18.1.8])

We aim at having better estimates for small $\varepsilon > 0$ and a control of the derivatives of C in terms of those of A and B. The following estimate and its proof are a particular case of [**6**, Theorem A.1].

THEOREM B.1. *For every $N \in \mathbb{N}$ and $\gamma \in \mathbb{N}^{2d}$, there exists a constant $K_{N,\gamma}$ such that for any $A \in \mathbf{P}(\mu_A)$, $B \in \mathbf{P}(\mu_B)$ the Moyal remainder*

$$R_N(A,B;z;\varepsilon) := (A \circledast B)(z) - \sum_{0\leq j\leq N} \varepsilon^j C_j(z) \tag{B.3}$$

satisfies for every $z \in \mathbb{R}^{2d}$ and $\varepsilon \in (0,1]$,

$$|\partial_z^\gamma R_N(A,B;z;\varepsilon)| \leq \varepsilon^{N+1} K_{N,\gamma} \sum_{N+1\leq|\alpha|,|\beta|\leq N+\kappa_0+|\gamma|} \|\partial_z^\alpha A\|_{L^\infty}\|\partial_z^\beta B\|_{L^\infty}, \tag{B.4}$$

with $\kappa_0 = 4d + 2$.

The estimate 4.4 allows to evaluate the norms of the operators involved in Theorem B.1.

COROLLARY B.2. If $A \in \mathbf{S}^{\mu}_{\varepsilon,\delta}$ and $B \in \mathbf{S}^{\mu'}_{\varepsilon,\delta}$, then $A \circledast B \in \mathbf{S}^{\mu+\mu'}_{\varepsilon,\delta}$ (see Remark 4.2) and for all $N, k \in \mathbb{N}$, there exists a constant $C_{N,k} > 0$ such that

$$\|\mathrm{op}_\varepsilon(R_N(A, B; z; \varepsilon))\|_{\Sigma^k_\varepsilon} \leq C_{N,k}\, \varepsilon^{N+1}\, \delta^{\mu+\mu'-2(N+1+k+\kappa_0)}.$$

PROOF. By Fourier transform computations and application of the Taylor formula, we get the following formula for the remainder,

$$R_N(A, B; z; \varepsilon) = \frac{1}{N!} \left(\frac{i\varepsilon}{2}\right)^{N+1} \int_0^1 (1-t)^N R_{N,t}(z; \varepsilon) dt, \tag{B.5}$$

where

$$R_{N,t}(z; \varepsilon) =$$
$$(2\pi\varepsilon t)^{-2d} \int\int_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} \exp\left(-\frac{i}{2t\varepsilon}\sigma(u, v)\right) \sigma^{N+1}(D_u, D_v) A(u + z) B(v + z) du dv.$$

Notice that the integral is an oscillating integral as we shall see below. We now use Lemma B.3 for $A, B \in \mathcal{S}(\mathbb{R}^{2d})$ with the integrand

$$F_{N,\gamma}(z; u, v) = \pi^{-2d}\, \partial^\gamma_z \left(\sigma^{N+1}(D_u, D_v) A(u + z) B(v + z)\right)$$

and the parameter $\lambda = 1/(2t\varepsilon)$. We then have

$$|\partial^\gamma_z R_{N,t}(z; \varepsilon)| \leq C_d \sup_{\substack{u,v\in\mathbb{R}^{2d} \\ |\alpha|+|\beta|\leq 4d+1}} |\partial^\alpha_u \partial^\beta_v F_{N,\gamma}(z; u, v)|.$$

Moreover, there holds the elementary estimate

$$|\sigma^{N+1}(D_u, D_v) A(u) B(v)| \leq (2d)^{N+1} \sup_{|\alpha|+|\beta|=N+1} |\partial^\alpha_x \partial^\beta_\xi A(x, \xi) \partial^\beta_y \partial^\alpha_\eta B(y, \eta)|.$$

Together with the Leibniz formula, we then get the claimed results with universal constants. For symbols $A \in \mathbf{P}(\mu_A)$ and $B \in \mathbf{P}(\mu_B)$ we argue by localisation. We use $A_\eta(u) = \mathrm{e}^{-\eta u^2} A(u)$ and $B_\eta(v) = \mathrm{e}^{-\eta v^2} B(v)$ for $\eta > 0$ and pass to the limit $\eta \to 0$. □

