Twisted Pseudodifferential Calculus and Application to the Quantum Evolution of Molecules

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Abstract

We construct an abstract pseudodifferential calculus with operator-valued symbol, adapted to the treatment of Coulomb-type interactions, and we apply it to study the quantum evolution of molecules in the Born-Oppenheimer approximation, in the case where the electronic Hamiltonian admits a local gap in its spectrum. In particular, we show that the molecular evolution can be reduced to the one of a system of smooth semiclassical operators, the symbol of which can be computed explicitely. In addition, we study the propagation of certain wave packets up to long time values of Ehrenfest order. (This work has been accepted for publication as part of the Memoirs of the American Mathematical Society and will be published in a future volume.)

1 Introduction

In quantum physics, the evolution of a molecule is described by the initial-value Schrödinger system,

$$\begin{cases} i\partial_t \varphi = H\varphi; \\ \varphi\,|_{t=0} = \varphi_0, \end{cases} \tag{1.1}$$

where φ_0 is the initial state of the molecule and H stands for the molecular Hamiltonian involving all the interactions between the particles that constitute the molecule (electron and nuclei). (In case the molecule is imbedded in an electromagnetic field, the corresponding potentials enter the expression of H, too.) Typically, the interaction between two particles of respective positions z and z' is of Coulomb type, that is, of the form $\alpha|z-z'|^{-1}$ with $\alpha \in I\!R$ constant.

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In the case of a free molecule, a first approach for studying the system (1.1) consists in considering bounded initial states only, that is, initial states that are eigenfunctions of the Hamiltonian after removal of the center of mass motion. More precisely, one can split the Hamiltonian into,

$$H = H_{\rm CM} + H_{\rm Rel},$$

where the two operators H_{CM} (corresponding to the kinetic energy of the center of mass) and H_{Rel} (corresponding to the relative motion of electrons and nuclei) commute. As a consequence, the quantum evolution factorizes into,

$$e^{-itH} = e^{-itH_{\rm CM}} e^{-itH_{\rm Rel}},$$

where the (free) evolution $e^{-itH_{\rm CM}}$ of the center of mass can be explicitly computed (mainly because $H_{\rm CM}$ has constant coefficients), while the relative motion $e^{-itH_{\rm Rel}}$ still contains all the interactions (and thus, all the difficulties of the problem). Then, taking φ_0 of the form,

$$\varphi_0 = \alpha_0 \otimes \psi_j \tag{1.2}$$

where α_0 depends on the position of the center of mass only, and ψ_j is an eigenfunction of $H_{\rm Rel}$ with eigenvalue E_j, the solution of (1.1) is clearly given by,

$$\varphi(t) = e^{-itE_j}(e^{-itH_{\rm CM}}\alpha_0) \otimes \psi_j.$$

Therefore, in this case, the only real problem is to know sufficiently well the eigenelements of H_{Rel}, in order to be able to produce initial states of the form (1.2).

In 1927, M. Born and R. Oppenheimer [BoOp] proposed a formal method for constructing such an approximation of eigenvalues and eigenfunctions of H_{Rel}. This method was based in the fact that, since the nuclei are much heavier than the electrons, their movement is slower and allows the electrons to adapt almost instantaneously to it. As a consequence, the movement of the electrons is not really perceived by the nuclei, except as a surrounding electric field created by their total potential energy (that becomes a function of the positions of the nuclei). In that way, the evolution of the molecule reduces to that of the nuclei imbedded in an effective electric potential created by the electrons. Such a reduction (that is equivalent to a separation of the problem into two different position-scales) permits, in a second moment, to use semiclassical tools in order to find the eigenelements of the final effective Hamiltonian.

At this point, it is important to observe that this method was formal only, in the sense that it permitted to produce formal series of functions that were (formally) solutions of the eigenvalue problem for H_{Rel}, but without any estimates on the remainder terms, and no information about the possible closeness of these functions to true eigenfunctions, nor to the possible exhaustivity of such approximated eigenvalues.

Many years later, a first attempt to justify rigorously (from the mathematical point of view) the Born-Oppenheimer approximation (in short: BOA) was made by J.-M. Combes, P. Duclos and R. Seiler [CDS] for the diatomic molecules, with an accuracy of order h^2, where $h := \sqrt{m/M}$ is the square-root of the ratio of the electron masses to nuclear masses. After that, full asymptotics in h were obtained by G. Hagedorn [Ha2, Ha3], both in the case of diatomic molecules with Coulomb interactions, and in the case of smooth interactions. In these two cases, these results have permitted to answer positively to the first question concerning the justification of the BOA, namely, the existence of satisfactory estimates on the remainder terms of the series. Later, by using completely different methods (mostly inspired by the microlocal treatment of semiclassical spectral problems, developed by B. Helffer and J. Sjöstrand in [HeSj11]), and in the case of smooth interactions, the first author [Ma1] extended this positive answer to the two remaining questions, that is, the exhaustivity and the closeness of the formal eigenfunctions to the true ones. Although such a method (based on microlocal analysis) seemed to require a lot of smoothness, it appeared that it could be adapted in the case of Coulomb interactions, too, giving rise to a first complete rigorous justification of the BOA in a work by M. Klein, A. Martinez, R. Seiler and X.P. Wang [KMSW]. The main trick, that has made possible such an adaptation, consists in a change of variables in the positions of the electrons, that depends in a convenient way of the position (say, x) of the nuclei. This permits to make the singularities of the interactions electron-nucleus independent of x, and thus, in some sense, to regularize these interactions with respect to x. Afterwards, the standard microlocal tools (in particular, the pseudodifferential calculus with operator-valued symbols, introduced in [Ba]) can be applied and permit to conclude.

Of course, all these justifications concerned the eigenvalue problem for H_{Rel}, not the general problem of evolution described in (1.1). In the general case, one could think about expanding any arbitrary initial state according to the eigenfunctions of H_{Rel}, and then apply the previous constructions to each term. However, this would lead to remainder terms quite difficult to estimate with respect to the small parameter h, mainly because one would have to mix two types of approximations that have nothing to do each other: The semiclassical one, and the eigenfunctions expansion one. In other words, this would correspond to handle both functional and microlocal analysis, trying to optimize both of them at the same time. It is folks that such a method is somehow contradictory, and does not produce good enough estimates. For this reason, several authors have looked for an alternative way of studying (1.1), by trying to adapt Born-Oppenheimer's ideas directly to the problem of evolution.

The first results in this direction are due to G. Hagedorn [Ha4, Ha5, Ha6], and provide complete asymptotic expansions of the solution of (1.1), in the case where the interactions are smooth and the initial state is a convenient perturbation of a single electronic-level state. More precisely, splitting the Hamiltonian into,

$$H = K_{\rm n}(hD_x) + H_{\rm el}(x),$$

where $K_{\rm n}(hD_x)$ stands for the quantum kinetic energy of the nuclei, and $H_{\rm el}(x)$ is the so-called electronic Hamiltonian (that may be viewed as acting on the position variables y of the electrons, and depending on the position x of the nuclei), one assumes that $H_{\rm el}(x)$ admits an isolated eigenvalue $\lambda(x)$ (say, for x in some open set of $\mathbb{R}^3$) with corresponding eigenfunction $\psi(x,y)$, and one takes φ_0 of the form,

$$\varphi_0(x,y) = f(x)\psi(x,y) + \sum_{k\geq 1} h^k \varphi_{0,k}(x,y) = f(x)\psi(x,y) + \mathcal{O}(h),$$

where $f(x)$ is a coherent state in the x-variables. Then, it is shown that, if the $\varphi_{0,k}$'s are well chosen, the solution of (1.1) (with a rescaled time $t \mapsto t/h$) admits an asymptotic expansion of the type,

$$\varphi_t(x,y) \sim f_t(x)\psi(x,y) + \sum_{k\geq 1} h^k \varphi_{t,k}(x,y),$$

where all the terms can be explicitly computed by means of the classical flow of the effective Hamiltonian $H_{\rm eff}(x,\xi) := K_{\rm n}(\xi) + \lambda(x)$.

Such a result is very encouraging, since it provides a case where the relevant information on the initial state is not anymore connected with the point spectrum of $H_{\rm rel}$, but rather with the localization in energy of the electrons and the localization in phase space of the nuclei. This certainly fits much better with the semiclassical intuition of this problem, in concomitance with the fact that the classical flow of $H_{\rm eff}(x,\xi)$ is involved.

Nevertheless, from a conceptual point of view, something is missing in the previous result. Namely, one would like to have an even closer relation between the complete quantum evolution $e^{-itH/h}$ and some *reduced quantum evolution* of the type $e^{-it\tilde{H}_{\rm eff}(x,hD_x)/h}$, for some $\tilde{H}_{\rm eff}$ close to $H_{\rm eff}$. In that way, one would be able to use all the well developed semiclassical (microlocal) machinery on the operator $\tilde{H}_{\rm eff}(x,hD_x)$, in order to deduce many results on its quantum evolution group $e^{-it\tilde{H}_{\rm eff}(x,hD_x)/h}$ (e.g., a representation of it as a Fourier integral operator). In the previous result, the presence of a coherent state in the expression of φ_0 has allowed the author to, somehow, by-pass this step, and to relate directly the complete quantum evolution to its semiclassical approximation (that is, to objects involving the underlying classical evolution). However, a preliminary link between $e^{-itH/h}$ and some $e^{-it\tilde{H}_{\rm eff}(x,hD_x)/h}$ would have the advantage of allowing more general initial states, and, by the use of more sophisticated results of semiclassical analysis, should permit to have a better understanding of the phenomena related to this approximation. Moreover, as we will see, this preliminary link is usually valid for very large time intervals of the form $[-h^{-N}, h^{-N}]$ with $N \geq 1$ arbitrary, while it is well known that the second step (that is, the semiclassical approximation of $e^{-it\tilde{H}_{\rm eff}(x,hD_x)/h}$) has, in the best cases, the Ehrenfest-time limitation $|t| = \mathcal{O}(\ln \frac{1}{h})$ (see (2.5) and Theorem 11.3 below).

The first results concerning a reduced quantum evolution have been obtained recently (and independently) by H. Spohn and S. Teufel in [SpTe], and by the present authors in [MaSo]. In both cases, it is assumed that, at time $t = 0$, the energy of the electrons is localized in some isolated part of the electronic Hamiltonian $H_{\rm el}(x)$. In [SpTe], the authors find an approximation of $e^{-itH/h}$ in terms of $e^{-itH_{\rm eff}(x,hD_x)/h}$, and prove an error estimate in $\mathcal{O}(h)$ (actually, it seems that such a result was already present in a much older, but unpublished, work by A. Raphaelian [Ra]). In [MaSo] (following a procedure of [NeSo, So], and later reproduced with further applications in [PST, Te]), a whole perturbation $\tilde{H}_{\rm eff} \sim H_{\rm eff} + \sum_{k\geq 1} h^k H_k$ of $H_{\rm eff}$ is constructed, allowing an error estimate in $\mathcal{O}(h^\infty)$ for the quantum evolution.

However, these two papers have the defect of assuming all the interactions smooth, and thus of excluding the physically interesting case of Coulomb interactions. Here, our goal is precisely to allow this case. More precisely, we plan to mix the arguments of [MaSo] and those of [KMSW] in order to include Coulomb-type (or, more generally, Laplace-compact) singularities of the potentials.

In [KMSW], the key-point consists in a refinement of the Hunziker distorsion method, that leads to a family of x-dependent unitary operators (where, for each operator, the nuclei-position variable x has to stay in some small open set) such that, once conjugated by these operators, the electronic Hamiltonian becomes smooth with respect to x. Then, by using local pseudodifferential calculus with operator-valued symbols, and various tricky patching techniques, a constructive Feshbach method (through a Grushin problem) is performed and leads to the required result.

When reading [KMSW], however, one has the impression that all the technical difficulties and tricky arguments actually hide a somewhat simpler concept, that should be related to some global pseudodifferential calculus adapted to the singularities of the interactions. In other words, it seems that interactions such as Coulomb electron-nucleus ones are indeed smooth with respect to x for some 'exotic' differential structure on the x-space, and that such a differential structure could be used to construct a complete pseudodifferential calculus (with operator-valued symbols). Such considerations (that are absent in [KMSW]) have naturally led us to the notion of *twisted pseudodifferential operator* that we describe in Sections 4 and 5. This new tool permits in particular to handle a certain type of partial differential operators with singular operator-valued coefficients, mainly as if their coefficients were smooth. To our opinion, the advantages are at least two. First of all, it simplifies considerably (making them clearer and closer to the smooth case) the arguments leading to the reduction of the quantum evolution of a molecule. Secondly, thanks to its abstract setting, we believe that it can be applied in other situations where singularities appear.

Roughly speaking, we say that an operator P on $L^2(I\!R^n_x;\mathcal{H})$ ($\mathcal{H}$ = abstract Hilbert space) is a twisted h-admissible pseudodifferential operator, if each operator $U_jPU_j^{-1}$ (where, for any j, $U_j = U_j(x)$ is a given unitary operator defined for x in some open set $\Omega_j \subset I\!R^n$) is h-admissible (e.g., in the sense of [Ba, GMS]). Then, under few general conditions on the finite family $(U_j, \Omega_j)_j$, we show that these operators enjoy all the nice properties of composition, inversion, functional calculus and symbolic calculus, similar to those present in the smooth case. Thanks to this, the general strategy of [MaSo] can essentially be reproduced, and leads to the required reduction of the quantum evolution. More precisely, we prove that, if the initial state φ_0 is conveniently localized in space, in energy, and on a L-levels isolated part of the electronic spectrum ($L \geq 1$), then, during a certain interval of time (that can be estimated), its quantum evolution can be described by that of a selfadjoint $L \times L$ matrix $A = A(x, hD_x)$ of smooth semiclassical pseudodifferential operators in the nuclei-variables, in the sense that one has,

$$e^{-itH/h}\varphi_0 = \mathcal{W}^* e^{-itA/h}\mathcal{W}\varphi_0 + \mathcal{O}(\langle t \rangle h^\infty),$$

where $\mathcal{W}$ is a bounded operator onto $L^2(\mathbb{R}^n)^{\oplus L}$, such that $\mathcal{W}\mathcal{W}^* = 1$ and $\mathcal{W}^*\mathcal{W}$ is an orthogonal projection (that projects onto a so-called almost-invariant subspace). We refer to Theorem 2.1 for a precise statement, and to Theorem 7.1 for an even better result in the case where the spectral gap of the electronic Hamiltonian is global. In the particular case $L = 1$, this also permits to give a geometrical description (involving the underlying classical Hamilton flow of A) of the time interval in which such a reduction is possible. Then, to make the paper more complete, we consider the case of coherent initial states (in the same spirit as in [Ha5, Ha6]) and, applying a semiclassical result of M. Combescure and D. Robert [CoRo], we justify the expansions given in [Ha6] up to times of order $\ln \frac{1}{h}$ (at least when the geometry makes it possible).

Outline of the paper:

In Section 2, we introduce our notations and assumptions, and we state our main results concerning the reduction of the quantum evolution in the case where the electronic Hamiltonian admits a local gap in its spectrum. In Section 3, we modify the electronic operator away from the relevant region in x, in order to deal with a globally nicer operator, admitting a global gap in its spectrum. Sections 4 and 5 are devoted to the settlement of an abstract singular pseudodifferential calculus (bounded in Section 4, and partial differential in Section 5). In Section 6, following [MaSo], we construct a quasi-invariant subspace that permits, in Section 7, to have a global reduction of the evolution associated with the modified operator constructed in Section 3. In Sections 8 and 9, we complete the proofs of our main results, and, in Section 10, we give a simple way of computing the effective Hamiltonian. Then, in Section 11, we apply these results to study the evolution of wave packets. Section 12 treats, more specifically, the case of polyatomic molecules, by showing how it can be inserted in our general framework. The remaining three sections are just appendices: Section 13 reviews standard results on pseudodifferential calculus; Section 14 gives an estimate on the propagation-speed of the support (up to $\mathcal{O}(h^\infty)$) for the solutions of (1.1); Section 15 contains two technical results used in the main text.

2 Assumptions and Main Results

The purpose of this paper is to investigate the asymptotic behavior as $h \to 0_+$ of the solutions of the time-dependent Schrödinger equation,

$$ih\frac{\partial \varphi}{\partial t} = P(h)\varphi \tag{2.1}$$

with

$$P(h) = \boldsymbol{\omega} + Q(x) + W(x), \tag{2.2}$$

where $Q(x)$ ($x \in I\!\!R^n$) is a family of selfadjoint operators on some fix Hilbert space $\mathcal{H}$ with same dense domain $\mathcal{D}_Q$, $\boldsymbol{\omega} = \sum_{|\alpha|\leq m} c_\alpha(x;h)(hD_x)^\alpha$ is a symmetric semiclassical differential operator of order 0 and degree m, with scalar coefficients depending smoothly on x, and $W(x)$ is a non negative function defined almost everywhere on $I\!\!R^n$.

Typically, in the case of a molecular system, x stands for the position of the nuclei, $Q(x)$ represents the electronic Hamiltonian that includes the electron-electron and nuclei-electron interactions (all of them of Coulomb-type), $\boldsymbol{\omega}$ is the quantized cinetic energy of the nuclei, and $W(x)$ represents the nuclei-nuclei interactions. Moreover, the parameter h is supposed to be small and, in the case of a molecular system, h^{-2} actually represents the quotient of electronic and nuclear masses. In more general systems, one can also include a magnetic potential and an exterior electric potential both in $\boldsymbol{\omega}$ and $Q(x)$. We refer to Section 12 for more details about this case.

We make the following assumptions:

$(H1)$ For all $\alpha, \beta \in Z\!\!\!Z_+^n$ with $|\alpha| \leq m$, $\partial^\beta c_\alpha(x,h) = \mathcal{O}(1)$ uniformly for $x \in I\!\!R^n$ and $h > 0$ small enough. Moreover, setting $\omega(x,\xi;h) := \sum_{|\alpha|\leq m} c_\alpha(x;h)\xi^\alpha$, we assume that there exists a constant $C_0 \geq 1$ such that, for all $(x,\xi) \in I\!\!R^{2n}$ and $h > 0$ small enough,

$$\mathrm{Re}\, \omega(x,\xi;h) \geq \frac{1}{C_0}\langle \xi \rangle^m - C_0.$$

In particular, Assumption $(H1)$ implies that m is even and $\boldsymbol{\omega}$ is well defined as a selfadjoint operator on $L^2(I\!\!R^n)$ (and, by extension, on $L^2(I\!\!R^n;\mathcal{H})$) with domain $H^m(I\!\!R^n)$. Moreover, by the Sharp Gårding Inequality (see, e.g., [Ma2]), it is uniformly semi-bounded from below.

$(H2)$ $W \geq 0$ is $\langle D_x \rangle^m$-compact on $L^2(I\!\!R^n)$, and there exists $\gamma \in I\!\!R$ such that, for all $x \in I\!\!R^n$, $Q(x) \geq \gamma$ on $\mathcal{H}$.

Assumptions $(H1)$ – $(H2)$ guarantee that, for h sufficiently small, $P(h)$ can be realized as a selfadjoint operator on $L^2(I\!\!R^n;\mathcal{H})$ with domain $\mathcal{D}(P) \subset H^m(I\!\!R^n;\mathcal{H}) \cap L^2(I\!\!R^n;\mathcal{D}_Q)$, and verifies $P(h) \geq \gamma_0$, with $\gamma_0 \in I\!\!R$ independent of h.

(Of course, in the case of a molecular system, $P(h)$ is essentially selfadjoint, and the domain of its selfadjoint extension is $H^2(I\!R^n \times Y)$, where Y stands for the space of electron positions.)

For $L \geq 1$ and $L' \geq 0$, we denote by $\lambda_1(x), \dots, \lambda_{L+L'}(x)$ the first $L + L'$ values given by the Min-Max principle for $Q(x)$ on $\mathcal{H}$, and we make the following local gap assumption on the spectrum $\sigma(Q(x))$ of $Q(x)$:

$(H3)$ There exists a contractible bounded open set $\Omega \subset I\!R^n$ and $L \geq 1$ such that, for all $x \in \Omega$, $\lambda_1(x), \dots, \lambda_{L+L'}(x)$ are discrete eigenvalues of $Q(x)$, and one has,

$$\inf_{x\in\Omega} \text{dist } (\sigma(Q(x))\backslash\{\lambda_{L'+1}(x), \dots, \lambda_{L'+L}(x)\}, \{\lambda_{L'+1}(x), \dots, \lambda_{L'+L}(x)\}) > 0.$$

Furthermore, the spectral projections $\Pi_0^-(x)$ associated with $\{\lambda_1(x), \dots, \lambda_{L'}(x)\}$ and $\Pi_0(x)$ associated with $\{\lambda_{L'+1}(x), \dots, \lambda_{L'+L}(x)\}$, both depend continuously on $x \in \Omega$.

Then, we assume that P can be "regularized" with respect to x in Ω, in the following sense:

$(H4)$ There exists a finite family of bounded open sets $(\Omega_j)_{j=1}^r$ in $I\!R^n$, a corresponding family of unitary operators $U_j(x)$ ($j = 1, \cdots, r$, $x \in \Omega_j$), and some fix selfadjoint operator $Q_0 \geq C_0$ on $\mathcal{H}$ with domain $\mathcal{D}_Q$, such that (denoting by U_j the unitary operator on $L^2(\Omega_j; \mathcal{H}) \simeq L^2(\Omega_j) \otimes \mathcal{H}$ induced by the action of $U_j(x)$ on $\mathcal{H}$),

- $\Omega = \cup_{j=1}^r \Omega_j$;
- For all $j = 1, \cdots, r$ and $x \in \Omega_j$, $U_j(x)$ leaves $\mathcal{D}_Q$ invariant;
- For all j, the operator $U_j \boldsymbol{\omega} U_j^{-1}$ is a semiclassical differential operator with operator-valued symbol, of the form,

$$U_j \boldsymbol{\omega} U_j^{-1} = \boldsymbol{\omega} + h \sum_{|\beta| \leq m-1} \omega_{\beta,j}(x; h)(hD_x)^\beta, \tag{2.3}$$

  where $\omega_{\beta,j} Q_0^{\frac{|\beta|}{m}-1} \in C^\infty(\Omega_j; \mathcal{L}(\mathcal{H}))$ for any $\gamma \in I\!N^n$ (here, $\mathcal{L}(\mathcal{H})$ stands for the Banach space of bounded operators on $\mathcal{H}$), and the quantity $\|\partial_x^\gamma \omega_{\beta,j}(x; h) Q_0^{\frac{|\beta|}{m}-1}\|_{\mathcal{L}(\mathcal{H})}$ is bounded uniformly with respect to h small enough and locally uniformly with respect to $x \in \Omega_j$;
- For all j, $U_j(x)Q(x)U_j(x)^{-1}$ and $U_j(x)Q_0U_j(x)^{-1}$ are in $C^\infty(\Omega_j; \mathcal{L}(\mathcal{D}_Q, \mathcal{H}))$ (where $\mathcal{L}(\mathcal{D}_Q, \mathcal{H})$ stands for the Banach space of bounded operators from $\mathcal{D}_Q$ to $\mathcal{H}$);
- $W \in C^\infty(\cup_{j=1}^r \Omega_j)$;

- There exists a dense subspace $\mathcal{H}_\infty \subset \mathcal{D}_Q \subset \mathcal{H}$, such that, for any $v \in \mathcal{H}_\infty$ and any $j = 1, \cdots, r$, the application $x \mapsto U_j(x)v$ is in $C^\infty(\Omega_j, \mathcal{D}_Q)$.

Note that, for physical molecular systems, a construction of such operators $U_j(x)$'s is made in [KMSW], and can be performed around any point of $I\!R^n$ where W is smooth. Moreover, in that case one can take $Q_0 = -\Delta_y + 1$ (where y stands for the position of the electrons), and the last point in (H4) can be realized by taking $\mathcal{H}_\infty = C_0^\infty(Y)$. Again, we refer the interested reader to Section 12. Let us also observe that, in the case $L' + L = 1$, one does not need to assume that Ω is contractible.

For any $\varphi_0 \in L^2(I\!R^n; \mathcal{H})$ (possibly h-dependent) such that $\|\varphi_0\|_{L^2(K_0^c;\mathcal{H})} = \mathcal{O}(h^\infty)$ for some compact set $K_0 \subset\subset I\!R^n$, and for any $\Omega' \subset\subset I\!R^n$ open neighborhood of K_0, we set,

$$T_{\Omega'}(\varphi_0) := \sup\{T > 0\,;\, \exists K_T \subset\subset \Omega',\ \sup_{t\in[0,T]} \|e^{-itP/h}\varphi_0\|_{L^2(K_T^c;\mathcal{H})} = \mathcal{O}(h^\infty)\}.$$

Then, $T_{\Omega'}(\varphi_0) \leq +\infty$, and, if one also assume that $\|(1 - f(P))\varphi_0\| = \mathcal{O}(h^\infty)$ for some $f \in C_0^\infty(I\!R)$, Theorem 14.1 in Appendix B shows that,

$$T_{\Omega'}(\varphi_0) \geq \frac{2 \text{ dist } (K_0, \partial\Omega')}{\|\nabla_\xi \omega(x, hD_x)g(P)\|},$$

for any $g \in C_0^\infty(I\!R)$ verifying $gf = f$.

As a main result, we obtain (denoting by $L^2(I\!R^n)^{\oplus L}$ the space $(L^2(I\!R^n))^L$ endowed with its natural Hilbert structure),

Theorem 2.1 *Assume (H1)-(H4) and let $\Omega' \subset\subset \Omega$ with Ω' open subset of $I\!R^n$. Then, for any $g \in C_0^\infty(I\!R)$, there exists an orthogonal projection Π_g on $L^2(I\!R^n;\mathcal{H})$, an operator $\mathcal{W} : L^2(I\!R^n;\mathcal{H}) \to L^2(I\!R^n)^{\oplus L}$, uniformly bounded with respect to h, and a selfadjoint $L \times L$ matrix A of h-admissible operators $H^m(I\!R^n) \to L^2(I\!R^n)$, with the following properties:*

- *For all $\chi \in C_0^\infty(\Omega')$,*
$$\Pi_g\chi = \Pi_0\chi + \mathcal{O}(h);$$
- *$\mathcal{W}\mathcal{W}^* = 1$ and $\mathcal{W}^*\mathcal{W} = \Pi_g$;*
- *For $x \in \Omega'$, the symbol $a(x, \xi; h)$ of A verifies,*
$$a(x, \xi; h) = \omega(x, \xi; h)\mathbf{I}_L + \mathcal{M}(x) + W(x)\mathbf{I}_L + hr(x, \xi; h)$$
where $\mathbf{I}_L$ stands for the L-dimensional identity matrix, $\mathcal{M}(x)$ is a $L\times L$ matrix depending smoothly on $x \in \Omega'$ and admitting $\lambda_{L'+1}(x), \dots, \lambda_{L'+L}(x)$ as eigenvalues, and where $\partial^\alpha r(x, \xi; h) = \mathcal{O}(\langle\xi\rangle^{m-1})$ for any multi-index α and uniformly with respect to $(x, \xi) \in \Omega' \times I\!R^n$ and $h > 0$ small enough;

- *For any $f \in C_0^\infty(I\!R)$ with $\operatorname{Supp} f \subset \{g=1\}$, and for any $\varphi_0 \in L^2(I\!R^n;\mathcal{H})$ such that $\|\varphi_0\| = 1$, and,*

$$\|\varphi_0\|_{L^2(K_0^c;\mathcal{H})} + \|(1-\Pi_g)\varphi_0\| + \|(1-f(P))\varphi_0\| = \mathcal{O}(h^\infty), \tag{2.4}$$

for some $K_0 \subset\subset \Omega'$, one has,

$$e^{-itP/h}\varphi_0 = \mathcal{W}^* e^{-itA/h}\mathcal{W}\varphi_0 + \mathcal{O}\left(\langle t\rangle h^\infty\right) \tag{2.5}$$

uniformly with respect to $h > 0$ small enough and $t \in [0, T_{\Omega'}(\varphi_0))$.

Remark 2.2 *Actually, much more informations are obtained on the operators Π_g, $\mathcal{W}$ and A, and we refer to Theorems 7.1 and 8.1 for more details, and to Section 10 for an explicit computation of A, up to $\mathcal{O}(h^4)$.*

Remark 2.3 *Condition (2.4) on the initial data may seems rather strong, but in fact, it will become clear from the proof that the operators Π_g, $f(\tilde{P})$ and χ (where $\chi \in C_0^\infty(I\!R^n)$ is supported in K_0) essentially commutes two by two (up to $\mathcal{O}(h)$). Indeed, in the case of a molecular system, they respectively correspond to a localization in energy for the electrons, a localization in energy for the whole molecule, and a localization in space for the nuclei.*

Remark 2.4 *Here, we have assumed that both $\Pi_0^-(x)$ and $\Pi_0(x)$ have finite rank, since this corresponds to the main applications that we have in mind. However, it will become clear from the proof that the case where one or both of them have infinite rank could be treated in a similar way, with the difference that, if $\operatorname{Rank}\Pi_0(x) = \infty$, then $\mathcal{W}^* e^{-itA/h}\mathcal{W}$ must be replaced by $e^{-it\Pi_g P\Pi_g/h}$ (there will not be any operator A anymore). Moreover, some assumption must be added in order to be able to construct a modified operator as in Section 3 (for instance, that both $\Pi_0^-(x)$ and $\Pi_0(x)$ admit extensions to all $x \in I\!R^n$ that depend smoothly on x away from a neighborhood of K).*

Remark 2.5 *In the next section, we modify the operator $Q(x)$ away from the interesting region, in such a way that the new operator $\tilde{Q}(x)$ admits a* global *gap in its spectrum. With such an operator, a much better result can be obtained, and permits to decouple completely the evolution in a somewhat more complete and abstract way: see Theorem 7.1 (in particular (7.2)). In particular, even if $\|(1-\Pi_g)\varphi_0\|$ is not small, Theorem 7.1 permits to have a description of the quantum evolution of φ_0 in terms of two independent reduced evolutions.*

As a corollary, in the case $L = 1$ we also obtain the following geometric lower bound on $T_{\Omega'}(\varphi_0)$, that relates it with the underlying classical Hamilton flow of the operator A:

Corollary 2.6 *Assume moreover that $L = 1$ and the coefficients $c_\alpha = c_\alpha(x;h)$ of $\boldsymbol{\omega}$ verify,*

$$c_\alpha(x;h) = c_{\alpha,0}(x) + \varepsilon(h)\tilde{c}_\alpha(x;h), \tag{2.6}$$

with $c_{\alpha,0}$ real-valued and independent of h, $\varepsilon(h) \to 0$ as $h \to 0$, and, for any β, $|\partial^\beta c_{\alpha,0}(x)| + |\partial^\beta \tilde{c}_\alpha(x,h)| = \mathcal{O}(1)$ uniformly, and set,

$$a_0(x,\xi) := \sum_{|\alpha|\le m} c_{\alpha,0}(x)\xi^\alpha + \lambda_{L'+1}(x) + W(x) \qquad (x \in \Omega').$$

Also, denote by $H_{a_0} := \partial_\xi a_0 \partial_x - \partial_x a_0 \partial_\xi$ the Hamilton field of a_0. Then, for any $f \in C_0^\infty(\mathbb{R})$ with $\operatorname{Supp} f \subset \{g = 1\}$, and for any $\varphi_0 \in L^2(\mathbb{R}^n;\mathcal{H})$ such that $\|\varphi_0\| = 1$, and,

$$\|\varphi_0\|_{L^2(K_0^c;\mathcal{H})} + \|(1-\Pi_g)\varphi_0\| + \|(1-f(P))\varphi_0\| = \mathcal{O}(h^\infty),$$

one has,

$$T_{\Omega'}(\varphi_0) \ge \sup\{T > 0\,;\, \pi_x(\cup_{t\in[0,T]} \exp tH_{a_0}(K(f))) \subset \Omega'\}, \tag{2.7}$$

where π_x stands for the projection $(x,\xi) \mapsto x$, and $K(f)$ is the compact subset of $\mathbb{R}^{2n}$ defined by,

$$K(f) := \{(x,\xi)\,;\, x \in K_0,\, \omega(x,\xi) + \gamma \le C_f\}$$

with $\gamma = \inf_{x\in\Omega'} \inf \sigma(Q(x))$ and $C_f := \operatorname{Max}|\operatorname{Supp} f|$.

Remark 2.7 *Thanks to (H1) and (H2), it is easy to see that $\exp tH_{a_0}(x,\xi)$ is well defined for all $(t,x,\xi) \in \mathbb{R} \times \mathbb{R}^{2n}$.*

Remark 2.8 *Actually, as it will be seen in the proof, in (2.7) one can replace the set $K(f)$ by $\cup_{j=1}^r FS(U_j\Pi_g\varphi_0)$, where FS stands for the Frequency Set of locally L^2 functions introduced in [GuSt] (we refer to Section 9 for more details).*

Remark 2.9 *Our proof would permit to state a similar result in the case $L > 1$, but under the additional assumption that the set $\{\lambda_{L'+1}(x), \dots, \lambda_{L'+L}(x)\}$ can be written as $\{E_1(x), \dots, E_{L''}(x)\}$, where the (possibly degenerate) eigenvalues $E_j(x)$ are such that $E_j(x) \ne E_{j'}(x)$ for $j \ne j'$ and $x \in \Omega$. In the general case where crossings may occur, such a type of result relies on the microlocal propagation of the Frequency Set for solutions of semiclassical matrix evolution problems (for which not much is known, in general).*

Remark 2.10 *The proof also provides a very explicit and somehow optimal bound on $T_{\Omega'}(\varphi_0)$ in the case where φ_0 is a coherent state with respect to the x-variables: see Theorem 11.3 and (11.8).*

3 A Modified Operator

In this section, we consider an arbitrary compact subset $K \subset\subset \Omega$ and an open neighborhood $\Omega_K \subset\subset \Omega$ of K. We also denote by Ω_0 an open subset of $\mathbb{R}^n$, with closure disjoint from $\overline{\Omega_K}$, and such that $(\Omega_j)_{j=0}^r$ covers all of $\mathbb{R}^n$, and we set $U_0 := \mathbf{1}$. The purpose of this section is to modify $Q(x)$ for x outside a neighborhood of K_0, in order to make it regular with respect to x there, and to deal with a global gap instead of a local one.

Due to the contractibility of Ω, we know that there exist $L'+L$ continuous functions $u_1, \dots, u_{L'+L}$ in $C(\Omega;\mathcal{H})$, such that the families $(u_1(x), \dots, u_{L'}(x))$ and $(u_{L'+1}(x), \dots, u_{L'+L}(x))$ span $\mathrm{Ran}\,\Pi_0^-(x)$ and $\mathrm{Ran}\,\Pi_0(x)$ respectively, for all $x \in \Omega$ (see, e.g., [KMSW]).

Then, following Lemma 1.1 in [KMSW], we first prove,

Lemma 3.1 *For all $x \in I\!R^n$, there exist $\tilde{u}_1(x), \dots, \tilde{u}_{L'+L}(x)$ in $\mathcal{D}_Q$, such that the family $(\tilde{u}_1(x), \dots, \tilde{u}_{L'+L}(x))$ is orthonormal in $\mathcal{H}$ for all $x \in I\!R^n$, the families $(\tilde{u}_1(x), \dots, \tilde{u}_{L'}(x))$ and $(\tilde{u}_{L'+1}(x), \dots, \tilde{u}_{L'+L}(x))$ span $\mathrm{Ran}\,\Pi_0^-(x)$ and $\mathrm{Ran}\,\Pi_0(x)$, respectively, when $x \in \Omega_K$, and, for all $j = 0, 1, \cdots, r$ and $k = 1, \dots, L'+L$,*

$$U_j(x)\tilde{u}_k(x) \in C^\infty(\Omega_j; \mathcal{D}_Q).$$

Proof Let $\zeta_1, \zeta_2 \in C^\infty(I\!R^n; [0,1])$, such that $\mathrm{Supp}\,\zeta_1 \subset \Omega_0^c$, $\zeta_1 = 1$ on Ω_K and $\zeta_1^2 + \zeta_2^2 = 1$ everywhere. Since $u_1(x), \dots, u_{L'+L}(x)$ depend continuously on x in Ω, for any $\varepsilon > 0$ one can find a finite number of points $x_1, \cdots, x_N \in \mathrm{Supp}\,\zeta_1$ and a partition of unity $\chi_1, \cdots, \chi_N \in C_0^\infty(\Omega)$ on $\mathrm{Supp}\,\zeta_1$, such that, for all $k = 1, \dots, L'+L$,

$$\sup_{x \in \mathrm{Supp}\,\zeta_1} \|u_k(x) - \sum_{\ell=1}^N \chi_\ell(x) u_k(x_\ell)\|_{\mathcal{H}} \leq \varepsilon.$$

On the other hand, using the last assertion of (H4), for any (k,ℓ) one can find $v_{k,\ell}$ in $\mathcal{D}_Q$, such that, $\|v_{k,\ell} - u_k(x_\ell)\|_{\mathcal{H}} \leq \varepsilon$ and $U_j(x)v_{k,\ell} \in C^\infty(\Omega_j, \mathcal{D}_Q)$ for all $j = 1, \dots, r$. Moreover, it follows from $(H3)$ and $(H4)$ that, for all $j = 1, \cdots, r$,

$$U_j(x)\Pi_0^-(x)U_j^*(x) \text{ and } U_j(x)\Pi_0(x)U_j^*(x) \in C^\infty(\Omega_j, \mathcal{L}(\mathcal{H}, \mathcal{D}_Q)).$$

Therefore, if we set,

$$v_k(x) := \Pi_0^-(x) \sum_{\ell=1}^N \chi_\ell(x) v_{k,\ell} \quad (k = 1, \dots, L');$$
$$v_k(x) := \Pi_0(x) \sum_{\ell=1}^N \chi_\ell(x) v_{k,\ell} \quad (k = L'+1, \dots, L'+L),$$

and since $\sum_{\ell=1}^N \chi_\ell(x) = 1$ on $\mathrm{Supp}\,\zeta_1$, we obtain (also using that $\Pi_0^-(x)u_k(x) = u_k(x)$ for $k \leq L'$, and $\Pi_0(x)u_k(x) = u_k(x)$ for $k \geq L'+1$),

$$\sup_{x \in \mathrm{Supp}\,\zeta_1} \|u_k(x) - v_k(x)\|_{\mathcal{H}} \leq 2\varepsilon$$
$$U_j(x)v_k(x) \in C^\infty(\Omega_j, \mathcal{D}_Q) \quad (j = 1, \dots, r).$$

In particular, by taking ε small enough, we see that the families $(v_1(x), \dots, v_{L'}(x))$ and $(v_{L'+1}(x), \dots, v_{L'+L}(x))$ span $\mathrm{Ran}\,\Pi_0^-(x)$ and $\mathrm{Ran}\,\Pi_0(x)$, respectively, for

$x \in \mathrm{Supp}\,\zeta_1$. Moreover, by Gram-Schmidt, this families can also be assumed to be orthonormal.