LEMMA B.3. *There exists a constant $C_d > 0$ such that for any $F \in \mathcal{S}(\mathbb{R}^{2d} \times \mathbb{R}^{2d}, \mathbb{C}^{m,m})$ the integral*

$$I(\lambda) = \lambda^{2d} \int_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} \exp[-i\lambda\sigma(u, v)] F(u, v) du dv. \tag{B.6}$$

satisfies

$$|I(\lambda)| \leq C_d \sup_{\substack{u,v\in\mathbb{R}^{2d} \\ |\alpha|+|\beta|\leq 4d+1}} |\partial^\alpha_u \partial^\beta_v F(u, v)|. \tag{B.7}$$

PROOF OF LEMMA B.3. The lemma is proved in a standard way, using integration by parts and stationary phase argument. For the sake of completeness, we give here a proof. We introduce a cut-off $\chi_0 \in \mathcal{C}^\infty_0(\mathbb{R})$ such that

$$\chi_0(x) = 1 \quad \text{for} \quad |x| \leq 1/2 \quad \text{and} \quad \chi_0(x) = 0 \quad \text{for} \quad |x| \geq 1.$$

We split $I(\lambda)$ into too pieces and write $I(\lambda) = I_0(\lambda) + I_1(\lambda)$ with

$$I_0(\lambda) = \lambda^{2d} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} \exp[-i\lambda\sigma(u,v)]\chi_0(u^2+v^2)F(u,v)dudv,$$
$$I_1(\lambda) = \lambda^{2d} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} \exp[-i\lambda\sigma(u,v)](1-\chi_0)(u^2+v^2))F(u,v)dudv.$$

We notice that $(u,v) \mapsto \sigma(u,u)$ is a quadratic non-degenerate real form on $\mathbb{R}^{4d}$.
Let us estimate $I_1(\lambda)$. We can integrate by parts with the differential operator

$$L = \frac{i}{|u|^2+|v|^2}\left(Ju\cdot\frac{\partial}{\partial v} - Jv\cdot\frac{\partial}{\partial u}\right),$$

using that $L\mathrm{e}^{-i\lambda\sigma(u,v)} = L\mathrm{e}^{-i\lambda Ju\cdot v} = \lambda\mathrm{e}^{-i\lambda\sigma(u,v)}$. For $I_1(\lambda)$, the integrand is supported outside the ball of radius $1/\sqrt{2}$ in $\mathbb{R}^{4d}$. Performing $4d+1$ integrations by parts for gaining enough decay to ensure integrability in $(u,v)\in\mathbb{R}^{4d}$, we get a constant c_d such that

$$|I_1(\lambda)| \leq c_d \sup_{\substack{u,v\in\mathbb{R}^{2d}\\ |\mu|+|\nu|\leq 4d+1}} |\partial_u^\mu \partial_v^\nu F(u,v)|.$$

To estimate $I_0(\lambda)$ we apply the stationary phase. The symmetric matrix of the quadratic form $\sigma(u,v)$ is

$$A_\sigma = \begin{pmatrix} 0 & -J \\ J & 0 \end{pmatrix}.$$

So the stationary phase Theorem ([**34**], Vol.I, section 7.7), we obtain the existence of two constants $c_1, c_2 > 0$ such that

$$|I_0(\lambda) - \lambda^{-2d}c_1| \leq c_2 \sup_{\substack{u,v\in\mathbb{R}^{2d}\\ |\alpha|\leq 2}} |\partial^\alpha(\chi_0(u^2+v^2)F(u,v)|. \tag{B.8}$$

□

APPENDIX C

Elements of semi-classical calculus: perturbation of scalar systems

In this Appendix, we revisit several well-known results concerning a Hamiltonian $K(t)$ valued in the set $\mathbb{C}^{m,m}$ of $m \times m$ matrices ($m \in \mathbb{N}$), and which is a perturbation of a scalar function $k(t)$. We consider an interval $I_\delta \subset \mathbb{R}$ that may depend on $\delta > 0$ and assume that $K(t)$ is defined on I_δ and of the form

$$K(t) = k(t)\mathbb{I}_m + \varepsilon K_1(t) + \cdots \varepsilon^N K_N(t) \tag{C.1}$$

with k scalar-valued and $k(t)\mathbb{I}_m + \varepsilon K_1(t)$ is subquadratic on the time interval I_δ according to Definition 1.1.

The difference with the classical setting is that we assume

$$\forall t \in I_\delta, \ \ \frac{1}{\varepsilon^2}\left(K(t) - k(t)\mathbb{I}_m - \varepsilon K_1(t)\right) \in \boldsymbol{S}^{-1}_{\varepsilon,\delta}(\mathcal{D}).$$

Therefore, we have to revisit the results to take care of the loss in δ and control all the classical estimates with respect to this parameter. We denote by $\mathcal{U}^\varepsilon_K(t_0, t)$ the unitary propagator associated with $K(t)$.

These assumptions are those satisfied by the Hamiltonian that we consider in the adiabatic region (see Section 5.2): by (3) of Theorem 4.9, the Hamiltonians $\widetilde{H}^{\mathrm{adia},N,\varepsilon}_\ell(t)$, defined for $\ell \in \{1, 2\}$ in (5.3), satisfy the assumptions made on the Hamiltonian $K(t)$ on the interval $[t_0, t^\flat - \delta]$ and on the interval $[t^\flat + \delta, t_0 + T]$, for adequate domains $\mathcal{D}$ given by the cut-offs. Therefore, the analysis below allows to deduce Theorem 5.9 from Proposition 5.8. In the gap region, we also use these results in the simpler case $\delta = 1$ (see Sections 5.3 and 5.4).

C.1. Egorov Theorem

The Egorov Theorem describes the evolution of an observable when it is conjugated by the propagator $\mathcal{U}^\varepsilon_K(t, s)$ associated with the operator $K(t)$. It is important to notice that this propagator maps Σ^k_ε in itself for all $k \in \mathbb{N}$. Indeed, for $1 \leq j \leq d$,

$$i\varepsilon\partial_t(x_j\psi^\varepsilon(t)) - \widehat{K}(t)(x_j\psi^\varepsilon(t)) = f^\varepsilon_j(t) \ \text{ and } \ i\varepsilon\partial_t(\varepsilon\partial_{x_j}\psi^\varepsilon(t)) - \widehat{K}(t)(\varepsilon\partial_{x_j}\psi^\varepsilon(t)) = g^\varepsilon_j(t),$$

with $f^\varepsilon_j(t) = [x_j, \widehat{K}(t)]\psi^\varepsilon(t)$ and $g^\varepsilon_j(t) = [\varepsilon D_{x_j}, \widehat{K}(t)]\psi^\varepsilon(t)$ uniformly bounded in L^2. Therefore, one deduces the L^2-boundedness of the families $(x_j\psi^\varepsilon(t))$ and $(\varepsilon D_{x_j}\psi^\varepsilon(t))$ for all $1 \leq j \leq d$, whence the boundedness of $\psi^\varepsilon(t)$ in Σ^1_ε for all $t \in \mathbb{R}$. The reader will have understood that a recursive process will give the boundedness of $\psi^\varepsilon(t)$ in any Σ^k_ε, for $t \in \mathbb{R}$ and $k \in \mathbb{N}$. In this setting, our aim is to revisit the evolution of $\mathcal{U}^\varepsilon_K(t_{\mathrm{in}}, t)\widehat{A}\mathcal{U}^\varepsilon_K(t, t_{\mathrm{in}})$ for matrix-valued observables $A \in \boldsymbol{S}_\delta$ and in spaces Σ^k_ε, with a precise estimate of the remainders.

PROPOSITION C.1. With the above notations, for any matrix-valued symbol $A \in \boldsymbol{S}_\delta$, there exists a formal series $(t, t_{\rm in}) \mapsto \sum_{j\geq 0} \varepsilon^j A_j(t, t_{\rm in})$ defined on $I_\delta \times I_\delta$ and such that for any $J \geq 1$, we have for all $t, t_{\rm in} \in I^\delta$,

$$\mathcal{U}_K^\varepsilon(t_{\rm in}, t)\widehat{A}\mathcal{U}_K^\varepsilon(t, t_{\rm in}) = \sum_{0\leq j\leq J} \varepsilon^j \widehat{A}_j(t, t_{\rm in}) + \varepsilon^{J+1}\widehat{R}_J^\varepsilon(t, t_{\rm in}),$$