Then, using again the last point of (H4), one can find an orthonormal family $w_1, \ldots, w_{L'+L} \in \mathcal{D}_Q$, such that $|\langle w_m, u_k(x_\ell)\rangle| \leq \varepsilon$ for all $1 \leq k, m \leq L' + L$, $1 \leq \ell \leq N$, and $U_j(x)w_m \in C^\infty(\Omega_j, \mathcal{D}_Q)$ $(j = 1, \ldots, r)$. Thus, setting,

$$\tilde{w}_k(x) := \zeta_1(x)v_k(x) + \zeta_2(x)w_k,$$

we see that, for all $k, k' \in \{1, \ldots, L' + L\}$,

$$\langle \tilde{w}_k(x), \tilde{w}_{k'}(x)\rangle_{\mathcal{H}} = \delta_{k,k'} + \mathcal{O}(\varepsilon).$$

As a consequence, taking $\varepsilon > 0$ sufficiently small and orthonormalizing the family $(\tilde{w}_1(x), \ldots, \tilde{w}_{L'+L}(x))$, we obtain a new family $(\tilde{u}_1(x), \ldots, \tilde{u}_{L'+L}(x))$ that verifies all the properties required in the lemma. •

Then, (with the usual convention $\sum_{k=1}^{L'} = 0$ if $L' = 0$) we set,

$$\tilde{\Pi}_0^-(x) = \sum_{k=1}^{L'} \langle \cdot, \tilde{u}_k(x)\rangle_{\mathcal{H}} \tilde{u}_k(x),$$

$$\tilde{\Pi}_0(x) = \sum_{k=L'+1}^{L'+L} \langle \cdot, \tilde{u}_k(x)\rangle_{\mathcal{H}} \tilde{u}_k(x)$$

so that $\tilde{\Pi}_0^-(x)$ and $\tilde{\Pi}_0(x)$ are orthogonal projections of rank L' and L respectively, are orthogonal each other, coincide with $\Pi_0^-(x)$ and $\Pi_0(x)$ for x in Ω_K, and verify,

$$U_j(x)\tilde{\Pi}_0^-(x)U_j(x)^* \text{ and } U_j(x)\tilde{\Pi}_0(x)U_j(x)^* \in C^\infty(\Omega_j, \mathcal{L}(\mathcal{H})), \qquad (3.1)$$

for all $j = 0, 1, \cdots, r$.

Now, with the help of $\tilde{\Pi}_0^-(x), \tilde{\Pi}_0(x)$, we modify $Q(x)$ outside a neighborhood of K as follows.

Proposition 3.2 *Let $\Omega'_K \subset\subset \Omega_K$ be an open neighborhood of K. Then, for all $x \in I\!R^n$, there exists a selfadjoint operator $\tilde{Q}(x)$ on $\mathcal{H}$, with domain $\mathcal{D}_Q$, and uniformly semi-bounded from below, such that,*

$$\tilde{Q}(x) = Q(x) \quad \text{if } x \in \Omega'_K; \qquad (3.2)$$

$$[\tilde{Q}(x), \tilde{\Pi}_0^-(x)] = [\tilde{Q}(x), \tilde{\Pi}_0(x)] = 0 \quad \text{for all } x \in I\!R^n, \qquad (3.3)$$

and the application $x \mapsto U_j(x)\tilde{Q}(x)U_j(x)^{-1}$ is in $C^\infty(\Omega_j; \mathcal{L}(\mathcal{D}_Q, \mathcal{H}))$ for all $j = 0, 1, \cdots, r$. Moreover, the bottom of the spectrum of $\tilde{Q}(x)$ consists in $L' + L$ eigenvalues $\tilde{\lambda}_1(x), \ldots, \tilde{\lambda}_{L'+L}(x)$, and $\tilde{Q}(x)$ admits a global gap in its spectrum, in the sense that,

$$\inf_{x \in I\!R^n} \text{dist}\,(\sigma(\tilde{Q}(x))\backslash\{\tilde{\lambda}_{L'+1}(x), \ldots, \tilde{\lambda}_{L'+L}(x)\}, \{\tilde{\lambda}_{L'+1}(x), \ldots, \tilde{\lambda}_{L'+L}(x)\}) > 0.$$

Proof We set $\tilde{\Pi}_0^+(x) = 1 - \tilde{\Pi}_0^-(x) - \tilde{\Pi}_0(x)$ and we choose a function $\zeta \in C_0^\infty(\Omega_K;[0,1])$ such that $\zeta = 1$ on Ω'_K. Then, with Q_0 as in (H4), we set,

$$\tilde{Q}(x) = \zeta(x)Q(x) + (1-\zeta(x))\tilde{\Pi}_0^+(x)Q_0\tilde{\Pi}_0^+(x) - (1-\zeta(x))\tilde{\Pi}_0^-(x).$$

Since $\tilde{\Pi}_0^-(x) = \Pi_0^-(x)$ and $\tilde{\Pi}_0(x) = \Pi_0(x)$ on $\mathrm{Supp}\,\zeta$, we see that $\tilde{\Pi}_0^-(x)$ and $\tilde{\Pi}_0(x)$ commute with $\tilde{Q}(x)$, and it is also clear that $\tilde{Q}(x)$ is selfadjoint with domain $\mathcal{D}_Q$. Moreover,

$$\begin{aligned}&\tilde{\Pi}_0^-(x)\tilde{Q}(x)\tilde{\Pi}_0^-(x) = \zeta(x)\Pi_0^-(x)Q(x)\Pi_0^-(x) - (1-\zeta(x))\Pi_0^-(x);\\&\tilde{\Pi}_0(x)\tilde{Q}(x)\tilde{\Pi}_0(x) = \zeta(x)\Pi_0(x)Q(x)\Pi_0(x),\end{aligned}$$

and, setting,

$$\lambda_{L+L'+1}(x) := \inf\left(\sigma(Q(x))\backslash\{\lambda_1(x),\dots,\lambda_{L+L'}(x)\}\right),$$

one has,

$$\tilde{\Pi}_0^+(x)\tilde{Q}(x)\tilde{\Pi}_0^+(x) \geq \left(\zeta(x)\lambda_{L+L'+1}(x) + (1-\zeta(x)\right)\tilde{\Pi}_0^+(x).$$

In particular, the bottom of the spectrum of $\tilde{Q}(x)$ consists in the $L+L'$ eigenvalues $\tilde{\lambda}_k(x) = \zeta(x)\lambda_k(x) - (1-\zeta(x))$ $(k=1,\dots,L')$, $\tilde{\lambda}_k(x) = \zeta(x)\lambda_k(x)$ $(k = L'+1,\dots,L'+L)$, and, due to (H3), one has,

$$\inf_{x\in I\!\!R^n}\left(\tilde{\lambda}_{L'+1}(x) - \tilde{\lambda}_{L'}(x)\right) = \inf_{x\in I\!\!R^n}\left(\zeta(x)(\lambda_{L'+1}(x) - \lambda_{L'}(x) + (1-\zeta(x))\right) > 0,$$

and

$$\begin{aligned}&\inf_{x\in\Omega}\ \mathrm{dist}\,(\sigma(\tilde{Q}(x))\backslash\{\tilde{\lambda}_1(x),\dots,\tilde{\lambda}_{L'+L}(x)\},\{\tilde{\lambda}_1(x),\dots,\tilde{\lambda}_{L'+L}(x)\})\\&\qquad\geq \inf_{x\in\Omega}|\zeta(x)(\lambda_{L'+L+1}(x) - \lambda_{L'+L}(x)) + (1-\zeta(x))| > 0,\end{aligned}$$

while, since $\mathrm{Supp}\,\zeta \subset \Omega$,

$$\inf_{x\in I\!\!R^n\backslash\Omega}\ \mathrm{dist}\,(\sigma(\tilde{Q}(x))\backslash\{\tilde{\lambda}_1(x),\dots,\tilde{\lambda}_{L'+L}(x)\},\{\tilde{\lambda}_1(x),\dots,\tilde{\lambda}_{L'+L}(x)\}) \geq 1.$$

In particular, $\tilde{Q}(x)$ admits a fix global gap in its spectrum as stated in the proposition. Finally, using (H4) and (3.1), we see that $U_j(x)\tilde{Q}(x)U_j^*(x)$ depends smoothly on x in Ω_j for all $j = 0,1,\cdots,r$. •

In the sequel, we also set,

$$\tilde{P} = \boldsymbol{\omega} + \boldsymbol{Q} := \boldsymbol{\omega} + \tilde{Q}(x) + \zeta(x)W(x), \tag{3.4}$$

and we denote by $\tilde{\Pi}_0$ the projection on $L^2(I\!\!R^n;\mathcal{H})$ induced by the action of $\tilde{\Pi}_0(x)$ on $\mathcal{H}$, i.e. the unique projection on $L^2(I\!\!R^n;\mathcal{H})$ that verifies

$$\tilde{\Pi}_0(f\otimes g)(x) = f(x)\tilde{\Pi}_0(x)g \quad \text{(a.e. on } I\!\!R^n \ni x)$$

for all $f \in L^2(I\!\!R^n)$ and $g \in \mathcal{H}$.

4 Twisted h-Admissible Operators

In order to construct (in the same spirit as in [BrNo, HeSj12, MaSo, NeSo, Sj2, So]) an orthogonal projection Π on $L^2(\mathbb{R}^n;\mathcal{H})$ such that $\Pi - \Pi_0 = \mathcal{O}(h)$ and $[\tilde{P},\Pi] = \mathcal{O}(h^\infty)$ (locally uniformly in energy), we need to generalize the notion of h-admissible operator with operator-valued symbol (see, e.g., [Ba, GMS] and the Appendix) by taking into account the possible singularities of $Q(x)$. To avoid complications, in this section we also restrict our attention to the case of bounded operators. The case of unbounded ones will be considered in the next section, at least from the point of view of *differential* operators.

Definition 4.1 *We call "regular covering" of $\mathbb{R}^n$ any finite family $(\Omega_j)_{j=0,\cdots,r}$ of open subsets of $\mathbb{R}^n$ such that $\cup_{j=0}^r \Omega_j = \mathbb{R}^n$ and such that there exists a family of functions $\chi_j \in C_b^\infty(\mathbb{R}^n)$ (the space of smooth functions on $\mathbb{R}^n$ with uniformly bounded derivatives of all order) with $\sum_{j=0}^r \chi_j = 1$, $0 \leq \chi_j \leq 1$, and* $\text{dist}\,(\,\text{Supp}\,(\chi_j), \mathbb{R}^n\backslash\Omega_j) > 0$ *$(j = 0,\cdots,r)$. Moreover, if $U_j(x)$ $(x \in \Omega_j$, $0 \leq j \leq r)$ is a family of unitary operators on $\mathcal{H}$, the family $(U_j,\Omega_j)_{j=0,\cdots,r}$ (where U_j denotes the unitary operator on $L^2(\Omega_j;\mathcal{H}) \simeq L^2(\Omega_j)\otimes\mathcal{H}$ induced by the action of $U_j(x)$ on $\mathcal{H}$) will be called a "regular unitary covering" of $L^2(\mathbb{R}^n;\mathcal{H})$.*

Remark 4.2 *Despite the terminology that we use, no assumption is made on any possible regularity of $U_j(x)$ with respect to x.*

Remark 4.3 *Possibly by shrinking a little bit Ω around the compact set K, one can always assume that the family $(U_j,\Omega_j)_{j=0,1,\cdots,r}$ defined in Section 2 is a regular unitary covering of $L^2(\mathbb{R}^n;\mathcal{H})$.*

In the sequels, we denote by $C_d^\infty(\Omega_j)$ the space of functions $\chi \in C_b^\infty(\mathbb{R}^n)$ such that $\text{dist}\,(\,\text{Supp}\,(\chi), \mathbb{R}^n\backslash\Omega_j) > 0$

Definition 4.4 (Twisted h-Admissible Operator) *Let $\mathcal{U} := (U_j,\Omega_j)_{j=0,\cdots,r}$ be a regular unitary covering (in the previous sense) of $L^2(\mathbb{R}^n;\mathcal{H})$. We say that an operator $A : L^2(\mathbb{R}^n;\mathcal{H}) \to L^2(\mathbb{R}^n;\mathcal{H})$ is a $\mathcal{U}$-twisted h-admissible operator, if there exists a family of functions $\chi_j \in C_d^\infty(\Omega_j)$ such that, for any $N \geq 1$, A can be written in the form,*

$$A = \sum_{j=0}^{r} U_j^{-1}\chi_j A_j^N U_j \chi_j + R_N, \tag{4.1}$$

where $\|R_N\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H}))} = \mathcal{O}(h^N)$, and, for any $j = 0,..,r$, A_j^N is a bounded h-admissible operator on $L^2(\mathbb{R}^n;\mathcal{H})$ with symbol $a_j^N(x,\xi) \in C_b^\infty(T^*\mathbb{R}^n;\mathcal{L}(\mathcal{H}))$, and, for any $\varphi_\ell \in C_d^\infty(\Omega_\ell)$ $(\ell = 0,..,r)$, the operator

$$U_\ell\varphi_\ell U_j^{-1}\chi_j A_j^N \chi_j U_j U_\ell^{-1}\varphi_\ell,$$

is still an h-admissible operator on $L^2(\mathbb{R}^n;\mathcal{H})$.

Remark 4.5 *In particular, by the Calderón-Vaillancourt theorem, the norm of A on $L^2(\mathbb{R}^n;\mathcal{H})$ is bounded uniformly with respect to $h \in (0,1]$.*

An equivalent definition is given by the following proposition:

Proposition 4.6 *An operator $A : L^2(\mathbb{R}^n;\mathcal{H}) \to L^2(\mathbb{R}^n;\mathcal{H})$ is a $\mathcal{U}$-twisted h-admissible operator if and only if the two following properties are verified:*

1. *For any $N \geq 1$ and any functions $\chi_1, \cdots, \chi_N \in C_b^\infty(\mathbb{R}^n)$, one has,*

$$\mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(A) = \mathcal{O}(h^N) \quad : \; L^2(\mathbb{R}^n;\mathcal{H}) \to L^2(\mathbb{R}^n;\mathcal{H})$$

   where we have used the notation $\mathrm{ad}_\chi(A) := [\chi, A] = \chi A - A\chi$.

2. *For any $\varphi_j \in C_d^\infty(\Omega_j)$, the operator $U_j \varphi_j A U_j^{-1} \varphi_j$ is a bounded h-admissible operator on $L^2(\mathbb{R}^n;\mathcal{H})$.*

Proof From Definition 4.4, it is clear that any $\mathcal{U}$-twisted h-admissible operator verifies the properties of the Proposition. Conversely, assume A verifies these properties, and denote by $(\chi_j)_{j=0,\cdots,r} \subset C_b^\infty(\mathbb{R}^n)$ a partition of unity on $\mathbb{R}^n$ such that $\mathrm{dist}\,(\,\mathrm{Supp}\,(\chi_j), \mathbb{R}^n \backslash \Omega_j) > 0$. Then, for all j one can construct $\varphi_j, \psi_j \in C_d^\infty(\Omega_j)$, such that $\varphi_j \chi_j = \chi_j$ and $\psi_j \varphi_j = \varphi_j$, and, for any $N \geq 1$, we can write,

$$\begin{aligned}
A &= \sum_{j=0}^{r} \chi_j A = \sum_{j=0}^{r} \big(\chi_j A \varphi_j + \chi_j \mathrm{ad}_{\varphi_j}(A)\big) \\
&= \sum_{j=0}^{r} \Big(\chi_j A \varphi_j + \chi_j \mathrm{ad}_{\varphi_j}(A)\varphi_j + \chi_j \mathrm{ad}_{\varphi_j}^2(A)\Big) \\
&= \cdots = \sum_{j=0}^{r} \left(\sum_{k=0}^{N-1} \chi_j \mathrm{ad}_{\varphi_j}^k(A)\varphi_j + \chi_j \mathrm{ad}_{\varphi_j}^N(A)\right) \\
&= \sum_{j=0}^{r} \left(\sum_{k=0}^{N-1} \psi_j \chi_j \mathrm{ad}_{\varphi_j}^k(A)\varphi_j \psi_j + \chi_j \mathrm{ad}_{\varphi_j}^N(A)\right).
\end{aligned}$$

In particular, since $\mathrm{ad}_{\varphi_j}^N(A) = \mathcal{O}(h^N)$, and U_j commutes with the multiplication by functions of x, we obtain

$$A = \sum_{j=0}^{r} U_j^{-1} \psi_j A_j^N U_j \psi_j + \mathcal{O}(h^N) \tag{4.2}$$

with

$$A_j^N := \sum_{k=0}^{N-1} U_j \chi_j \mathrm{ad}_{\varphi_j}^k(A) U_j^{-1} \varphi_j = \sum_{k=0}^{N-1} \chi_j \mathrm{ad}_{\varphi_j}^k(U_j \varphi_j A U_j^{-1} \varphi_j). \tag{4.3}$$

Therefore, A_j^N is a bounded h-admissible operator, and for any $\tilde{\psi}_l \in C_d^\infty(\Omega_l)$, it verifies,

$$U_l\tilde{\psi}_l U_j^{-1}\psi_j A_j^N \psi_j U_j \tilde{\psi}_l U_l^{-1} = \sum_{k=0}^{N-1} \chi_j \mathrm{ad}_{\varphi_j}^k (U_l\tilde{\psi}_l A U_l^{-1}\tilde{\psi}_l)\varphi_j,$$

that is still an h-admissible operator. Thus, the proposition follows. •

In the sequel, if A is a $\mathcal{U}$-twisted h-admissible operator, then an expression of A as in (4.1) will be said "adapted" to $\mathcal{U}$.

One also has at disposal a notion of (full) symbol for such operators. In the sequels, we denote by $S(\Omega_j \times I\!R^n; \mathcal{L}(\mathcal{H}))$ the space of (h-dependent) operator-valued symbols $a_j \in C^\infty(\Omega_j \times I\!R^n; \mathcal{L}(\mathcal{H}))$ such that, for any $\alpha \in I\!N^{2n}$, the quantity $\|\partial^\alpha a_j(x,\xi)\|_{\mathcal{L}(\mathcal{H})}$ is bounded uniformly for h small enough and for (x,ξ) in any set of the form $\Omega_j' \times I\!R^n$, with $\Omega_j' \subset \Omega_j$, $\mathrm{dist}\left(\Omega_j', I\!R^n \backslash \Omega_j\right) > 0$. We also set,

$$\Omega := (\Omega_j)_{j=0,\dots,r};$$
$$\mathbf{S}(\Omega; \mathcal{L}(\mathcal{H})) := S(\Omega_0 \times I\!R^n; \mathcal{L}(\mathcal{H})) \times \ldots \times S(\Omega_r \times I\!R^n; \mathcal{L}(\mathcal{H})),$$

and we write $a = \mathcal{O}(h^\infty)$ in $\mathbf{S}(\Omega; \mathcal{L}(\mathcal{H}))$ when $\|\partial^\alpha a_j(x,\xi)\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(h^\infty)$ uniformly in any set $\Omega_j' \times I\!R^n$ as before.

Lemma 4.7 *Let A be a $\mathcal{U}$-twisted h-admissible operator, where $\mathcal{U} = (U_j, \Omega_j)_{0\le j\le r}$ is some regular unitary covering. Then, for all $j = 0, \dots, r$, there exists an operator-valued symbol $a_j \in S(\Omega_j \times I\!R^n; \mathcal{L}(\mathcal{H}))$, unique up to $\mathcal{O}(h^\infty)$, such that, for any $\chi_j = \chi_j(x) \in C_d^\infty(\Omega_j)$, the symbol of the h-admissible operator $U_j\chi_j A U_j^{-1}\chi_j$ is $\chi_j \sharp a_j \sharp \chi_j$ (where $\sharp$ stands for the standard symbolic composition: see Appendix A).*

Proof Indeed, given two functions $\chi_j, \varphi_j \in C_d^\infty(\Omega_j)$ with $\varphi_j\chi_j = \chi_j$, one has

$$U_j\chi_j A U_j^{-1}\chi_j = \chi_j \left(U_j\varphi_j A U_j^{-1}\varphi_j\right)\chi_j,$$

and thus, denoting by a_j^χ the symbol of $U_j\chi A U_j^{-1}\chi$, one obtains

$$a_j^{\chi_j} = \chi_j \sharp a_j^{\varphi_j} \sharp \chi_j.$$

In particular, using the explicit expression of $\sharp$ (see Appendix A, Proposition 13.2), we see that $a_j^{\varphi_j} = a_j^{\chi_j} + \mathcal{O}(h^\infty)$ in the interior of $\{\chi_j(x) = 1\}$. Then, the result follows by taking a non-decreasing sequence $(\varphi_{j,k})_{k\ge 1}$ in $C_d^\infty(\Omega_j)$, such that $\bigcup_{k\ge 0}\{x \in \Omega_j\,;\, \varphi_{j,k}(x) = 1\} = \Omega_j$, and, for any $(x,\xi) \in \Omega_j \times I\!R^n$, by defining $a_j(x,\xi)$ as the common value of the $a_j^{\varphi_{j,k}}(x,\xi)$'s for k large enough. •

Definition 4.8 (Symbol) *Let A be a $\mathcal{U}$-twisted h-admissible operator, where $\mathcal{U} = (U_j, \Omega_j)_{0\le j\le r}$ is some regular unitary covering. Then, the family of* *operator-valued functions* $\sigma(A) := (a_j)_{0\leq j\leq r} \in \mathbf{S}(\Omega;\mathcal{L}(\mathcal{H}))$*, defined in the previous lemma, is called the (full) symbol of* A*. Moreover,* A *is said to be elliptic if, for any* $j = 0,\cdots,r$ *and* $(x,\xi) \in \Omega_j \times I\!R^n$*, the operator* $a_j(x,\xi)$ *is invertible on* $\mathcal{H}$*, and verifies,*

$$\|a_j(x,\xi)^{-1}\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(1), \tag{4.4}$$

uniformly for h *small enough and for* (x,ξ) *in any set of the form* $\Omega'_j \times I\!R^n$*, with* $\Omega'_j \subset \Omega_j$, $\mathrm{dist}\left(\Omega'_j, I\!R^n\backslash\Omega_j\right) > 0$.