with $A_j(t, t_{\rm in}) \in \boldsymbol{S}_\delta^{-2j}$ uniformly in $\varepsilon \in]0, 1]$. Besides, for all $k \in \mathbb{N}$, there exists a constant $C_{k,J}$ such that

$$\|\widehat{R_J^\varepsilon}(t, t_{\rm in})\|_{\Sigma_\varepsilon^k} \leq c_k \delta^{-2(J+1+\kappa_0)},$$

and the matrix $A_0(t, t_{\rm in})$ is given by

$$A_0(t, t_{\rm in}, z) = (\mathcal{R}^*(t, t_{\rm in})A\mathcal{R}(t, t_{\rm in})) \circ (\Phi_k^{t,t_{\rm in}})(z), \tag{C.2}$$

where the unitary matrices $\mathcal{R}(t, t_{\rm in}, z)$ solve the transport equation

$$i\partial_t \mathcal{R}(t, t_{\rm in}, z) = K_1\left(t, \Phi_k^{t,t_{\rm in}}(z)\right)\mathcal{R}(t, t_{\rm in}, z),\ \mathcal{R}(t_{\rm in}, t_{\rm in}, z) = \mathbb{I}_m. \tag{C.3}$$

REMARK C.2. In particular we have the propagation law of the supports:

$$\mathrm{supp}(A_j(t, t_{\rm in})) = \Phi_k^{t_{\rm in},t}(\mathrm{supp}(A)) \quad \text{for any } \ j \geq 0.$$

In the scalar time independent case case ($k = k(z)$ and $K_j = 0$ for $j \geq 1$), the Egorov theorem

$$\mathcal{U}_K^\varepsilon(t_{\rm in}, t)\widehat{A}\mathcal{U}_K^\varepsilon(t, t_{\rm in}) = \widehat{A \circ \Phi_k^{t,t_{in}}} + O(\varepsilon)$$

is well-known (see [**13, 14, 64**] for example). In the time-dependent matrix-valued case considered here, the dynamics on the observable is driven by the classical flow twisted by the precession $\mathcal{R}$ (see also Section 1.3.3 where such terms appear). The proof also requires a careful treatment of the time.

PROOF. We perform a recursive argument. The starting point comes from the analysis of the auxiliary map defined for $\tau, t \in I_\delta$ and valued in $\mathbf{S}_\delta$ by

$$A \mapsto A(t, \tau) := (\mathcal{R}(\tau, t)A\,\mathcal{R}(\tau, t)^*) \circ \Phi_k^{t,\tau}.$$

Because we are going to differentiate in τ, we use the relation

$$i\partial_\tau \Phi_k^{t,\tau} = -J\nabla k(\tau, \Phi_k^{t,\tau}),$$

(where J is the matrix defined in (1.10)), which implies for all $z \in \mathbb{R}^{2d}$, using also that the flow map is symplectic and preserves the Poisson bracket,

$$\partial_\tau A(t, \tau, z) + \{k(\tau), A(t, \tau)\}(z) = \frac{1}{i}[K_1(\tau, z), A(t, \tau, z)],\ \ A(t, t) = A.$$

Let us know starts with the proof of the result for $J = 0$. We choose $s, \tau, t \in I_\delta$ and consider the quantity

$$Q_A^\varepsilon(t, s, \tau) = \mathcal{U}_K^\varepsilon(s, \tau)\widehat{A}(t, \tau)\mathcal{U}_K^\varepsilon(\tau, s).$$

The times s, τ, t can be understood as $s \leq \tau \leq t$ with s an initial time (that will be taken as $s = t_{\rm in}$) and t the time at which we want to prove the property. We then have the boundary properties

$$Q_A^\varepsilon(t, s, t) = \mathcal{U}_K^\varepsilon(s, t)\widehat{A}\mathcal{U}_K^\varepsilon(t, s) \ \text{ and } \ Q_A^\varepsilon(t, s, s) = \widehat{A}(t, s).$$

Differentiating in τ, we have

$$\begin{aligned}\frac{d}{d\tau}Q_A^\varepsilon(t,s,\tau) &= \mathcal{U}_K^\varepsilon(s,\tau)\left(\left[-\frac{1}{i\varepsilon}\widehat{K}(\tau),\widehat{A}(t,\tau)\right]+\partial_\tau\widehat{A}(t,\tau)\right)\mathcal{U}_K^\varepsilon(\tau,s)\\ &= \mathcal{U}_K^\varepsilon(s,\tau)\left(\left[-\frac{1}{i\varepsilon}\widehat{K}(\tau),\widehat{A}(t,\tau)\right]-\{k,\widehat{A(t,\tau)}\}+\frac{1}{i}[K_1(\tau),\widehat{A(t,\tau)}]\right)\mathcal{U}_K^\varepsilon(\tau,s)\\ &= \varepsilon\,\mathcal{U}_K^\varepsilon(s,\tau)\,\widehat{B_1^\varepsilon}(t,\tau)\,\mathcal{U}_K^\varepsilon(\tau,s)\end{aligned}$$

where the matrix $B_1^\varepsilon \in \mathbf{S}^{-2}_{\varepsilon,\delta}$ stems from the Moyal product (see Corollary B.2). We deduce by integration between the times s and t

$$\mathcal{U}_K^\varepsilon(s,t)\widehat{A}\mathcal{U}_K^\varepsilon(t,s) = \widehat{A}(t,s)+\varepsilon\int_s^t \mathcal{U}_K^\varepsilon(s,\tau)\,\widehat{B_1^\varepsilon}(t,\tau)\,\mathcal{U}_K^\varepsilon(\tau,s)d\tau,$$

which gives the first step of the recursive argument.

We now assume that we have obtained for $J\geq 0$

$$\mathcal{U}_K^\varepsilon(s,t)\widehat{A}\mathcal{U}_K^\varepsilon(t,s) = \sum_{j=0}^J \varepsilon^j\,\widehat{A}_j(t,s)+\varepsilon^{J+1}\int_s^t \mathcal{U}_K^\varepsilon(s,\tau)\,\widehat{B_{J+1}^\varepsilon}(t,\tau)\,\mathcal{U}_K^\varepsilon(\tau,s)d\tau$$

with $B_{J+1}^\varepsilon \in \mathbf{S}_\delta^{-2(J+1)}$. We write

$$B_{J+1}^\varepsilon = B_{J+1}+B_{J+2}^{1,\varepsilon}$$

with $B_{J+1}\in\mathbf{S}_\delta^{-2(J+1)}$ and $B_{J+2}^\varepsilon\in\mathbf{S}_{\varepsilon,\delta}^{-2(J+2)}$. Then, the preceding equation writes

$$\begin{aligned}\mathcal{U}_K^\varepsilon(s,t)\widehat{A}\mathcal{U}_K^\varepsilon(t,s) &= \sum_{j=0}^J \varepsilon^j\,\widehat{A}_j(t,s)\\ &\quad+\varepsilon^{J+1}\int_s^t Q^\varepsilon_{B_{J+1}}(t,s,\tau)d\tau+\varepsilon^{J+2}\int_s^t \mathcal{U}_K^\varepsilon(s,\tau)\,\widehat{B_{J+2}^{1,\varepsilon}}(t,\tau)\,\mathcal{U}_K^\varepsilon(\tau,s)d\tau.\end{aligned}\tag{C.4}$$

We focus on the term involving $Q^\varepsilon_{B_{J+1}}(t,s,\tau)$ that we treat as in the preceding step. We obtain

$$Q^\varepsilon_{B_{J+1}}(t,s,\tau) = \mathcal{R}(s,\tau)B_{J+1}(t,\tau)\mathcal{R}(\tau,s)^*+\varepsilon\int_s^\tau \mathcal{U}_K^\varepsilon(s,\tau')\widehat{B}^{2,\varepsilon}_{J+2}(\tau,\tau')\mathcal{U}_K^\varepsilon(\tau',s)d\tau'$$

with $B_{J+2}^{2,\varepsilon}\in\mathbf{S}^{-2(J+2)}_{\varepsilon,\delta}$. We set

$$A_{J+1}(s,t) = \int_s^t \mathcal{R}(s,\tau)B_{J+1}(t,\tau)\mathcal{R}(\tau,s)^*\in\mathbf{S}_\delta^{-2(J+1)}$$

and

$$B^\varepsilon_{J+2}(t,\tau) = B^{1,\varepsilon}_{J+2}(t,\tau)+\int_s^\tau B^{2,\varepsilon}_{J+2}(\tau',\tau)d\tau'\in\mathbf{S}^{-2(J+1)}_{\varepsilon,\delta}.$$