In particular, it follows from the proof of Proposition 4.6 that, if such an operator A is elliptic, then it can be written in the form (4.1), with A_j^N elliptic on $\{\chi_j \neq 0\}$ for all j, N. Moreover, we have the two following result on composition and parametrices:

Proposition 4.9 (Composition) *Let* $\mathcal{U}$ *be a regular covering of* $L^2(I\!R^n;\mathcal{H})$*, and let* A *and* B *be two* $\mathcal{U}$*-twisted* h*-admissible operators. Then, the composition* AB *is a* $\mathcal{U}$*-twisted* h*-admissible operator, too. Moreover, its symbol is given by,*

$$\sigma(AB) = \sigma(A)\sharp\sigma(B),$$

where the operation $\sharp$ *is defined component by component, that is,*

$$(a_j)_{0\leq j\leq r}\sharp(b_j)_{0\leq j\leq r} := (a_j\sharp b_j)_{0\leq j\leq r}.$$

Proof First of all, since

$$\mathrm{ad}_{\chi}(AB) = \mathrm{ad}_{\chi}(A)B + A\,\mathrm{ad}_{\chi}(B),$$

one easily sees, by induction on N, that the first condition in Proposition 4.6 is satisfied. Moreover, if $\chi_j \in C_d^\infty(\Omega_j)$, let $\varphi_j \in C_d^\infty(\Omega_j)$ such that $\varphi_j\chi_j = \chi_j$. Then, if, for any operator C, we set $C_j := U_j\varphi_jCU_j^{-1}\varphi_j$, we have,

$$\begin{aligned} U_j\chi_jABU_j^{-1}\chi_j &= \chi_jA_jB_j\chi_j + U_j\chi_j\mathrm{ad}_{(\varphi_j^2)}(A)BU_j^{-1}\chi_j \\ &= \chi_jA_jB_j\chi_j + \chi_j[\mathrm{ad}_{(\varphi_j^2)}(A)]_jB_j\chi_j + U_j\chi_j\mathrm{ad}^2_{(\varphi_j^2)}(A)BU_j^{-1}\chi_j \\ &= \cdots \\ &= \sum_{k=0}^{N-1}\chi_j[\mathrm{ad}^k_{(\varphi_j^2)}(A)]_jB_j\chi_j + U_j\chi_j\mathrm{ad}^N_{(\varphi_j^2)}(A)BU_j^{-1}\chi_j \end{aligned} \tag{4.5}$$

for all $N \geq 1$. Therefore, since $U_j\chi_j\mathrm{ad}^N_{(\varphi_j^2)}(A)BU_j^{-1}\chi_j = \mathcal{O}(h^N)$, and the operator $[\mathrm{ad}^k_{(\varphi_j^2)}(A)]_j = \mathrm{ad}^k_{(\varphi_j^2)}(A_j)$ is a bounded h-admissible operator, we deduce from (4.5) that AB is a $\mathcal{U}$-twisted h-admissible operator. Moreover, since $\varphi_j = 1$ on the support of χ_j, we see that the symbol of $\chi_j\mathrm{ad}^k_{(\varphi_j^2)}(A_j)$ vanishes identically for $k \geq 1$, and thus, we also deduce from (4.5) that the symbol $(c_j)_{0\leq j\leq r}$ of AB verifies,

$$\chi_j\sharp c_j\sharp\chi_j = \chi_j\sharp a_j\sharp b_j\sharp\chi_j,$$

for any $\chi_j \in C_d^\infty(\Omega_j)$, and the result follows. •

Proposition 4.10 (Parametrix) *Let A be a $\mathcal{U}$-twisted h-admissible operator, and assume that A is elliptic. Then, A is invertible on $L^2(I\!R^n;\mathcal{H})$, and its inverse A^{-1} is a $\mathcal{U}$-twisted h-admissible operator. Moreover, its symbol $\sigma(A^{-1})$ is related to the one $\sigma(A)=(a_j)_{0\leq j\leq r}$ of A by the following formula:*

$$\sigma(A^{-1})=(\sigma(A))^{-1}+hb,$$

where $(\sigma(A))^{-1}:=(a_j^{-1})_{0\leq j\leq r}$ and $b\in\mathbf{S}(\Omega;\mathcal{L}(\mathcal{H}))$.

Proof We first prove that A is invertible by following an idea of [KMSW] (proof of Theorem 1.2).

For $j=0,\cdots,r$, let $\chi_j,\varphi_j\in C_d^\infty(\Omega_j)$ such that $\varphi_j\chi_j=\chi_j$, and $\sum_{j=0}^r\chi_j=1$. Then, by assumption, the symbol of $U_j\varphi_jAU_j^{-1}\varphi_j$ can be written on the form $\varphi_j(x)\sharp a_j(x,\xi)\sharp\varphi_j(x)$ with $a_j(x,\xi)$ invertible, and the operator,

$$B:=\sum_{j=0}^r U_j^{-1}\varphi_j^3\mathrm{Op}_h(\varphi_ja_j^{-1})U_j\chi_j$$

is well defined and bounded on $L^2(I\!R^n;\mathcal{H})$. Moreover, using the standard symbolic calculus, we compute,

$$\begin{aligned}AB &= \sum_{j=0}^r AU_j^{-1}\varphi_j^3\mathrm{Op}_h(\varphi_ja_j^{-1})U_j\chi_j\\ &= \sum_{j=0}^r U_j^{-1}\varphi_jU_j\varphi_jAU_j^{-1}\varphi_j\mathrm{Op}_h(\varphi_ja_j^{-1})U_j\chi_j\\ &\qquad\qquad +[A,\varphi_j^2]U_j^{-1}\varphi_j\mathrm{Op}_h(\varphi_ja_j^{-1})U_j\chi_j\\ &= \sum_{j=0}^r U_j^{-1}\varphi_j\mathrm{Op}_h(\varphi_j^2a_j)\mathrm{Op}_h(\varphi_ja_j^{-1})U_j\chi_j+\mathcal{O}(h)\\ &= \sum_{j=0}^r U_j^{-1}\varphi_j^4U_j\chi_j+\mathcal{O}(h)=\sum_{j=0}^r\chi_j+\mathcal{O}(h)=1+\mathcal{O}(h).\end{aligned}\tag{4.6}$$

In the same way, defining,

$$B':=\sum_{j=0}^r U_j^{-1}\chi_j\mathrm{Op}_h(\varphi_ja_j^{-1})U_j\varphi_j^3,$$

we obtain $B'A=1+\mathcal{O}(h)$, and this proves the invertibility of A for h small enough. It remains to verify that A^{-1} is a $\mathcal{U}$-twisted h-admissible operator. We first prove,

Lemma 4.11 *Let A be a $\mathcal{U}$-twisted h-admissible operator, and let $\chi,\psi\in C_b^\infty(I\!R^n)$ such that* $\mathrm{dist}\,(\,\mathrm{Supp}\,\chi,\ \mathrm{Supp}\,\psi)>0$. *Then,* $\|\chi A\psi\|=\mathcal{O}(h^\infty)$.

Proof Given $N \geq 1$, let $\varphi_1, \cdots, \varphi_N \in C_b^\infty(\mathbb{R}^n)$, such that $\varphi_1 \chi = \chi$, $\varphi_{k+1}\varphi_k = \varphi_k$ $(k = 1, \cdots, N-1)$, and $\varphi_N \psi = 0$. Then, one has,

$$\begin{aligned} \chi A \psi &= \varphi_1 \mathrm{ad}_\chi(A)\psi = \varphi_2 \mathrm{ad}_{\varphi_1} \circ \mathrm{ad}_\chi(A)\psi \\ &= \cdots = \mathrm{ad}_{\varphi_N} \circ \cdots \circ \mathrm{ad}_{\varphi_1} \circ \mathrm{ad}_\chi(A)\psi = \mathcal{O}(h^{N+1}). \end{aligned}$$

•

Now, since,

$$\mathrm{ad}_\chi(A^{-1}) = -A^{-1}\mathrm{ad}_\chi(A)A^{-1},$$

it is easy to see, by induction on N, that A^{-1} satisfies to the first property of Proposition 4.6. Moreover, for $v \in L^2(\mathbb{R}^n; \mathcal{H})$ and for $\chi_j \in C_d^\infty(\Omega_j)$, let us set,

$$u = A^{-1}U_j^{-1}\chi_j v,$$

and choose $\varphi_j, \in C_d^\infty(\Omega_j; \mathbb{R})$, $\psi_j \in C_b^\infty(\mathbb{R}^n; \mathbb{R})$, such that $\psi_j \chi_j = 0$, $\varphi_j^4 + \psi_j^2 \geq 1$, and $\mathrm{dist}\,(\,\mathrm{Supp}\,(\varphi_j - 1),\, \mathrm{Supp}\,\chi_j) > 0$. Then, since the symbol of $A_j := U_j \varphi_j A U_j^{-1} \varphi_j$ is of the form $\varphi_j \sharp a_j \sharp \varphi_j$ with $a_j(x,\xi)$ invertible for x in $\mathrm{Supp}\,\varphi_j$, we see that the bounded h-admissible operator $B_j := A_j^* A_j + \psi_j^2$ is globally elliptic, and one has,

$$\begin{aligned} B_j U_j \chi_j u &= A_j^* A_j U_j \chi_j u = A_j^* U_j \varphi_j A \chi_j u = A_j^* U_j \chi_j A u + A_j^* U_j \varphi_j [A, \chi_j] u \\ &= A_j^* \chi_j^2 v + A_j^* U_j \varphi_j [A, \chi_j] \varphi_j^2 u + A_j^* U_j \chi_j A(\varphi_j^2 - 1) u \\ &= A_j^* \chi_j^2 v + A_j^* [A_j, \chi_j] U_j \varphi_j u + \mathcal{O}(h^\infty \|v\|), \end{aligned} \tag{4.7}$$

where the last estimate comes from Lemma 4.11. In particular, since B_j^{-1} is an h-admissible operator, we obtain that $U_j \chi_j u$ can be written on the form,

$$U_j \chi_j u = C_j v + h C_j' U_j \varphi_j u + \mathcal{O}(h^\infty \|v\|)$$

where C_j, C_j' are bounded h-admissible operators. Repeating the same argument with $U_j \varphi_j u$ instead of $U_j \chi_j u$, and iterating the procedure, it follows that $U_j \chi_j A^{-1} U_j^{-1} \chi_j$ is an h-admissible operator. Moreover, we see on (4.7) that the symbol of $U_j \chi_j A^{-1} U_j^{-1} \chi_j$ coincides, up to $\mathcal{O}(h)$, with that of $B_j^{-1} A_j^* \chi_j^2$, that is,

$$(\varphi_j^4(x) a_j^*(x,\xi) a_j(x,\xi) + \psi_j^2(x))^{-1} a_j^*(x,\xi) \chi_j(x)^2 = a_j(x,\xi)^{-1} \chi_j(x)^2,$$

since $\varphi_j = 1$ and $\psi_j = 0$ on the support of χ_j. Thus, the proposition follows. •

Proposition 4.12 (Functional Calculus) *Let A be a selfadjoint $\mathcal{U}$-twisted h-admissible operator, and let $f \in C_0^\infty(\mathbb{R})$. Then, the operator $f(A)$ is a $\mathcal{U}$-twisted h-admissible operator, and its symbol is related to that of A by the formula,*

$$\sigma(f(A)) = f(\,\mathrm{Re}\,\sigma(A)) + hb,$$

where $f(\,\mathrm{Re}\,(a_j)_{j=0,\dots,r}) := (f(\,\mathrm{Re}\,a_j))_{j=0,\dots,r}$ and $b \in \mathbf{S}(\Omega; \mathcal{L}(H))$.

Proof We use a formula of representation of $f(A)$ due to B. Helffer and J. Sjöstrand. Denote by $\tilde{f} \in C_0^\infty(\mathbb{C})$ an almost analytic extension of f, that is, a function verifying $\tilde{f}\,|_{\mathbb{R}} = f$ and $|\overline{\partial}\tilde{f}(z)| = \mathcal{O}(|\,\mathrm{Im}\, z|^\infty)$ uniformly on $\mathbb{C}$. Then, we have (see, e.g., [DiSj1, Ma2]),

$$f(A) = \frac{1}{\pi}\int \overline{\partial}\tilde{f}(z)(A-z)^{-1}dz\, d\bar{z}. \tag{4.8}$$

Now, by Proposition 4.10, we see that, for $z \in \mathbb{C}\setminus\mathbb{R}$, the operator $(A-z)^{-1}$ is a $\mathcal{U}$-twisted h-admissible operator. Moreover, by standard rules on the operations ad_χ, if A and B are two bounded operators, then, for any $N \geq 1$ and any $\chi_1, \cdots, \chi_N \in C_b^\infty(\mathbb{R}^n)$, one has,

$$\mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(AB) = \sum_{\substack{I\cup J=\{1,\dots,N\}\\ I\cap J=\emptyset}} \left(\prod_{i\in I}\mathrm{ad}_{\chi_i}\right)(A)\left(\prod_{j\in J}\mathrm{ad}_{\chi_j}\right)(B).$$

In particular, replacing A and B by $A-z$ and $(A-z)^{-1}$ respectively, one obtains,

$$\begin{aligned}&\mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}((A-z)^{-1})\\ &= -(A-z)^{-1}\sum_{\substack{I\cup J=\{1,\dots,N\}\\ I\cap J=\emptyset,\, I\neq\emptyset}} \left(\prod_{i\in I}\mathrm{ad}_{\chi_i}\right)(A-z)\left(\prod_{j\in J}\mathrm{ad}_{\chi_j}\right)((A-z)^{-1}),\end{aligned}$$

and thus, an easy induction gives,

$$\mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}((A-z)^{-1}) = \mathcal{O}(h^N|\,\mathrm{Im}\, z|^{-(N+1)}),$$

uniformly with respect to h and z. Therefore, it is easy to deduce from (4.8) that $f(A)$ is a $\mathcal{U}$-twisted h-admissible operator. Moreover, since $(a_j)_{0\leq j\leq r} := \sigma(A) = \mathrm{Re}\,(\sigma(A)) + \mathcal{O}(h)$, a computation similar to that of (4.6) shows that,

$$(A-z)^{-1} = \sum_{j=0}^{r} U_j^{-1}\varphi_j^3\mathrm{Op}_h(\varphi_j(\,\mathrm{Re}\, a_j - z)^{-1})U_j\chi_j + hR$$

where φ_j and χ_j are as in (4.6), and R verifies,

$$U_j\tilde{\chi}_jRU_j^{-1}\tilde{\chi}_j = \mathrm{Op}_h(\sum_{k=0}^{N} h^k r_{k,j}(z)) + \mathcal{O}(h^N|\,\mathrm{Im}\, z|^{-N_1(N)},$$

for any $\tilde{\chi}_j \in C_0^\infty(\Omega_j)$ such that $\tilde{\chi}_j\varphi_j = \tilde{\chi}_j\chi_j = \tilde{\chi}_j$, any $N \geq 1$, and for some $N_1(N) \geq 1$ and $r_{k,j}(z) \in C^\infty(T^*\Omega_j)$, $\partial^\alpha r_{k,j}(z) = \mathcal{O}(|\,\mathrm{Im}\, z|^{-N_{\alpha,k,j}})$ uniformly. Then, one easily concludes that the symbol b_j of $U_j\tilde{\chi}_jf(A)U_j\tilde{\chi}_j$ verifies,

$$bj = \tilde{\chi}_j(\,\mathrm{Re}\, a_j - z)^{-1}\tilde{\chi}_j + \mathcal{O}(h),$$

and since the previous construction can be made for $\tilde{\chi}_j \in C_0^\infty(\Omega_j)$ arbitrary, the result on the symbol of $f(A)$ follows. •

In order to complete the theory of bounded $\mathcal{U}$-twisted h-admissible operators, it remains to generalize the notion of quantization. To this purpose, we first observe that, if $a = (a_j)_{j=0,\dots,r} \in \mathbf{S}(\Omega; \mathcal{L}(H))$, then, the two operators $\varphi_j \mathrm{Op}_h(a_j)\varphi_j$ and $U_j^{-1}\varphi_j \mathrm{Op}_h(a_j) U_j \varphi_j$ are well defined for any $\varphi_j \in C_d^\infty(\Omega_j)$. Moreover, if $a = \sigma(A)$ is the symbol of a $\mathcal{U}$-twisted h-admissible operator A, then, by construction, it necessarily verifies the following condition of compatibility:

$$U_j^{-1}\varphi \mathrm{Op}_h(a_j) U_j \varphi = U_k^{-1}\varphi \mathrm{Op}_h(a_k) U_k \varphi, \tag{4.9}$$

for any $\varphi \in C_d^\infty(\Omega_j) \cap C_d^\infty(\Omega_k)$. Then, we have,

Theorem 4.13 (Quantization) *Let $a = (a_j)_{j=0,\dots,r} \in \mathbf{S}(\Omega; \mathcal{L}(H))$ satisfying to the compatibility condition (4.9). Then, there exists a $\mathcal{U}$-twisted h-admissible operator A, unique up to $\mathcal{O}(h^\infty)$, such that $a = \sigma(A)$. Moreover, A is given by the formula,*

$$A = \sum_{j=0}^{r} U_j^{-1}\chi_j \mathrm{Op}_h(a_j) U_j \varphi_j, \tag{4.10}$$

where $\chi_j, \varphi_j \in C_d^\infty(\Omega_j) (j = 0, \dots, r)$ is any family of functions such that $\sum_{j=0}^r \chi_j = 1$ and $\mathrm{dist}\,(\,\mathrm{Supp}\,(\varphi_j - 1),\ \mathrm{Supp}\,\chi_j) > 0$.