The equation (C.4) then becomes

$$\mathcal{U}_K^\varepsilon(s,t)\widehat{A}\mathcal{U}_K^\varepsilon(t,s) = \sum_{j=0}^{J+1}\varepsilon^j\,\widehat{A}_j(t,s)+\varepsilon^{J+2}\int_s^t \mathcal{U}_K^\varepsilon(s,\tau)\,\widehat{B^\varepsilon_{J+2}}(t,\tau)\,\mathcal{U}_K^\varepsilon(\tau,s)d\tau$$

and this concludes the proof. □

C.2. Asymptotic behavior of the propagator

In this section, we analyze the propagator $\mathcal{U}_K^\varepsilon(t,t_{\rm in})$ and compare it with $\mathcal{U}_{KS}^\varepsilon(t,t_{\rm in})$ the propagator for

$$KS(t)=k(t)\mathbb{I}_m+\varepsilon K_1(t).$$

LEMMA C.3. *For all $J\in\mathbb{N}$, there exists*

$$W^\varepsilon(t,t_{\rm in})=\sum_{0\leq j\leq J}\varepsilon^j\,W_j(t,t_{\rm in})+\varepsilon^{J+1}R_J^\varepsilon(t,t_{\rm in})$$

with $W_j(t,t_{\rm in})\in\boldsymbol{S}_\delta^{-2j}$ such that for all $t\in\mathbb{R}$,

$$\mathcal{U}_K^\varepsilon(t,t_{\rm in})=\widehat{W}^\varepsilon(t,t_{\rm in})\mathcal{U}_{KS}^\varepsilon(t,t_{\rm in}).$$

Besides, $W_0(t,t_{\rm in})=\mathbb{I}_m$ and for all $\gamma\in\mathbb{N}^{2d}$, there exists $C_{J,\gamma}>0$ such that

$$\sup_{z\in\mathbb{R}^d}|\partial_z^\gamma R_J^\varepsilon(t,t_{\rm in},z)|\leq C_{J,\gamma}\,\delta^{-2(J+1+|\gamma|+\kappa_0)}$$

where κ_0 is the universal constant of Theorem B.1.

REMARK C.4. Using the estimate (4.4), we deduce that for all $k\in\mathbb{N}$, there exists $C_k>0$ such that

$$\|{\rm op}_\varepsilon(R_J^\varepsilon(t,t_{\rm in}))\|_{\mathcal{L}(\Sigma_\varepsilon^k)}\leq C_k\left(\frac{\varepsilon}{\delta^2}\right)^{\frac{|\gamma|}{2}}\,\delta^{-2(J+1+k+\kappa_0)}.$$

As a consequence, for $\delta=\varepsilon^\alpha$ with $\alpha\in(0,\frac12]$, we have

$$\|{\rm op}_\varepsilon(R_J^\varepsilon(t,t_{\rm in}))\|_{\mathcal{L}(\Sigma_\varepsilon^k)}\leq C_k\,\delta^{-2(J+1+k+\kappa_0)}. \tag{C.5}$$

Similarly, by (4.5), for such δ,

$$\|{\rm op}_\varepsilon(W_j(t,t_{\rm in}))\|_{\mathcal{L}(\Sigma_\varepsilon^k)}\leq C_k\,\delta^{-2j-k},\quad j\in\mathbb{N}. \tag{C.6}$$

PROOF. If such a $W^\varepsilon(t,t_{\rm in})$ exists, it must satisfy the following equation

$$i\varepsilon\partial_t\widehat{W}^\varepsilon(t,t_{\rm in})\widehat{W}^\varepsilon(t,t_{\rm in})\mathcal{U}_{KS}^\varepsilon(t_{\rm in},t)\left(\widehat{K}(t)-\widehat{KS}(t)\right)\mathcal{U}_{KS}^\varepsilon(t,t_{\rm in})^*,\ \ \widehat{W}^\varepsilon(t_{\rm in},t_{\rm in})=\mathbb{I}_m$$

Applying Egorov Theorem of Propostion C.1, we know that

$$\mathcal{U}_{KS}^\varepsilon(t_{\rm in},t)\left(\widehat{K}(t)-\widehat{KS}(t)\right)\mathcal{U}_{KS}^\varepsilon(t_{\rm in},t)^*=\varepsilon^2\widehat{L}^\varepsilon(t,t_{\rm in})$$

where

$L^\varepsilon(t,t_{\rm in})=\sum_{j\geq0}\varepsilon^jL_j(t,t_{\rm in})\in\mathbf{S}_{\varepsilon,\delta}^{-1}$ with estimates on $L_j(t,t_{\rm in})$ and on the remainder term in the asymptotic expansion. Using the estimates proved in Appendices A and B, it is enough to solve as formal series in ε the equation

$$i\partial_t\left(\sum_{j\geq0}\varepsilon^jW_j(t,t_{\rm in})\right)=\varepsilon\left(\sum_{j\geq0}\varepsilon^jW_j(t,t_{\rm in})\right)\circledast\left(\sum_{k\geq0}\varepsilon^jL_j(t,t_{\rm in})\right). \tag{C.7}$$

□

C.3. Propagation of wave packets

When ψ_0^ε is a wave packet, the action of $\mathcal{U}_{KS}^\varepsilon(t,t_1)\psi_0^\varepsilon$ on ψ_0^ε can be described precisely. Following Section 14.2 of [**13**], Theorem 77, we have the following result.

PROPOSITION C.5. Assume we have $\psi^\varepsilon = \mathrm{WP}_{z_0}^\varepsilon(f^\varepsilon)\vec{V}$ with $\vec{V}\in\mathbb{C}^m$,

$$f^\varepsilon = \sum_{0\le j\le J} \varepsilon^{j/2} f_j, \quad f_j \in \mathcal{S}(\mathbb{R}^d).$$

There exists a family $(\vec{U}_j(t))_{j\ge 0}$ defined on the interval I_δ such that

(i) For all $j\in\mathbb{N}$ and $t\in I_\delta$, $\vec{U}_j(t)\in\mathcal{S}(\mathbb{R}^d)$,
(ii) For all $k,j\in\mathbb{N}$, there exists a constant $C_{k,j}$ such that

$$\sup_{t\in I_\delta}\sup_{|\alpha|+|\beta|=k} \|x^\alpha \partial_x^\beta U_j(t)\|_{L^\infty} \le C_{k,j}\delta^{-j}.$$

(iii) For all $k\in\mathbb{N}$ and $N\in\mathbb{N}$, there exists $C_{k,N}$ and N_k such that for all $t\in\mathbb{R}$, we have

$$\left\| \mathcal{U}_K^\varepsilon(t,t_{\rm in})\psi^\varepsilon - \mathrm{e}^{\frac{i}{\varepsilon}S(t,t_{\rm in},z_0)}\mathrm{WP}^\varepsilon_{\Phi_k^{t,t_{\rm in}}(z_0)}\left(\sum_{j=0}^{2N}\varepsilon^{\frac{j}{2}}\vec{U}_j(t)\right)\right\|_{\Sigma_\varepsilon^k} \le C_{k,N}\left(\frac{\varepsilon}{\delta^2}\right)^N \delta^{-N-N_k}.$$

Besides

$$\vec{U}_0(t) = \mathcal{R}(t,t_{\rm in})\,\mathcal{M}[F(t,t_{\rm in})]f_0\vec{V} \ \text{ and } \ \vec{U}_1(t) = \mathcal{R}(t,t_{\rm in})\,\mathcal{M}[F(t,t_{\rm in})]\mathbf{b}_1(t,t_{\rm in})f_0\vec{V} \tag{C.8}$$

where

$$\begin{aligned}\mathbf{b}_1(t,t_{\rm in}) &= \frac{1}{i}\sum_{|\alpha|=3}\frac{1}{\alpha!}\int_{t_{\rm in}}^t \partial_z^\alpha h(s,z_s)\mathrm{op}_1^w((F(t_{\rm in},s)z)^\alpha)ds \\ &\quad + \frac{1}{i}\int_{t_{\rm in}}^t \partial_z H_1(s,z_s)\mathrm{op}_1(F(t_{\rm in},s)z)ds,\end{aligned} \tag{C.9}$$

$F(t,t_{\rm in})$ is the stability matrix for the flow $z_t := \Phi_k^{t,t_{\rm in}}(z_0)$ (see (1.12)) and $\mathcal{R}(t,t_{\rm in})$ satisfies the equation (C.3).