Proof The unicity up to $\mathcal{O}(h^\infty)$ is a direct consequence of the formulas (4.2)-(4.3), where A is expressed in terms of $U_j\varphi_j A U_j^{-1}\varphi_j$ and is clearly $\mathcal{O}(h^\infty)$ if these operators have identically vanishing symbols. For the existence, we define A as in (4.10) and we observe that, thanks to (4.9), for any $k \in \{0, \dots, r\}$ and $\psi_k \in C_d^\infty(\Omega_k)$, one has,

$$\begin{aligned} U_k\psi_k A U_k^{-1}\psi_k &= \sum_{j=0}^{r} \chi_j \psi_k \mathrm{Op}_h(a_k)\varphi_j\psi_k = \sum_{j=0}^{r} \chi_j \psi_k \mathrm{Op}_h(a_k)\psi_k + \mathcal{O}(h^\infty) \\ &= \psi_k \mathrm{Op}_h(a_k)\psi_k + \mathcal{O}(h^\infty). \end{aligned}$$

Thus, A admits $(a_k)_{k=0,\dots,r}$ as its symbol, and the result follows. •

To end this section, let us go back to our operator $\tilde{P}$ defined at the end of Section 3. We have,

Proposition 4.14 *Assume (H1)-(H4). Then, the operator $\tilde{P}$ defined in (3.4) is such that $\tilde{P}(\boldsymbol{\omega} + Q_0)^{-1}$ is a $\mathcal{U}$-twisted h-admissible operator on $L^2(I\!R^n; \mathcal{H})$, where $\mathcal{U} = (U_j, \Omega_j)_{j=0,1,\cdots,r}$ is the regular covering defined in Section 2. Moreover, its symbol $\tilde{p} = (\tilde{p}_j)_{j=0,1,\cdots,r}$ verifies,*

$$\tilde{p}_j(x,\xi) = (\omega(x,\xi) + \tilde{Q}_j(x) + \zeta(x)W(x))(\omega(x,\xi) + Q_{0,j}(x))^{-1} + hb_j,$$

where $(\tilde{Q}_j(x))_{j=0,1,\cdots,r}$ (resp. $(Q_{0,j}(x))_{j=0,1,\cdots,r}$ is the symbol of $\tilde{Q}(x)$ (resp. $Q_0(x)$), and $(b_j)_{j=0,\dots,r} \in \mathbf{S}(\Omega; \mathcal{L}(H))$.

Proof We must verify the two conditions of Proposition 4.6. We have,

$$\begin{aligned}&\mathrm{ad}_\chi(\tilde P(\boldsymbol{\omega}+Q_0)^{-1})\\&\quad=\mathrm{ad}_\chi(\tilde P)(\boldsymbol{\omega}+Q_0)^{-1}+\tilde P\mathrm{ad}_\chi((\boldsymbol{\omega}+Q_0)^{-1})\\&\quad=\mathrm{ad}_\chi(\boldsymbol{\omega})(\boldsymbol{\omega}+Q_0)^{-1}-\tilde P(\boldsymbol{\omega}+Q_0)^{-1}\mathrm{ad}_\chi(\boldsymbol{\omega})(\boldsymbol{\omega}+Q_0)^{-1}\\&\quad=\mathcal{O}(h),\end{aligned}$$

and an easy iteration shows that the first condition of Proposition 4.6 is satisfied. Moreover, if $\chi_j,\tilde\chi_j\in C_b^\infty(I\!\!R^n)$ are supported in Ω_j $(j=1\cdots,r)$ and verify $\mathrm{Supp}\,\chi_j\cap\mathrm{Supp}\,(1-\tilde\chi_j)=\emptyset$, and if we set $P_j:=U_j\chi_j\tilde PU_j^{-1}\tilde\chi_j$, we have,

$$\begin{aligned}&U_j\chi_j\tilde P(\boldsymbol{\omega}+Q_0)^{-1}U_j^{-1}\chi_j\\&\quad=U_j\chi_j\tilde P\tilde\chi_j^2(\boldsymbol{\omega}+Q_0)^{-1}U_j^{-1}\chi_j+U_j\chi_j\boldsymbol{\omega}(1-\tilde\chi_j^2)(\boldsymbol{\omega}+Q_0)^{-1}U_j^{-1}\chi_j\\&\quad=P_jU_j\tilde\chi_j(\boldsymbol{\omega}+Q_0)^{-1}U_j^{-1}\chi_j+\mathcal{O}(h^\infty),\end{aligned}$$

and a slight generalization of the last argument in the proof of Proposition 4.10 (this time with $B_j=U_j\varphi_j(\boldsymbol{\omega}+Q_0)U_j^{-1}\varphi_j+\psi_j(\boldsymbol{\omega}+Q_0)\psi_j$), shows that $P_jU_j\tilde\chi_j(\boldsymbol{\omega}+Q_0)^{-1}U_j^{-1}\chi_j$ is a bounded h-admissible operator on $L^2(I\!\!R^n;\mathcal{H})$. Therefore, the second condition of Proposition 4.6 is satisfied, too, and the result follows. •

Corollary 4.15 *The two operators $(\tilde P+i)^{-1}$ and $(\boldsymbol{\omega}+Q_0)^{-1}$ are $\mathcal{U}$-twisted h-admissible operators on $L^2(I\!\!R^n;\mathcal{H})$.*

Proof First observe that the previous proof is still valid if $\tilde P$ is changed into $\tilde P+1$. This proves that $(\boldsymbol{\omega}+Q_0)^{-1}=(\tilde P+1)(\boldsymbol{\omega}+Q_0)^{-1}-\tilde P(\boldsymbol{\omega}+Q_0)^{-1}$ is a $\mathcal{U}$-twisted h-admissible operator. Moreover, since $(\tilde P+i)(\boldsymbol{\omega}+Q_0)^{-1}$ is elliptic, by Proposition 4.10 its inverse $(\boldsymbol{\omega}+Q_0)(\tilde P+i)^{-1}$ is a $\mathcal{U}$-twisted h-admissible operator, too. Therefore, so is $(\tilde P+i)^{-1}=(\boldsymbol{\omega}+Q_0)^{-1}\left[(\boldsymbol{\omega}+Q_0)(\tilde P+i)^{-1}\right]$. •

Proposition 4.16 *For any $f\in C_0^\infty(I\!\!R)$, the operator $f(\tilde P)$ is a $\mathcal{U}$-twisted h-admissible.*

Proof By Proposition 4.14 and Corollary 4.15, we see that the operator $(\tilde P-z)(\boldsymbol{\omega}+Q_0)^{-1}$ is a $\mathcal{U}$-twisted h-admissible operator, and it is elliptic for $z\in\mathbb{C}\setminus I\!\!R$. Therefore, by Proposition 4.10, its inverse $(\boldsymbol{\omega}+Q_0)(\tilde P-z)^{-1}$ is a $\mathcal{U}$-twisted h-admissible operator, too. Moreover, for any $N\geq 1$ and any $\chi_1,\cdots,\chi_N\in C_b^\infty(I\!\!R^n)$, one has,

$$\mathrm{ad}_{\chi_1}\circ\cdots\circ\mathrm{ad}_{\chi_N}((\boldsymbol{\omega}+Q_0)(\tilde P-z)^{-1})=\mathcal{O}(h^N|\,\mathrm{Im}\,z|^{-(N+1)})$$

uniformly with respect to h and z. Therefore, we deduce again from (4.8) that $(\boldsymbol{\omega}+Q_0)f(\tilde P)$, too, is a $\mathcal{U}$-twisted h-admissible operator. As a consequence, so is $f(\tilde P)$. •

5 Twisted Partial Differential Operators

For $\mu \geq 0$, we set,

$$H_d^\mu(\Omega_j) := \{u \in L^2(\Omega_j;\mathcal{H})\,;\, \forall \chi_j \in C_d^\infty(\Omega_j),\, \chi_j u \in H^\mu(\mathbb{R}^n;\mathcal{H})\},$$

where $H^\mu(\mathbb{R}^n;\mathcal{H})$ stands for the usual Sobolev space of order μ on $\mathbb{R}^n$ with values in $\mathcal{H}$. Moreover, if $\mathcal{U} := (U_j,\Omega_j)_{j=0,\cdots,r}$ is a regular unitary covering (in the previous sense) of $L^2(\mathbb{R}^n;\mathcal{H})$, we introduce the vector-space,

$$\mathcal{H}_d^\mu(\mathcal{U}) := \{u \in L^2(\mathbb{R}^n;\mathcal{H})\,;\, \forall\, j = 0,\dots,r,\, U_j u\left|_{\Omega_j}\right. \in H_d^\mu(\Omega_j)\},$$

endowed with the family of semi-norms,

$$\|u\|_{\mu,\chi} := \|u\|_{L^2} + \sum_{j=0}^{r} \|U_j\chi_j u\|_{H^\mu},$$

where $\chi := (\chi_j)_{j=0,\dots,r}$ is such that $\chi_j \in C_d^\infty(\Omega_j)$ for all j. In particular, we have a notion of continuity for operators $A : \mathcal{H}_d^\mu(\mathcal{U}) \to \mathcal{H}_d^\nu(\mathcal{U})$.

Let us also remark that, for $\mu = 0$, we recover $\mathcal{H}_d^0(\mathcal{U}) = L^2(\mathbb{R}^n;\mathcal{H})$, and, if $\mu \geq \nu$, then $\mathcal{H}_d^\mu(\mathcal{U}) \subset \mathcal{H}_d^\nu(\mathcal{U})$ with a continuous injection.

Definition 5.1 *Let $\mathcal{U} := (U_j,\Omega_j)_{j=0,\cdots,r}$ be a regular unitary covering (in the previous sense) of $L^2(\mathbb{R}^n;\mathcal{H})$, and let $\mu \in \mathbb{Z}_+$. We say that an operator $A : \mathcal{H}_d^\mu(\mathcal{U}) \to L^2(\mathbb{R}^n;\mathcal{H})$ is a (semiclassical) $\mathcal{U}$-twisted partial differential operator up to regularizing unitary conjugation (in short: $\mathcal{U}$-twisted PDO) of degree μ, if A is local with respect to the variable x (that is,* Supp $(Au) \subset$ Supp u *for all u, where* Supp *stands for the support with respect to x), and, for all $j = 0,\dots,r$, the operator $U_jAU_j^{-1}$ (well defined on $H_d^\mu(\Omega_j)$) is of the form,*

$$U_jAU_j^{-1} = \sum_{|\alpha|\leq\mu} a_{\alpha,j}(x;h)(hD_x)^\alpha$$

with $a_{\alpha,j} \in S(\Omega_j;\mathcal{L}(\mathcal{H}))$.

In particular, for any partition of unity $(\chi_j)_{j=0,\dots,r}$ on $\mathbb{R}^n$ with $\chi_j \in C_d^\infty(\Omega_j)$, A can be written as,

$$A = \sum_{j=0}^{r} U_j^{-1}A_jU_j\chi_j, \tag{5.1}$$

with $A_j := U_jAU_j^{-1}$. As a consequence, one also has $\mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_{\mu+1}}(A) = 0$ for any functions $\chi_1,\cdots,\chi_{\mu+1} \in C_b^\infty(\mathbb{R}^n)$.

Of course, we also have an obvious notion of (full) symbol for such operators, namely, the family,

$$\sigma(A) := (a_j)_{0\leq j\leq r}, \quad a_j(x,\xi;h) := \sum_{|\alpha|\leq\mu} a_{\alpha,j}(x;h)\xi^\alpha.$$

Moreover, if A and B are two $\mathcal{U}$-twisted PDO's on $L^2(I\!R^n;\mathcal{H})$, of respective degrees μ and μ', by writing $U_jABU_j^{-1} = (U_jAU_j^{-1})(U_jBU_j^{-1})$ and by using a partition of unity as before, we immediately see that AB is well defined on $\mathcal{H}_d^{\mu+\mu'}(\mathcal{U})$, and is a $\mathcal{U}$-twisted PDO, too, with symbol,

$$\sigma(AB) = \sigma(A)\sharp\sigma(B).$$

Now, we turn back again to the operator $\tilde{P}$ defined at the end of Section 3, and the regular covering defined in Section 2.

Proposition 5.2 *Let A be a $\mathcal{U}$-twisted PDO on $L^2(I\!R^n;\mathcal{H})$ of degree μ, where $\mathcal{U}$ is the regular covering defined in Section 2. Then, for any integers k,ℓ such that $k+\ell \geq \mu/m$, the operator $(\tilde{P}+i)^{-k}A(\tilde{P}+i)^{-\ell}$ is a $\mathcal{U}$-twisted h-admissible operator.*

Proof We first consider the case $k = 0$. For $\varphi_j, \psi_j \in C_d^\infty(\Omega_j)$, such that $\operatorname{dist}(\operatorname{Supp}(\psi_j - 1), \operatorname{Supp}\varphi_j) > 0$, we have,

$$U_j\varphi_jA(\tilde{P}+i)^{-\ell}U_j^{-1}\varphi_j = U_j\varphi_jAU_j^{-1}\psi_jU_j\psi_j(\tilde{P}+i)^{-\ell}U_j^{-1}\varphi_j, \tag{5.2}$$

and, as in the proof of Proposition 4.10, we see that the inverse of $(\tilde{P}+i)^\ell$ can be written as,

$$(\tilde{P}+i)^{-\ell} = B(1+hR) \tag{5.3}$$

where R is uniformly bounded, and B is of the form,

$$B = \sum_{\nu=0}^{r} U_\nu^{-1}\tilde{\chi}_\nu \mathrm{Op}_h((p_\nu+i)^{-\ell})U_\nu\chi_\nu, \tag{5.4}$$

where $(\chi_\nu)_{\nu=0,\dots,r}$ is an arbitrary partition of unity with $\chi_\nu \in C_d^\infty(\Omega_\nu)$, $\tilde{\chi}_\nu \in C_d^\infty(\Omega_\nu)$ is such that $\tilde{\chi}_\nu\chi_\nu = \chi_\nu$, and $p_\nu(x,\xi;h) = \omega(x,\xi;h)+\tilde{Q}_\nu(x)+\zeta(x)W(x)$.

Lemma 5.3 *Let $j \in \{0,\dots,r\}$ and $\psi_j \in C_d^\infty(\Omega_j)$ be fixed. Then, there exists a partition of unity $(\chi_\nu)_{\nu=0,\dots,r}$ of $I\!R^n$ with $\chi_\nu \in C_d^\infty(\Omega_\nu)$, and there exists $\tilde{\chi}_\nu \in C_d^\infty(\Omega_\nu)$ with $\tilde{\chi}_\nu\chi_\nu = \chi_\nu$ ($\nu = 0,\dots,r$), such that $\chi_j\psi_j = \psi_j$ and $\tilde{\chi}_\nu\psi_j = 0$ if $\nu \neq j$.*

Proof It is enough to construct a partition of unity in such a way that $\operatorname{dist}(\operatorname{Supp}\psi_j, \operatorname{Supp}(\chi_j - 1)) > 0$ (and thus, automatically, one will also have $\operatorname{dist}(\operatorname{Supp}\psi_j, \operatorname{Supp}\chi_\nu) > 0$ for $\nu \neq j$). Let $(\chi'_\nu)_{\nu=0,\dots,r}$ be a partition of unity as in Definition 4.1, and let $\chi''_j \in C_d^\infty(\Omega_j;[0,1])$ such that $\chi''_j = 1$ in a neighborhood of $\operatorname{Supp}\psi_j \cup \operatorname{Supp}\chi_j$. Then, the result is obtained by taking $\chi_\nu := (1-\chi''_j)\chi'_\nu$ if $\nu \neq j$, and $\chi_j := \chi''_j$. •

Taking the χ_ν's and $\tilde{\chi}_\nu$'s as in the previous lemma, we obtain from (5.3)-(5.4),

$$U_j\psi_j(\tilde{P}+i)^{-\ell} = \psi_j\mathrm{Op}_h((p_j+i)^{-\ell})U_j\chi_j(1+hR),$$

and thus, since $U_j\varphi_j A U_j^{-1}\psi_j$ is a differential operator of degree μ with operator-valued symbol, we easily deduce from (5.2) that if $m\ell \geq \mu$, then $A(\tilde{P}+i)^{-\ell}$ is bounded on $L^2(I\!R^n;\mathcal{H})$, uniformly with respect to $h>0$. Moreover, writing,

$$U_j\varphi_j A(\tilde{P}+i)^{-\ell}U_j^{-1}\varphi_j = [U_j\varphi_j A U_j^{-1}\psi_j\langle hD_x\rangle^{-m\ell}][\langle hD_x\rangle^{m\ell}U_j\psi_j(\tilde{P}+i)^{-\ell}U_j^{-1}\varphi_j],$$

and using the standard pseudodifferential calculus with operator-valued symbol for the first factor, and a slight refinement of (4.7) for the second one, we see that $U_j\varphi_j A(\tilde{P}+i)^{-\ell}U_j^{-1}\varphi_j$ is an h-admissible operator on $L^2(I\!R^n);\mathcal{H})$. Then, it only remains to verify the first property of Proposition 4.6. We first prove,

Lemma 5.4 *For any $\alpha_1,\dots,\alpha_N \in C_b^\infty(I\!R^n)$, one has,*

$$\mathrm{ad}_{\alpha_1}\circ\dots\circ\mathrm{ad}_{\alpha_N}((\tilde{P}+i)^{-\ell}) = h^N(\tilde{P}+i)^{-\ell}R_N, \tag{5.5}$$

with $R_N=\mathcal{O}(1)$ on $L^2(I\!R^n;\mathcal{H})$.

Proof Since $\mathrm{ad}_{\alpha_N}((\tilde{P}+i)^{-\ell}) = -(\tilde{P}+i)^{-\ell}\mathrm{ad}_{\alpha_N}((\tilde{P}+i)^{\ell})(\tilde{P}+i)^{-\ell}$, by an easy iteration we see that it is enough to prove that $h^{-N}\mathrm{ad}_{\alpha_1}\circ\dots\circ\mathrm{ad}_{\alpha_N}((\tilde{P}+i)^{\ell})(\tilde{P}+i)^{-\ell}$ is uniformly bounded. Moreover, since $\mathrm{ad}_{\alpha_N}((\tilde{P}+i)^{\ell})(\tilde{P}+i)^{-\ell}$ is a sum of terms of the type $(\tilde{P}+i)^k\mathrm{ad}_{\alpha_N}(\boldsymbol{\omega})(\tilde{P}+i)^{-k-1}$ $(0\leq k\leq \ell-1)$, another easy iteration shows that it is enough to prove that $h^{-N}(\tilde{P}+i)^{\ell}\mathrm{ad}_{\alpha_1}\circ\dots\circ\mathrm{ad}_{\alpha_N}(\boldsymbol{\omega})(\tilde{P}+i)^{-\ell-1}$ is uniformly bounded. Now, by (H4), we see that, for any partition of unity (χ_j) as before, $(\tilde{P}+i)^{\ell}$ can be written as,

$$(\tilde{P}+i)^{\ell} = \sum_{j=0}^{r} U_j^{-1}P_{j,\ell}U_j\chi_j,$$

where $P_{j,\ell}$ is of the form,

$$P_{j,\ell} = \sum_{|\alpha|\leq m\ell}\rho_{j,\ell,\alpha}(x;h)(hD_x)^{\alpha},$$

with $\rho_{j,\ell,\alpha}Q_0^{\frac{|\alpha|}{m}-\ell}\in C^\infty(\Omega_j;\mathcal{H})$. Moreover, by (2.3), the operator $U_j\mathrm{ad}_{\alpha_1}\circ\dots\circ\mathrm{ad}_{\alpha_N}(\boldsymbol{\omega})U_j^{-1} = \mathrm{ad}_{\alpha_1}\circ\dots\circ\mathrm{ad}_{\alpha_N}(U_j\boldsymbol{\omega}U_j^{-1})$ is of the form,

$$U_j\mathrm{ad}_{\alpha_1}\circ\dots\circ\mathrm{ad}_{\alpha_N}(\boldsymbol{\omega})U_j^{-1} = h^N\sum_{|\alpha|\leq(m-N)_+}\tau_{j,\alpha}(x;h)(hD_x)^{\alpha},$$

with $\tau_{j,\alpha}Q_0^{\frac{|\alpha|}{m}-1}\in C^\infty(\Omega_j;\mathcal{H})$. In particular, we obtain,

$$(\tilde{P}+i)^{\ell}\mathrm{ad}_{\alpha_1}\circ\dots\circ\mathrm{ad}_{\alpha_N}(\boldsymbol{\omega}) = h^N\sum_{j=0}^{r}\sum_{|\alpha|\leq m(\ell+1)}U_j^{-1}\lambda_{j,\ell,\alpha}(x;h)(hD_x)^{\alpha}U_j\varphi_j,$$

with $\varphi_j\in C_d^\infty(\Omega_j)$ and $\lambda_{j,\ell,\alpha}Q_0^{\frac{|\alpha|}{m}-\ell-1}\in C^\infty(\Omega_j;\mathcal{H})$, and the result follows as before by using (5.3)-(5.4), and by observing that, for $|\alpha|\leq m(\ell+1)$, the operator $Q_0^{1+\ell-\frac{|\alpha|}{m}}(hD_x)^\alpha(\langle hD_x\rangle^m+Q_0)^{-\ell-1}$ is uniformly bounded, and thus so is the operator $Q_0^{1+\ell-\frac{|\alpha|}{m}}(hD_x)^\alpha\varphi_j\mathrm{Op}_h((p_j+i)^{-\ell-1})U_j\chi_j$. •

On the other hand, we see on (5.1) that $\mathrm{ad}_{\chi_1}\circ\ldots\circ\mathrm{ad}_{\chi_N}(A)$ is a $\mathcal{U}$-twisted PDO of degree $(\mu-N)_+$, and the first property of Proposition 4.6 for $A(\tilde P+i)^{-\ell}$ follows easily.

For the case $k>0$, by taking a partition of unity, we first observe that,

$$(\tilde P+i)^{-k}A(\tilde P+i)^{-\ell}=\sum_{j=0}^{r}(\tilde P+i)^{-k}U_j^{-1}A_jU_j\chi_j(\tilde P+i)^{-\ell}$$

where $A_j=U_jAU_j^{-1}$ can be written as,

$$A_j=\sum_{\substack{|\alpha|\leq mk\\|\beta|\leq m\ell}}(hD_x)^\alpha a_{\alpha,\beta,j}(x;h)(hD_x)^\beta.$$

Then, by using (in addition to (5.3)-(5.4)) that,

$$(\tilde P+i)^{-k}=(1+hR')B'$$

where R' is uniformly bounded, and B' is of the form,

$$B'=\sum_{\nu=0}^{r}U_\nu^{-1}\chi_\nu\mathrm{Op}_h((p_\nu+i)^{-\ell})U_\nu\tilde\chi_\nu,$$

the same previous arguments show that $(\tilde P+i)^{-k}A(\tilde P+i)^{-\ell}$ is bounded on $L^2(I\!R^n;\mathcal{H})$, uniformly with respect to $h>0$.

Then, let $N\geq 1$ and $\alpha_1\ldots,\alpha_N\in C_d^\infty(\Omega_j)$, such that $\alpha_1\varphi_j=\varphi_j$, $\alpha_2\alpha_1=\alpha_1$, ... , $\alpha_N\alpha_{N-1}=\alpha_{N-1}$, and $\alpha_N(\psi_j-1)=0$. We have,

$$\begin{aligned}&U_j\varphi_j(\tilde P+i)^{-k}A(\tilde P+i)^{-\ell}U_j^{-1}\varphi_j\\&\quad=U_j\varphi_j(\tilde P+i)^{-k}A\psi_j(\tilde P+i)^{-\ell}U_j^{-1}\varphi_j\\&\qquad+U_j\varphi_j(\tilde P+i)^{-k}A(\psi_j-1)\mathrm{ad}_{\alpha_1}\circ\ldots\circ\mathrm{ad}_{\alpha_N}((\tilde P+i)^{-\ell})U_j^{-1}\varphi_j\end{aligned}$$

and thus, by (5.5),

$$\begin{aligned}&U_j\varphi_j(\tilde P+i)^{-k}A(\tilde P+i)^{-\ell}U_j^{-1}\varphi_j\\&\qquad=U_j\varphi_j(\tilde P+i)^{-k}A\psi_j(\tilde P+i)^{-\ell}U_j^{-1}\varphi_j+\mathcal{O}(h^N).\end{aligned}$$

Then, writing $A\psi_j=U_j^{-1}\tilde\psi_jA_jU_j\psi_j$, with $A_j=U_jAU_j^{-1}$ and $\tilde\psi_j\in C_d^\infty(\Omega_j)$ such that $\tilde\psi_j\psi_j=\psi_j$, the result is obtained along the same lines as before. •

Proposition 5.5 *The two operators $\boldsymbol{\omega}Q_0^{-1}$ and $Q_0^{-1}\boldsymbol{\omega}$ are $\mathcal{U}$-twisted PDO's of degree m. Moreover, if A is a $\mathcal{U}$-twisted PDO such that Q_0A and AQ_0 are $\mathcal{U}$-twisted PDO's, too, of degree μ, then the operator $h^{-1}[\boldsymbol{\omega},A]$ is a $\mathcal{U}$-twisted PDO of degree at most $\mu+m-1$.*

Proof Thank to (H4), the fact that $\boldsymbol{\omega} Q_0^{-1}$ and $Q_0^{-1}\boldsymbol{\omega}$ are $\mathcal{U}$-twisted PDO's of degree m is obvious. Moreover, the fact that Q_0A and AQ_0 are both $\mathcal{U}$-twisted PDO's implies that $U_jAU_j^{-1}$ can be written as,

$$U_jAU_j^{-1} = \sum_{|\alpha|\leq\mu} a_{\alpha,j}(x;h)(hD_x)^\alpha$$

with $Q_0a_{\alpha,j}$ and $a_{\alpha,j}Q_0$ in $S(\Omega_j;\mathcal{L}(\mathcal{H}))$. Then, using (H4), we have,

$$\begin{aligned} U_j\boldsymbol{\omega} AU_j^{-1} &= \sum_{\substack{|\alpha|\leq m\\ |\beta|\leq\mu}} c_\alpha(x;h)(hD_x)^\alpha a_{\beta,j}(x;h)(hD_x)^\beta \\ &\quad +h\sum_{\substack{|\alpha|\leq m-1\\ |\beta|\leq\mu}} \omega_{\alpha,j}(x;h)(hD_x)^\alpha a_{\beta,j}(x;h)(hD_x)^\beta \end{aligned}$$

and

$$\begin{aligned} U_jA\boldsymbol{\omega} U_j^{-1} &= \sum_{\substack{|\alpha|\leq m\\ |\beta|\leq\mu}} a_{\beta,j}(x;h)(hD_x)^\beta c_\alpha(x;h)(hD_x)^\alpha \\ &\quad +h\sum_{\substack{|\alpha|\leq m-1\\ |\beta|\leq\mu}} a_{\beta,j}(x;h)(hD_x)^\beta\omega_{\alpha,j}(x;h)(hD_x)^\alpha. \end{aligned}$$

Moreover, by (H4) (and the fact that $U_j\boldsymbol{\omega} U_j^{-1}$ is symmetric), we know that c_α is scalar-valued, and $Q_0^{-1}\omega_{\alpha,j}$, $\omega_{\alpha,j}Q_0^{-1}$ are bounded operators on $\mathcal{H}$ (together with all their derivatives). Thus, it is clear that $h^{-1}U_j[\boldsymbol{\omega},A]U_j^{-1}$ is a PDO of degree $\leq \mu+m-1$, and the result follows. •

6 Construction of a Quasi-Invariant Subspace

Theorem 6.1 *Assume (H1)-(H4), and denote by* $\mathcal{U} := (U_j,\Omega_j)_{j=0,\cdots,r}$ *the regular unitary covering of* $L^2(I\!R^n;\mathcal{H})$ *constructed from the operators* U_j *and the open sets* Ω_j *defined in Section 2. Then, for any* $g\in C_0^\infty(I\!R)$*, there exists a* $\mathcal{U}$*-twisted* h*-admissible operator* Π_g *on* $L^2(I\!R^n;\mathcal{H})$*, such that* Π_g *is an orthogonal projection that verifies,*

$$\Pi_g = \tilde{\Pi}_0 + \mathcal{O}(h) \tag{6.1}$$

and, for any $f\in C_0^\infty(I\!R)$ *with* Supp $f\subset\{g=1\}$*, and any* $\ell\geq 0$*,*

$$\tilde{P}^\ell[f(\tilde{P}),\Pi_g] = \mathcal{O}(h^\infty). \tag{6.2}$$

Moreover, Π_g *is uniformly bounded as an operator :* $L^2(I\!R^n;\mathcal{H})\to L^2(I\!R^n;\mathcal{D}_Q)$ *and, for any* $\ell\geq 0$*, any* $N\geq 1$*, and any functions* $\chi_1,\cdots,\chi_N\in C_b^\infty(I\!R^n)$*, one has,*

$$\tilde{P}^\ell \mathrm{ad}_{\chi_1}\circ\cdots\circ\mathrm{ad}_{\chi_N}(\Pi_g) = \mathcal{O}(h^N). \tag{6.3}$$

Proof: We first perform a formal construction, by essentially following a procedure taken from [Ne1] (see also [BrNo] in the case $L = 1$). In the sequel, all the twisted PDO's that are involved are associated with the regular covering $\mathcal{U}$ constructed in Section 2, and we will omit to specify it all the time. We say that a twisted PDO is symmetric when it is formally selfadjoint with respect to the scalar product in $L^2(\mathbb{R}^n;\mathcal{H})$.

Since $\boldsymbol{Q} = \tilde{Q}(x) + \zeta(x)W(x)$ commutes with $\tilde{\Pi}_0$, we have,

$$[\tilde{P}, \tilde{\Pi}_0] = [\boldsymbol{\omega}, \tilde{\Pi}_0]. \tag{6.4}$$

Moreover, denoting by $\gamma(x)$ a complex oriented single loop surrounding the set $\{\tilde{\lambda}_{L'+1}(x), \dots, \tilde{\lambda}_{L'+L}(x)\}$ and leaving the rest of the spectrum of $\tilde{Q}(x)$ in its exterior, we have,

$$\tilde{\Pi}_0(x) = \frac{1}{2i\pi}\int_{\gamma(x)} (z - \tilde{Q}(x))^{-1} dz, \tag{6.5}$$

and thus, it results from Proposition 3.2 and assumption (H4) that $Q_0\tilde{\Pi}_0(x)$ is a $\mathcal{U}$-twisted PDO of degree 0. Therefore, applying Proposition 5.5, we immediately obtain,

$$[\tilde{P}, \tilde{\Pi}_0] = -ihS_0, \tag{6.6}$$

where S_0 is a symmetric twisted PDO (of degree $m-1$). Moreover, setting $\tilde{\Pi}_0^{\perp} := 1 - \tilde{\Pi}_0$, we observe that,

$$S_0 = \tilde{\Pi}_0 S_0 \tilde{\Pi}_0^{\perp} + \tilde{\Pi}_0^{\perp} S_0 \tilde{\Pi}_0. \tag{6.7}$$

Then, we set,

$$\tilde{\Pi}_1 := -\frac{1}{2\pi}\oint_{\gamma(x)} (z-\tilde{Q}(x))^{-1}\left[\tilde{\Pi}_0^{\perp}(x)S_0\tilde{\Pi}_0(x) - \tilde{\Pi}_0(x)S_0\tilde{\Pi}_0^{\perp}(x)\right](z-\tilde{Q}(x))^{-1}dz. \tag{6.8}$$

Thus, $\tilde{\Pi}_1$ is a symmetric $\mathcal{U}$-twisted PDO (of degree $m-1$), and is such that $Q_0\tilde{\Pi}_1$ is a twisted PDO, too. Therefore, using Proposition 5.5 again, we have,

$$[\tilde{P}, \tilde{\Pi}_1] = [\boldsymbol{Q}, \tilde{\Pi}_1] + hB,$$

where B is a twisted PDO (of degree $2(m-1)$). Then, using that $\tilde{Q}(x)(z - \tilde{Q}(x))^{-1} = (z - \tilde{Q}(x))^{-1}\tilde{Q}(x) = z(z - \tilde{Q}(x))^{-1} - 1$, one computes,

$$\begin{aligned}
[\tilde{Q}(x), \tilde{\Pi}_1] &= \frac{1}{2\pi}\oint_{\gamma(x)}\left[\tilde{\Pi}_0^{\perp}(x)S_0\tilde{\Pi}_0(x) - \tilde{\Pi}_0(x)S_0\tilde{\Pi}_0^{\perp}(x)\right](z - \tilde{Q}(x))^{-1}dz \\
&\quad -\frac{1}{2\pi}\oint_{\gamma(x)}(z - \tilde{Q}(x))^{-1}\left[\tilde{\Pi}_0^{\perp}(x)S_0\tilde{\Pi}_0(x) - \tilde{\Pi}_0(x)S_0\tilde{\Pi}_0^{\perp}(x)\right]dz \\
&= i\left[\tilde{\Pi}_0^{\perp}(x)S_0\tilde{\Pi}_0(x) - \tilde{\Pi}_0(x)S_0\tilde{\Pi}_0^{\perp}(x)\right]\tilde{\Pi}_0(x) \\
&\qquad -i\tilde{\Pi}_0(x)\left[\tilde{\Pi}_0^{\perp}(x)S_0\tilde{\Pi}_0(x) - \tilde{\Pi}_0(x)S_0\tilde{\Pi}_0^{\perp}(x)\right] \\
&= i(\tilde{\Pi}_0^{\perp}S_0\tilde{\Pi}_0 + \tilde{\Pi}_0 S_0\tilde{\Pi}_0^{\perp}),
\end{aligned}$$

that gives,

$$[\boldsymbol{Q}, \tilde{\Pi}_1] = i(\tilde{\Pi}_0^\perp S_0 \tilde{\Pi}_0 + \tilde{\Pi}_0 S_0 \tilde{\Pi}_0^\perp) + [\zeta W, \tilde{\Pi}_1], \tag{6.9}$$

and thus, using (6.7), one obtains,

$$[\tilde{P}, \tilde{\Pi}_1] = iS_0 - ihS_1, \tag{6.10}$$

where S_1 is a symmetric twisted PDO (of degree $2(m-1)$). Hence, setting,

$$\Pi^{(1)} := \tilde{\Pi}_0 + h\tilde{\Pi}_1,$$

we deduce from (6.6) and (6.10),

$$[\tilde{P}, \Pi^{(1)}] = -ih^2 S_1. \tag{6.11}$$

Moreover,

$$(\Pi^{(1)})^2 - \Pi^{(1)} = h(\tilde{\Pi}_0\tilde{\Pi}_1 + \tilde{\Pi}_1\tilde{\Pi}_0 - \tilde{\Pi}_1) + h^2\tilde{\Pi}_1^2 = h^2\tilde{\Pi}_1^2 =: h^2 T_1,$$

where T_1 is a symmetric twisted PDO (of degree $2(m-1)$), such that $Q_0 T_1$ is a twisted PDO, too.

Now, by induction on M, suppose that we have constructed a symmetric twisted PDO $\Pi^{(M)}$ as,

$$\Pi^{(M)} = \sum_{k=0}^{M} h^k \tilde{\Pi}_k,$$

where the $Q_0\tilde{\Pi}_k$'s are twisted PDO's, such that,

$$(\Pi^{(M)})^2 - \Pi^{(M)} = h^{M+1} T_M; \tag{6.12}$$

$$[\tilde{P}, \Pi^{(M)}] = -ih^{M+1} S_M, \tag{6.13}$$

with S_M and $Q_0 T_M$ twisted PDO's.

We set,

$$\Pi^{(M+1)} = \Pi^{(M)} + h^{M+1}\tilde{\Pi}_{M+1},$$

with,

$$\begin{aligned} \tilde{\Pi}_{M+1} \quad := \quad & -\frac{1}{2\pi}\oint_{\gamma(x)} (z - \tilde{Q}(x))^{-1}\left[\tilde{\Pi}_0^\perp S_M \tilde{\Pi}_0 - \tilde{\Pi}_0 S_M \tilde{\Pi}_0^\perp\right](z - \tilde{Q}(x))^{-1} dz \\ & + \tilde{\Pi}_0^\perp T_M \tilde{\Pi}_0^\perp - \tilde{\Pi}_0 T_M \tilde{\Pi}_0. \end{aligned} \tag{6.14}$$

Then, $\Pi^{(M+1)}$ is again a symmetric twisted PDO, and, using the induction assumption, we immediately see that $\tilde{Q}(x)\tilde{\Pi}_{M+1}$ (and thus also $Q_0\tilde{\Pi}_{M+1}$) is a twisted PDO. Moreover, since T_M and $\Pi^{(M)}$ commute, we have,

$$\Pi^{(M)} T_M (1 - \Pi^{(M)}) = (1 - \Pi^{(M)}) T_M \Pi^{(M)} = -h^{M+1} T_M^2,$$

and thus, since $\Pi^{(M)} = \tilde{\Pi}_0 + hR_M$ with $Q_0 R_M$ twisted PDO, we first obtain,

$$\tilde{\Pi}_0^\perp T_M \tilde{\Pi}_0 + \tilde{\Pi}_0 T_M \tilde{\Pi}_0^\perp = hR'_M, \tag{6.15}$$

with $Q_0 R'_M$ twisted PDO. On the other hand, one can check that,

$$\tilde{\Pi}_{M+1} - (\tilde{\Pi}_0 \tilde{\Pi}_{M+1} + \tilde{\Pi}_{M+1} \tilde{\Pi}_0) = \tilde{\Pi}_0 T_M \tilde{\Pi}_0 + \tilde{\Pi}_0^\perp T_M \tilde{\Pi}_0^\perp,$$

and thus, with (6.15),

$$\tilde{\Pi}_{M+1} - (\tilde{\Pi}_0 \tilde{\Pi}_{M+1} + \tilde{\Pi}_{M+1} \tilde{\Pi}_0) = T_M - hR'_M.$$

As a consequence, we obtain,

$$(\Pi^{(M+1)})^2 - \Pi^{(M+1)} = h^{M+2} T_{M+1}, \tag{6.16}$$

where $Q_0 T_{M+1}$ is a twisted PDO. Applying Proposition 5.5, we also have,

$$[\boldsymbol{\omega}, \tilde{\Pi}_{M+1}] = hR''_M,$$

with R''_M twisted PDO, and thus,

$$\begin{aligned} [\tilde{P}, \tilde{\Pi}_{M+1}] &= [\boldsymbol{Q}, \tilde{\Pi}_{M+1}] + hR''_M \\ &= i(\tilde{\Pi}_0 S_M \tilde{\Pi}_0^\perp + \tilde{\Pi}_0^\perp S_M \tilde{\Pi}_0) \\ &\qquad + \tilde{\Pi}_0^\perp [\boldsymbol{Q}, T_M] \tilde{\Pi}_0^\perp - \tilde{\Pi}_0 [\boldsymbol{Q}, T_M] \tilde{\Pi}_0 + hR_M^{(3)} \end{aligned} \tag{6.17}$$

with $R_M^{(3)}$ twisted PDO, and, using the hypothesis of induction (and, again, the twisted symbolic calculus),

$$\begin{aligned} &\tilde{\Pi}_0^\perp [\boldsymbol{Q}, T_M] \tilde{\Pi}_0^\perp \\ &\quad = \tilde{\Pi}_0^\perp [\tilde{P}, T_M] \tilde{\Pi}_0^\perp + hR_M^{(4)} \\ &\quad = h^{-(M+1)} \tilde{\Pi}_0^\perp [\tilde{P}, (\Pi^{(M)})^2 - \Pi^{(M)}] \tilde{\Pi}_0^\perp + hR_M^{(4)} \\ &\quad = h^{-(M+1)} \tilde{\Pi}_0^\perp ([\tilde{P}, \Pi^{(M)}] \Pi^{(M)} + \Pi^{(M)} [\tilde{P}, \Pi^{(M)}] - [\tilde{P}, \Pi^{(M)}]) \tilde{\Pi}_0^\perp + hR_M^{(4)} \\ &\quad = -i \tilde{\Pi}_0^\perp (S_M \Pi^{(M)} + \Pi^{(M)} S_M - S_M) \tilde{\Pi}_0^\perp + hR_M^{(4)} \\ &\quad = i \tilde{\Pi}_0^\perp S_M \tilde{\Pi}_0^\perp + hR_M^{(5)}, \end{aligned} \tag{6.18}$$

and, in the same way,

$$\tilde{\Pi}_0 [\boldsymbol{Q}, T_M] \tilde{\Pi}_0 = -i \tilde{\Pi}_0 S_M \tilde{\Pi}_0 + hR_M^{(6)}, \tag{6.19}$$

where the operators $R_M^{(k)}$'s are all twisted PDO's. Inserting (6.18)-(6.19) into (6.17), we finally obtain,

$$[\tilde{P}, \tilde{\Pi}_{M+1}] = iS_M + hR_M^{(7)},$$

that implies,

$$[\tilde{P}, \Pi^{(M+1)}] = -ih^{M+2} S_{M+1},$$

where S_{M+1} is a twisted PDO. Therefore, the induction is established.