PROOF. Let $k\in\mathbb{N}$. Using Lemma C.3 and the estimate (C.5), we obtain

$$\begin{aligned}\mathcal{U}_K^\varepsilon(t,t_{\rm in})\psi^\varepsilon &= \widehat{W}^\varepsilon(t,t_{\rm in})\mathcal{U}_{KS}^\varepsilon(t,t_{\rm in})\psi^\varepsilon \\ &= \sum_{0\le j\le J}\varepsilon^j\,\widehat{W}_j(t,t_{\rm in})\mathcal{U}_{KS}^\varepsilon(t,t_{\rm in})\psi^\varepsilon + \varepsilon^{J+1}\widehat{R}_J^\varepsilon(t,t_{\rm in})\mathcal{U}_{KS}^\varepsilon(t,t_{\rm in})\psi^\varepsilon \\ &= \sum_{0\le j\le J}\varepsilon^j\,\widehat{W}_j(t,t_{\rm in})\mathcal{U}_{KS}^\varepsilon(t,t_{\rm in})\psi^\varepsilon + O\left(\varepsilon^{J+1}\delta^{-2(J+1+\kappa_0)}\right)\end{aligned}$$

in $\Sigma_\varepsilon^k(\mathbb{R}^d)$. We then use the standard result of propagation of wave packets for $KS(t)$ (see [**13**])

$$\mathcal{U}_{KS}^\varepsilon(t,t_{\rm in})\psi^\varepsilon = \mathrm{e}^{\frac{i}{\varepsilon}S(t,t_{\rm in},z_0)}\mathrm{WP}^\varepsilon_{z_t}\left(\sum_{j=1}^{2J}\varepsilon^{\frac{j}{2}}\vec{B}_j(t)\right) + O(\varepsilon^{J+1})$$

with $\vec{B}_j(t) = \vec{U}_j(t)$ as in (C.8) for $j = 0, 1$, and $\vec{B}_j(t)$ is determined by a recursive equation in terms of $\vec{B}_0(t), \cdots, \vec{B}_{j-1}(t)$. This description relies on the observation that setting

$$\varphi_j^\varepsilon(t) = \mathrm{e}^{\frac{i}{\varepsilon}S(t,t_{\mathrm{in}},z_0)}\mathrm{WP}_{z_t}^\varepsilon\left(\vec{B}_j(t)\right)$$

we have the two relations

$$i\varepsilon\partial_t\varphi_j^\varepsilon(t) = \mathrm{e}^{\frac{i}{\varepsilon}S}\mathrm{WP}_{z_t}^\varepsilon\left(-\partial_t(S+\xi_t\cdot x_t)\vec{B}_j + \sqrt{\varepsilon}\dot{z}_t\cdot\widehat{z}\vec{B}_j + i\varepsilon\partial_t\vec{B}_j\right)$$

$$\begin{aligned}\widehat{KS(t)}\varphi_j^\varepsilon(t) &= \mathrm{e}^{\frac{i}{\varepsilon}S}\mathrm{WP}_{z_t}^\varepsilon\left(\widehat{KS(t,z_t+\sqrt{\varepsilon}z)}\vec{B}_j(t)\right)\\ &= \mathrm{e}^{\frac{i}{\varepsilon}S}\mathrm{WP}_{z_t}^\varepsilon\left(\mathrm{op}_1\left(k(t,z_t)+\sqrt{\varepsilon}\nabla k(t,z_t)\cdot z + \frac{\varepsilon}{2}\mathrm{Hess}\,k(t,z_t)z\cdot z + \varepsilon K_1(t,z_t) + O(\varepsilon^{\frac{3}{2}})\right)\vec{B}_j\right)\end{aligned}$$

where we have set $z_t = (x_t, \xi_t)$. These relations also prove (C.8) with the additional remark that $W_0(t, t_{\mathrm{in}}) = \mathbb{I}$ and, for $j \in \mathbb{N}$,

$$\widehat{W}_j(t,t_{\mathrm{in}})\mathrm{WP}_{z_t}^\varepsilon\left(\vec{B}_j(t)\right) = \mathrm{WP}_{z_t}^\varepsilon\left(\mathrm{op}_1\left(W_j(t,t_{\mathrm{in}},z_t+\sqrt{\varepsilon}z)\right)\vec{B}_j(t)\right)$$

and using the estimate (C.6) with $\varepsilon = 1$. □

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