From this point, we follow an idea of [So]. Let $g \in C_0^\infty(I\!R)$. Using Propositions 5.2 and 4.16, and writing $g(\tilde{P})\tilde{\Pi}_k = g(\tilde{P})(\tilde{P} + i)^N (\tilde{P} + i)^{-N} \tilde{\Pi}_k$, we see that the operators $g(\tilde{P})\tilde{\Pi}_k$ $(k \geq 0)$ are all twisted h-admissible operators. In particular, they are all bounded, uniformly with respect to h. Moreover, for any $\ell, \ell' \geq 0$, any $N \geq 1$, and any functions $\chi_1, \cdots, \chi_N \in C_b^\infty(\mathbb{R}^n)$, by construction, $h^{-N}\mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(\tilde{\Pi}_k)$ is a twisted PDO, and thus, by Propositions 5.2 and 4.16, $h^{-N}\tilde{P}^\ell g(\tilde{P})\mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(\tilde{\Pi}_k)\tilde{P}^{\ell'}$ is uniformly bounded. It is also easy to show (e.g., by using (6.24) hereafter) that,

$$\tilde{P}^\ell \mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(g(\tilde{P}))\tilde{P}^{\ell'} = \mathcal{O}(h^N), \tag{6.20}$$

and therefore, we obtain,

$$h^{-N}\tilde{P}^\ell \mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(g(\tilde{P})\tilde{\Pi}_k)\tilde{P}^{\ell'} = \mathcal{O}(1),$$

uniformly with respect to h. As a consequence, we can resum in a standard way the formal series of operators $\sum_{k=0}^\infty h^k g(\tilde{P})\tilde{\Pi}_k$ (see, e.g., [Ma2] Lemma 2.3.3), in such a way that, if we denote by $\Pi(g)$ such a resummation, we have,

$$\|\tilde{P}^\ell \mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(\Pi(g) - \sum_{k=0}^{M-1} h^k g(\tilde{P})\tilde{\Pi}_k)\tilde{P}^{\ell'}\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H}))} = \mathcal{O}(h^{M+N}), \tag{6.21}$$

for any $\ell, \ell' \geq 0$, $M, N \geq 0$ and any $\chi_1, \cdots, \chi_N \in C_b^\infty(\mathbb{R}^n)$ (with the conventions $\mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(\Pi(g)) = \Pi(g)$ if $N = 0$, and $\sum_{k=0}^{M-1} = 0$ if $M = 0$).

Then, we prove,

Lemma 6.2 *For any $\ell \geq 0$, one has,*

$$\|\tilde{P}^\ell(\Pi(g) - \Pi(g)^*)\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H}))} = \mathcal{O}(h^\infty). \tag{6.22}$$

Proof In view of (6.21), it is enough to show that, for any $M \geq 1$, one has,

$$(\tilde{P} + i)^\ell [g(\tilde{P}), \Pi^{(M)}] = \mathcal{O}(h^{M+1}). \tag{6.23}$$

For $N \geq 1$ large enough, we set $g_N(s) := g(s)(s+i)^N \in C_0^\infty(\mathbb{R})$, and we observe that,

$$g(\tilde{P}) = g_N(\tilde{P})(\tilde{P} + i)^{-N} = \frac{1}{\pi}\int \overline{\partial}\tilde{g}_N(z)(\tilde{P} - z)^{-1}(\tilde{P} + i)^{-N} dz\, d\bar{z}, \tag{6.24}$$

where $\tilde{g}_N$ is an almost analytic extension of g_N. Therefore, we obtain,

$$(\tilde{P} + i)^\ell [g(\tilde{P}), \Pi^{(M)}]$$

$$= \frac{1}{\pi}\int \overline{\partial}\tilde{g}_N(z)(\tilde{P}-z)^{-1}(\tilde{P}+i)^{\ell-N}[\Pi^{(M)}, (\tilde{P}-z)(\tilde{P}+i)^N](\tilde{P}-z)^{-1}(\tilde{P}+i)^{-N} dz\, d\bar{z}, \tag{6.25}$$

and it follows from (6.13) and the twisted PDO calculus, that,

$$[\Pi^{(M)}, (\tilde{P} - z)(\tilde{P} + i)^N] = h^{M+1}R_{M,N} \tag{6.26}$$

where $R_{M,N}$ is a twisted PDO of degree $\mu_M + mN$, with μ_M the degree of S_M. Therefore, if we choose N such that $2mN - m\ell \geq \mu_M + mN$, that is, $N \geq \ell + \mu_M/m$, then (6.25)-(6.26) and Proposition 5.2 tell us that $h^{-(M+1)}[g(\tilde{P}), \Pi^{(M)}]$ is a twisted h-admissible operator, and the result follows. •

We set,

$$\tilde{\Pi}_g := \Pi(g)+\Pi(g)^* - \frac{1}{2}(g(\tilde{P}))\Pi(g)^* + \Pi(g)g(\tilde{P})) + (1-g(\tilde{P}))\tilde{\Pi}_0(1-g(\tilde{P})). \quad (6.27)$$

Then, $\tilde{\Pi}_g$ is a selfadjoint twisted h-admissible operator, and since $\Pi(g) = g(\tilde{P})\tilde{\Pi}_0 + \mathcal{O}(h)$, we have,

$$\|\tilde{\Pi}_g - \tilde{\Pi}_0\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H}))} + \|\tilde{\Pi}_g^2 - \tilde{\Pi}_g\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H}))} = \mathcal{O}(h). \quad (6.28)$$

By construction, we also have $\tilde{P}^\ell(g(\tilde{P})\Pi(g)^* - \Pi(g)g(\tilde{P})) = \mathcal{O}(h^\infty)$ for all $\ell \geq 0$, and thus, by Lemma 6.2,

$$\tilde{P}^\ell\tilde{\Pi}_g = \tilde{P}^\ell\left[\Pi(g) + (1-g(\tilde{P}))\left(\Pi(g) + \tilde{\Pi}_0(1-g(\tilde{P}))\right)\right] + \mathcal{O}(h^\infty). \quad (6.29)$$

Moreover, if $f \in C_0^\infty(\mathbb{R})$ is such that $\mathrm{Supp}\, f \subset \{g = 1\}$, and if we denote by $\Pi(f)$ a resummation of the formal series $\sum_{k\geq 0} h^k f(\tilde{P})\tilde{\Pi}_k$ as before, since $f(\tilde{P})(1-g(\tilde{P})) = 0$, $f(\tilde{P})\Pi(g) - \Pi(f) = \mathcal{O}(h^\infty)$, and $\tilde{P}^\ell(1-g(\tilde{P})\Pi(g)f(\tilde{P}) = \tilde{P}^\ell(1-g(\tilde{P})\Pi(g)^*f(\tilde{P}) + \mathcal{O}(h^\infty) = \tilde{P}^\ell(1-g(\tilde{P})\Pi(f) + \mathcal{O}(h^\infty) = \mathcal{O}(h^\infty)$, we deduce from (6.29) and Lemma 6.2,

$$\tilde{P}^\ell[f(\tilde{P}), \tilde{\Pi}_g] = \tilde{P}^\ell\left(\Pi(f) - \Pi(g)^*f(\tilde{P})\right) + \mathcal{O}(h^\infty) = \tilde{P}^\ell\left(\Pi(f) - \Pi(f)^*\right) + \mathcal{O}(h^\infty),$$

and thus,

$$\|\tilde{P}^\ell[f(\tilde{P}), \tilde{\Pi}_g]\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H}))} = \mathcal{O}(h^\infty). \quad (6.30)$$

On the other hand, we deduce from Lemma 6.2 and (6.12),

$$\begin{aligned}
\tilde{P}^\ell(\Pi(g)^2 - \Pi(g^2)) &= \tilde{P}^\ell(\Pi(g)\Pi(g)^* - \Pi(g^2)) + \mathcal{O}(h^\infty) \\
&= \tilde{P}^\ell(\Pi(g)g(\tilde{P}) - \Pi(g^2)) + \mathcal{O}(h^\infty) \\
&= \mathcal{O}(h^\infty), \quad (6.31)
\end{aligned}$$

and thus, using (6.29)-(6.31),

$$\tilde{P}^\ell(\tilde{\Pi}_g^2 - \tilde{\Pi}_g)f(\tilde{P}) = \mathcal{O}(h^\infty). \quad (6.32)$$

Then, following the arguments of [Ne1, Ne2, NeSo, So], for h small enough we can define the following orthogonal projection:

$$\Pi_g := \frac{1}{2i\pi}\int_{|z-1|=\frac{1}{2}} (\tilde{\Pi}_g - z)^{-1}\, dz, \quad (6.33)$$

and it verifies (see [So], Formula (3.9), and [Ne1], Proposition 3),

$$\Pi_g - \tilde\Pi_g = \frac{1}{2i\pi}(\tilde\Pi_g^2 - \tilde\Pi_g)\int_{|z-1|=\frac12}(\tilde\Pi_g - z)^{-1}(2\tilde\Pi_g - 1)(1-\tilde\Pi_g - z)^{-1}(1-z)^{-1}\,dz. \tag{6.34}$$

In particular, we obtain from (6.32) and (6.34),

$$\tilde P^\ell(\Pi_g - \tilde\Pi_g)f(\tilde P) = \mathcal{O}(h^\infty), \tag{6.35}$$

and thus, we deduce from (6.28) and (6.30) that (6.1) and (6.2) hold.

In order to prove (6.3), we first observe that, by using (6.20), (6.21) and the fact that $\mathrm{ad}_{\chi_k}(\tilde\Pi_0) = 0$, we obtain,

$$\tilde P^\ell \mathrm{ad}_{\chi_1}\circ\cdots\circ\mathrm{ad}_{\chi_N}(\tilde\Pi_g) = \mathcal{O}(h^N), \tag{6.36}$$

for any $N \geq 1$. On the other hand, we have,

Lemma 6.3 *For any $\ell \geq 0$ and $z \in \mathbb{C}$ such that $|z-1| = 1/2$, the operator $\tilde P^\ell(\tilde\Pi_g - z)^{-1}(\tilde P + i)^{-\ell}$ is uniformly bounded on $L^2(\mathbb{R}^n;\mathcal{H})$.*

Proof Writing, for $\ell > 0$,

$$\begin{aligned} H_\ell : &= (\tilde P + i)^\ell(\tilde\Pi_g - z)^{-1}(\tilde P + i)^{-\ell} \\ &= H_{\ell-1} + (\tilde P + i)^{\ell-1}[\tilde P, (\tilde\Pi_g - z)^{-1}](\tilde P + i)^{-\ell} \\ &= H_{\ell-1} + H_{\ell-1}(\tilde P + i)^{\ell-1}[\tilde\Pi_g, \tilde P](\tilde P + i)^{-\ell}H_\ell, \end{aligned}$$

and performing an easy induction, we see that it is enough to prove that $(\tilde P + i)^{\ell-1}[\tilde\Pi_g, \tilde P](\tilde P + i)^{-\ell}$ is $\mathcal{O}(h)$. Due to (6.29), it is enough to study the two terms $(\tilde P + i)^{\ell-1}[\tilde\Pi(g), \tilde P](\tilde P + i)^{-\ell}$ and $(\tilde P + i)^{\ell-1}[\tilde\Pi_0, \tilde P](\tilde P + i)^{-\ell}$. By (6.13), the first one is $\mathcal{O}(h^\infty)$, while the second one is equal to $(\tilde P + i)^{\ell-1}[\tilde\Pi_0, \boldsymbol{\omega}](\tilde P + i)^{-\ell}$ and thus, by Propositions 5.5 and 5.2, is $\mathcal{O}(h)$. •

Combining (6.36), (6.33) and Lemma 6.3, we easily obtain (6.3), and this completes the proof of Theorem 6.1. •

Remark 6.4 *Observe that the previous proof also provides a way of computing the full symbol of $\tilde\Pi_g$ (and thus of Π_g, too) up to $\mathcal{O}(h^M)$, for any $M \geq 1$. Indeed, formulas (6.12), (6.13), and (6.14) permit to do it inductively.*

Remark 6.5 *For this proof, we did not succeed in adapting the elegant argument of [Sj2] (as this was done for smooth interactions in [So]), because of a technical problem. Namely, this argument involves a translation in the spectral variable z, of the type $z \mapsto z + \omega(x,\xi)$, inside the symbol of the resolvent of $\tilde P$. In our case, this would have led to consider a symbol $\tilde a = (\tilde a_j)_{0\leq j\leq r}$ of the type $\tilde a_j = a_j(x,\xi,z+\omega_j(x,\xi))$, where ω_j is the symbol of $U_j\boldsymbol{\omega}U_j^{-1}$ and $a(x,\xi,z) = (a_j(x,\xi,z))_{0\leq j\leq r}$ is the symbol of $(z-\tilde P)^{-1}$. But then, it is not clear to us (and probably may be wrong) that the compatibility conditions (4.9) are verified by $\tilde a$, and this prevents us from quantizing it in order to continue the argument.*

7 Decomposition of the Evolution for the Modified Operator

In this section we prove a general result on the quantum evolution of $\tilde{P}$.

Theorem 7.1 *Under the same assumtions as for Theorem 6.1, let $g \in C_0^\infty(I\!R)$. Then, one has the following results:*
1) Let $\varphi_0 \in L^2(I\!R^n; \mathcal{H})$ verifying,

$$\varphi_0 = f(\tilde{P})\varphi_0, \tag{7.1}$$

for some $f \in C_0^\infty(I\!R)$ such that $\operatorname{Supp} f \subset \{g = 1\}$. Then, with the projection Π_g constructed in Theorem 6.1, one has,

$$e^{-it\tilde{P}/h}\varphi_0 = e^{-it\tilde{P}^{(1)}/h}\Pi_g\varphi_0 + e^{-it\tilde{P}^{(2)}/h}(1-\Pi_g)\varphi_0 + \mathcal{O}(|t|h^\infty\|\varphi_0\|) \tag{7.2}$$

uniformly with respect to h small enough, $t \in I\!R$ and φ_0 verifying (7.1), with,

$$\tilde{P}^{(1)} := \Pi_g\tilde{P}\Pi_g \quad ; \quad \tilde{P}^{(2)} := (1-\Pi_g)\tilde{P}(1-\Pi_g).$$

2) Let $\varphi_0 \in L^2(I\!R^n; \mathcal{H})$ (possibly h-dependent) verifying $\|\varphi_0\| = 1$, and,

$$\varphi_0 = f(\tilde{P})\varphi_0 + \mathcal{O}(h^\infty), \tag{7.3}$$

for some $f \in C_0^\infty(I\!R)$ such that $\operatorname{Supp} f \subset \{g = 1\}$. Then, one has,

$$e^{-it\tilde{P}/h}\varphi_0 = e^{-it\tilde{P}^{(1)}/h}\Pi_g\varphi_0 + e^{-it\tilde{P}^{(2)}/h}(1-\Pi_g)\varphi_0 + \mathcal{O}(\langle t\rangle h^\infty) \tag{7.4}$$

uniformly with respect to h small enough and $t \in I\!R$.
3) There exists a bounded operator $\mathcal{W} : L^2(I\!R^n; \mathcal{H}) \to L^2(I\!R^n)^{\oplus L}$ with the following properties:

- *For any $j \in \{0, 1, \dots, r\}$, and any $\varphi_j \in C_d^\infty(\Omega_j)$, the operator $\mathcal{W}_j := \mathcal{W}U_j^{-1}\varphi_j$ is an h-admissible operator from $L^2(I\!R^n; \mathcal{H})$ to $L^2(I\!R^n)^{\oplus L}$;*
- *$\mathcal{W}\mathcal{W}^* = 1$ and $\mathcal{W}^*\mathcal{W} = \Pi_g$;*
- *The operator $A := \mathcal{W}\tilde{P}\mathcal{W}^* = \mathcal{W}\tilde{P}^{(1)}\mathcal{W}^*$ is an h-admissible operator on $L^2(I\!R^n)^{\oplus L}$ with domain $H^m(I\!R^n)^{\oplus L}$, and its symbol $a(x,\xi;h)$ verifies,*

  $$a(x,\xi;h) = \omega(x,\xi;h)\mathbf{I}_L + \mathcal{M}(x) + \zeta(x)W(x)\mathbf{I}_L + hr(x,\xi;h)$$

  where $\mathcal{M}(x)$ is a $L \times L$ matrix depending smoothly on x, with spectrum $\{\tilde{\lambda}_{L'+1}(x), \dots, \tilde{\lambda}_{L'+L}(x)\}$, and $r(x,\xi : h)$ verifies,

  $$\partial^\alpha r(x,\xi;h) = \mathcal{O}(\langle\xi\rangle^{m-1})$$

  for any multi-index α and uniformly with respect to $(x,\xi) \in T^*I\!R^n$ and $h > 0$ small enough.

In particular, $\mathcal{W}\big|_{\mathrm{Ran}\,\Pi_g} : \mathrm{Ran}\,\Pi_g \to L^2(\mathbb{R}^n)^{\oplus L}$ *is unitary, and* $e^{-it\tilde{P}^{(1)}/h}\Pi_g = \mathcal{W}^* e^{-itA/h}\mathcal{W}\Pi_g = \mathcal{W}^* e^{-itA/h}\mathcal{W}$ *for all* $t \in \mathbb{R}$*.*

Remark 7.2 *In Section 10, we give a way of computing easily the expansion of* A *up to any power of* h*. As an example, we compute explicitly its first three terms (that is, up to* $\mathcal{O}(h^4)$*).*

Proof 1) Setting $\varphi := e^{-it\tilde{P}/h}\varphi_0$, we have $f(\tilde{P})\varphi = \varphi$, and thus

$$ih\partial_t \Pi_g \varphi = \Pi_g \tilde{P} f(\tilde{P})\varphi = \Pi_g^2 \tilde{P} f(\tilde{P})\varphi. \tag{7.5}$$

Moreover, writing $[\Pi_g, \tilde{P}]f(\tilde{P}) = [\Pi_g, \tilde{P}f(\tilde{P})] + \tilde{P}[f(\tilde{P}), \Pi_g]$, Theorem 6.1 tells us that $\|[\Pi_g, \tilde{P}]f(\tilde{P})\| = \mathcal{O}(h^\infty)$. Therefore, we obtain from (7.5),

$$ih\partial_t \Pi_g \varphi = \Pi_g \tilde{P}\Pi_g f(\tilde{P})\varphi + \mathcal{O}(h^\infty\|\varphi\|) = \tilde{P}^{(1)}\Pi_g\varphi + \mathcal{O}(h^\infty\|\varphi_0\|),$$

uniformly with respect to h and t. This equation can be re-written as,

$$ih\partial_t (e^{it\tilde{P}^{(1)}/h}\Pi_g\varphi) = \mathcal{O}(h^\infty\|\varphi_0\|),$$

and thus, integrating from 0 to t, we obtain,

$$\Pi_g\varphi = e^{-it\tilde{P}^{(1)}/h}\Pi_g\varphi_0 + \mathcal{O}(|t|h^\infty\|\varphi_0\|),$$

uniformly with respect to h, t and φ_0.

Reasoning in the same way with $1 - \Pi_g$ instead of Π_g, we also obtain,

$$(1-\Pi_g)\varphi = e^{-it\tilde{P}^{(2)}/h}(1-\Pi_g)\varphi_0 + \mathcal{O}(|t|h^\infty\|\varphi_0\|),$$

and (7.2) follows.

2) Formula (7.4) follows exactly in the same way.

3) Since $\Pi_g - \tilde{\Pi}_0 = \mathcal{O}(h)$, for h small enough we can consider the operator $\mathcal{V}$ defined by the Nagy formula,

$$\mathcal{V} = \left(\tilde{\Pi}_0\Pi_g + (1-\tilde{\Pi}_0)(1-\Pi_g)\right)\left(1 - (\Pi_g - \tilde{\Pi}_0)^2\right)^{-1/2}. \tag{7.6}$$

Then, $\mathcal{V}$ is a twisted h-admissible operator, it differs from the identity by $\mathcal{O}(h)$, and standard computations (using that $(\Pi_g - \tilde{\Pi}_0)^2$ commutes with both $\tilde{\Pi}_0\Pi_g$ and $(1-\tilde{\Pi}_0)(1-\Pi_g)$: see, e.g., [Ka] Chap.I.4) show that,

$$\mathcal{V}^*\mathcal{V} = \mathcal{V}\mathcal{V}^* = 1 \quad \text{and} \quad \tilde{\Pi}_0\mathcal{V} = \mathcal{V}\Pi_g.$$

Now, with $\tilde{u}_k$ as in Lemma 3.1, we define $Z_L : L^2(\mathbb{R}^n;\mathcal{H}) \to L^2(\mathbb{R}^n)^{\oplus L}$ by,

$$Z_L\psi(x) = \bigoplus_{k=L'+1}^{L'+L} \langle \psi(x), \tilde{u}_k(x)\rangle_{\mathcal{H}},$$

and we set,

$$\mathcal{W} := Z_L \circ \mathcal{V} = Z_L + \mathcal{O}(h). \tag{7.7}$$

Thanks to the properties of $\mathcal{V}$, we see that $\mathcal{W}\Pi_g = \mathcal{W}$, and, since $Z_L^* Z_L = \tilde{\Pi}_0$ and $Z_L Z_L^* = 1$, we also obtain:

$$\mathcal{W}^*\mathcal{W} = \mathcal{V}^*\tilde{\Pi}_0\mathcal{V} = \Pi_g \ ; \ \mathcal{W}\mathcal{W}^* = 1.$$

Moreover, for any $\varphi_j, \chi_j \in C_d^\infty(\Omega_j)$ such that $\chi_j = 1$ near $\operatorname{Supp}\varphi_j$, and for any $\psi \in L^2(I\!\!R^n;\mathcal{H})$, we have,

$$\mathcal{W}U_j^{-1}\varphi_j\psi(x) = \bigoplus_{k=L'+1}^{L'+L} \langle \mathcal{V}_j\psi(x), \tilde{u}_{k,j}(x)\rangle_{\mathcal{H}},$$

with $\mathcal{V}_j := U_j\chi_j\mathcal{V}U_j^{-1}\varphi_j$ and $\tilde{u}_{k,j}(x) := U_j(x)\tilde{u}_k(x) \in C^\infty(\Omega_j,\mathcal{H})$. Therefore, $\mathcal{W}U_j^{-1}\varphi_j$ is an h-admissible operator from $L^2(I\!\!R^n;\mathcal{H})$ to $L^2(I\!\!R^n)^{\oplus L}$, and the first two properties stated on $\mathcal{W}$ are proved. (Actually, one can easily see that $\mathcal{W}$ also verifies a property analog to the first one in Proposition 4.6, and thus, with an obvious extension of the notion of twisted operator, that $\mathcal{W}$ is, indeed, a twisted h-admissible operator from $L^2(I\!\!R^n;\mathcal{H})$ to $L^2(I\!\!R^n)^{\oplus L}$.)

Then, defining

$$A := \mathcal{W}\tilde{P}\mathcal{W}^* = \mathcal{W}\tilde{P}^{(1)}\mathcal{W}^*, \tag{7.8}$$

we want to prove that A is an h-admissible operator and study its symbol. We first need the following result:

Lemma 7.3 *For any $\ell \geq 0$, any $N \geq 1$ and any $\chi_1, \cdots, \chi_N \in C_b^\infty(I\!\!R^n)$, one has,*

$$\|\tilde{P}^\ell \mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(\mathcal{W}^*)\|_{\mathcal{L}(L^2(I\!\!R^n);L^2(I\!\!R^n;\mathcal{H})} = \mathcal{O}(h^N). \tag{7.9}$$

Proof Since $\mathcal{W}^* = \mathcal{V}^* Z_L^*$ and Z_L^* commutes with the multiplication by any function of x, it is enough to prove,

$$\tilde{P}^\ell \mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(\mathcal{V}^*) = \mathcal{O}(h^N),$$

on $L^2(I\!\!R^n;\mathcal{H})$. Moreover, using (6.3) and and the fact that $\tilde{\Pi}_0$ commutes with the multiplication by any function of x, too, we see on (7.6) that it is enough to show that,

$$(\tilde{P}+i)^\ell(1-(\Pi_g-\tilde{\Pi}_0)^2)^{-1/2}(\tilde{P}+i)^{-\ell} = \mathcal{O}(1); \tag{7.10}$$

$$\tilde{P}^\ell \mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}\left((1-(\Pi_g-\tilde{\Pi}_0)^2)^{-1/2}\right) = \mathcal{O}(h^N). \tag{7.11}$$

By construction, we have $\tilde{P}^\ell(\Pi(g)-g(\tilde{P})\tilde{\Pi}_0) = \mathcal{O}(h)$, and thus, we immediately see on (6.29) that $\tilde{P}^\ell(\tilde{\Pi}_g - \tilde{\Pi}_0) = \mathcal{O}(h)$. Then, writing

$$\Pi_g - \tilde{\Pi}_0 = \frac{1}{2i\pi}\int_{|z-1|=\frac{1}{2}} (\tilde{\Pi}_g - z)^{-1}(\tilde{\Pi}_0 - \tilde{\Pi}_g)(\tilde{\Pi}_0 - z)^{-1}\, dz,$$

and using Lemma 6.3, we also obtain,

$$\tilde{P}^\ell(\Pi_g - \tilde{\Pi}_0) = \mathcal{O}(h), \tag{7.12}$$

for all $\ell \geq 0$. In particular, $(\tilde{P}+i)^\ell(\Pi_g - \tilde{\Pi}_0)(\tilde{P}+i)^{-\ell} = \mathcal{O}(h)$, and therefore, for h sufficiently small, we can write,

$$(\tilde{P}+i)^\ell(1-(\Pi_g-\tilde{\Pi}_0)^2)^{-1/2}(\tilde{P}+i)^{-\ell} = \Big(1 - [(\tilde{P}+i)^\ell(\Pi_g - \tilde{\Pi}_0)(\tilde{P}+i)^{-\ell}]^2\Big)^{-1/2},$$

and (7.10) follows.

To prove (7.11), we write $(1-(\Pi_g - \tilde{\Pi}_0)^2)^{-1/2}$ as,

$$(1-(\Pi_g - \tilde{\Pi}_0)^2)^{-1/2} = 1 + \sum_{k=1}^{\infty} \alpha_k (\Pi_g - \tilde{\Pi}_0)^k,$$

where the radius of convergence of the power series $\sum_{k=1}^\infty \alpha_k z^k$ is 1. Thus,

$$\tilde{P}^\ell \mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N} \Big((1-(\Pi_g - \tilde{\Pi}_0)^2)^{-1/2}\Big) = \sum_{k=1}^{\infty} \alpha_k \mathcal{A}_{N,k}$$

where $\mathcal{A}_{N,k} := \tilde{P}^\ell \mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}((\Pi_g - \tilde{\Pi}_0)^k)$ is the sum of k^N terms of the form,

$$\tilde{P}^\ell[\mathrm{ad}_{\chi_{i_{1,1}}} \cdots \mathrm{ad}_{\chi_{i_{1,n_1}}}(\Pi_g - \tilde{\Pi}_0)] \dots [\mathrm{ad}_{\chi_{i_{k,1}}} \cdots \mathrm{ad}_{\chi_{i_{k,n_k}}}(\Pi_g - \tilde{\Pi}_0)],$$

with $n_1, \dots, n_k \geq 0$, $n_1 + \ldots + n_k = N$. Then, using (6.21) together with (7.12), we see that all these terms have a norm bounded by $(C_N)^k h^{k+N}$, for some constant $C_N > 0$ independent of k. Therefore, $\|\mathcal{A}_{N,k}\| \leq k^N (C_N)^k h^{k+N}$, and (7.11) follows. •

Then, proceeding as in the proof of Lemma 4.11, we deduce from Lemma 7.9 that, if $\chi, \psi \in C_b^\infty(\mathbb{R}^n)$ are such that $\mathrm{dist}(\mathrm{Supp}\,\chi, \mathrm{Supp}\,\psi) > 0$, then $\|\tilde{P}^\ell \chi \mathcal{W}^* \psi\| = \mathcal{O}(h^\infty)$. As a consequence, taking a partition of unity $(\chi_j)_{j=0,\dots,r}$ on $\mathbb{R}^n$ with $\chi_j \in C_d^\infty(\Omega_j)$, and choosing $\varphi_j \in C_d^\infty(\Omega_j)$ such that $\mathrm{dist}(\mathrm{Supp}\,(\varphi_j - 1), \mathrm{Supp}\,\chi_j) > 0$ $(j = 0, \dots, r)$, we have (using also that $\tilde{P}$ is local in the variable x),

$$A = \sum_{j=0}^{r} \mathcal{W}\chi_j \tilde{P} \mathcal{W}^* = \sum_{j=0}^{r} \varphi_j \mathcal{W} \chi_j \tilde{P} \varphi_j^2 \mathcal{W}^* \varphi_j + R(h),$$

with $\|R(h)\|_{\mathcal{L}(L^2(\mathbb{R}^n))} = \mathcal{O}(h^\infty)$. Thus,

$$A = \sum_{j=0}^{r} \varphi_j \mathcal{W} U_j^{-1} \chi_j \tilde{P}_j U_j \varphi_j \mathcal{W}^* \varphi_j + R(h),$$

where $\tilde{P}_j = U_j \tilde{P} U_j^{-1} \varphi_j$ is an h-admissible (differential) operator from $H^m(\mathbb{R}^n; \mathcal{D}_Q)$ to $L^2(\mathbb{R}^n; \mathcal{H})$, while $U_j \varphi_j \mathcal{W}^* \varphi_j$ is an h-admissible operator from

$H^m(\mathbb{R}^n)^{\oplus L}$ to $H^m(\mathbb{R}^n;\mathcal{D}_Q)$ and $\varphi_j\mathcal{W}U_j^{-1}\chi_j$ is an h-admissible operator from $L^2(\mathbb{R}^n;\mathcal{H})$ to $L^2(\mathbb{R}^n)^{\oplus L}$. Therefore, A is an h-admissible operator from $H^m(\mathbb{R}^n)^{\oplus L}$ to $L^2(\mathbb{R}^n)^{\oplus L}$, and, if we set,

$$\tilde{p}_j(x,\xi;h)=\omega(x,\xi;h)+\tilde{Q}_j(x)+\zeta(x)W(x)+h\sum_{|\beta|\leq m-1}\omega_{\beta,j}(x;h)\xi^\beta,$$

and if we denote by $v_j(x,\xi)$ (resp. $v_j^*(x,\xi)$) the symbol of $U_j\mathcal{V}U_j^{-1}$) (resp. $U_j\mathcal{V}U_j^{-1}$), then, the (matrix) symbol $a=(a_{k,\ell})_{1\leq k,\ell\leq L}$ of A, is given by,

$$a_{k,\ell}(x,\xi,h)=\sum_{j=0}^r\langle\chi_j(x)v_j(x,\xi)\sharp\tilde{p}_j(x,\xi)\sharp v_j^*(x,\xi)\sharp\tilde{u}_{L'+k,j}(x),\tilde{u}_{L'+\ell,j}(x)\rangle_{\mathcal{H}}.$$

In particular, since $\partial^\alpha(v_j-1)$ and $\partial^\alpha(v_j^*-1)$ are $\mathcal{O}(h)$, we obtain,

$$a_{k,\ell}(x,\xi,h)=\sum_{j=0}^r\langle\chi_j(x)(\omega(x,\xi)+\tilde{Q}_j(x)+\zeta(x)W(x))\tilde{u}_{L'+k,j}(x),\tilde{u}_{L'+\ell,j}(x)\rangle_{\mathcal{H}}+r_{k,\ell}(h)$$

with $\partial^\alpha r_{k,\ell}(h)=\mathcal{O}(h\langle\xi\rangle^{m-1})$, and thus, using the fact that

$$\langle\tilde{Q}_j(x)\tilde{u}_{L'+k,j}(x),\tilde{u}_{L'+\ell,j}(x)\rangle=\varphi_j(x)\langle\tilde{Q}(x)\tilde{u}_{L'+k}(x),\tilde{u}_{L'+\ell}(x)\rangle,$$

this finally gives,

$$\begin{aligned}a_{k,\ell}(x,\xi,h)&=\sum_{j=0}^r\chi_j(x)(\omega(x,\xi)\delta_{k,\ell}+m_{k,\ell}(x)+\zeta(x)W(x)\delta_{k,\ell})+r_{k,\ell}(h)\\&=(\omega(x,\xi)+\zeta(x)W(x))\delta_{k,\ell}+m_{k,\ell}(x)+r_{k,\ell}(h),\end{aligned}$$

with $m_{k,\ell}(x):=\langle\tilde{Q}(x)\tilde{u}_{L'+k}(x),\tilde{u}_{L'+\ell}(x)\rangle$. This completes the proof of Theorem 7.1. •

8 Proof of Theorem 2.1

In view of Theorem 7.1, it is enough to prove,

Theorem 8.1 *Let $\varphi_0\in L^2(\mathbb{R}^n;\mathcal{H})$ such that $\|\varphi_0\|=1$, and,*

$$\|\varphi_0\|_{L^2(K_0^c;\mathcal{H})}+\|(1-\Pi_g)\varphi_0\|+\|(1-f(P))\varphi_0\|=\mathcal{O}(h^\infty),\tag{8.1}$$

for some $K_0\subset\subset\Omega'\subset\subset\Omega$, $f,g\in C_0^\infty(\mathbb{R})$, $gf=f$, and let $\tilde{P}$ be the operator constructed in Section 2 with $K=\overline{\Omega'}$, and Π_g be the projection constructed in Theorem 6.1. Then, with the notations of Theorem 7.1, we have,

$$e^{-itP/h}\varphi_0=\mathcal{W}^*e^{-itA/h}\mathcal{W}\varphi_0+\mathcal{O}\left(\langle t\rangle h^\infty\right),\tag{8.2}$$

uniformly with respect to $h>0$ small enough and $t\in[0,T_{\Omega'}(\varphi_0))$.

Proof : Denote by $\chi \in C_0^\infty(\Omega'_K)$ (where Ω'_K is the same as in Proposition 3.2) a cutoff function such that $\chi = 1$ on K. We first prove,

Lemma 8.2

$$\|(f(P) - f(\tilde{P}))\chi\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H})} = \mathcal{O}(h^\infty).$$

Proof Using (4.8), we obtain,

$$(f(P) - f(\tilde{P}))\chi = \frac{1}{\pi}\int \overline{\partial}\tilde{f}(z)(P-z)^{-1}(\tilde{P}-P)(\tilde{P}-z)^{-1}\chi dz\, d\bar{z}.$$

Moreover, if $\psi \in C_0^\infty(\Omega'_K)$ is such that $\psi = 1$ on a neighborhood of $\operatorname{Supp}\chi$, Corollary 4.15 and Lemma 4.11 tell us,

$$(\psi - 1)(\tilde{P}-z)^{-1}\chi = \mathcal{O}(h^N|\operatorname{Im} z|^{-(N+1)}),$$

for any $N \geq 1$. As a consequence,

$$(f(P) - f(\tilde{P}))\chi = \frac{1}{\pi}\int \overline{\partial}\tilde{f}(z)(P-z)^{-1}(\tilde{P}-P)\psi(\tilde{P}-z)^{-1}\chi dz\, d\bar{z} + \mathcal{O}(h^\infty),$$

and since $(\tilde{P}-P)\psi = (\tilde{Q}-Q)\psi = 0$, the result follows. •

Now, by (8.1), we have,

$$\varphi_0 = f(P)\varphi_0 + \mathcal{O}(h^\infty) = f(P)\chi\varphi_0 + \mathcal{O}(h^\infty),$$

and thus, by Lemma 8.2,

$$\varphi_0 = f(\tilde{P})\chi\varphi_0 + \mathcal{O}(h^\infty) = f(\tilde{P})\varphi_0 + \mathcal{O}(h^\infty).$$

This means that (7.3) is satisfied, and thus, by Theorem 7.1, the decomposition (7.4) is true. Using (8.1) again, this gives,

$$e^{-it\tilde{P}/h}\varphi_0 = e^{-it\tilde{P}^{(1)}/h}\Pi_g\varphi_0 + \mathcal{O}(|t|h^\infty) = \mathcal{W}^* e^{-itA/h}\mathcal{W}\varphi_0 + \mathcal{O}(\langle t\rangle h^\infty), \quad (8.3)$$

uniformly with respect to h and t.

On the other hand, if we set $\varphi(t) := e^{-itP/h}\varphi_0$, then, by assumption, $\varphi(t) = f(P)\varphi(t) + \mathcal{O}(h^\infty)$ and $\varphi(t) = \chi\varphi(t) + \mathcal{O}(h^\infty)$ uniformly for $t \in [0, T_{\Omega'}(\varphi_0)]$. Therefore, applying Lemma 8.2 again, we obtain as before, $\varphi(t) = f(\tilde{P})\varphi(t) + \mathcal{O}(h^\infty)$, and thus also,

$$\varphi(t) = f(\tilde{P})\chi\varphi(t) + \mathcal{O}(h^\infty), \quad (8.4)$$

uniformly with respect to h and $t \in [0, T_{\Omega'}(\varphi_0)]$. Moreover, since P and $\tilde{P}$ coincide on the support of χ, we can write,

$$ih\partial_t f(\tilde{P})\chi\varphi(t) = f(\tilde{P})\chi P\varphi(t) = f(\tilde{P})\tilde{P}\chi\varphi(t) + f(\tilde{P})[\chi, \tilde{P}]\varphi(t),$$

and thus, since $f(\tilde{P})[\chi, \tilde{P}] = f(\tilde{P})[\chi, \boldsymbol{\omega}]$ is bounded, and $[\chi, \boldsymbol{\omega}]$ is a differential operator with coefficients supported in $\operatorname{Supp}\nabla\chi$ (where φ is $\mathcal{O}(h^\infty)$), we obtain,

$$ih\partial_t f(\tilde{P})\chi\varphi(t) = f(\tilde{P})\chi P\varphi(t) = \tilde{P}f(\tilde{P})\chi\varphi(t) + \mathcal{O}(h^\infty).$$

As a consequence,

$$f(\tilde{P})\chi\varphi(t) = e^{-it\tilde{P}/h} f(\tilde{P})\chi\varphi_0 + \mathcal{O}(|t|h^\infty),$$

and therefore, by (8.4),

$$\varphi(t) = e^{-it\tilde{P}/h}\varphi_0 + \mathcal{O}(\langle t\rangle h^\infty), \tag{8.5}$$

uniformly with respect to h and $t \in [0, T_{\Omega'}(\varphi_0))$. Then, Theorem 8.1 follows from (8.3) and (8.5). •

9 Proof of Corollary 2.6

First of all, let us recall the (standard) notion of frequency set $FS(v)$ of some (possibly h-dependent) $v \in L^2_{\rm loc}(\Omega)$ (see, e.g., [Ma2] and references therein). It is said that a point $(x_0, \xi_0) \in T^*\Omega$ is not in $FS(v)$ if there exist $\chi_1 \in C_0^\infty(\omega)$ and $\chi_2 \in C_0^\infty(I\!R^n)$ such that $\chi_1(x_0) = \chi_2(\xi_0) = 1$ and $\Vert\chi_2(hD_x)\chi_1 v\Vert_{L^2(I\!R^n)} = \mathcal{O}(h^\infty)$. This is also equivalent to say that there exists an open neighborhood $\mathcal{N}$ of (x_0, ξ_0) in $T^*I\!R^n$, such that, for *any* $\chi \in C_0^\infty(\mathcal{N})$ and any $\chi_1 \in C_0^\infty(\Omega)$, one has $\Vert{\rm Op}_h(\chi)\chi_1 v\Vert_{L^2(I\!R^n)} = \mathcal{O}(h^\infty)$.

As one can see, this notion can be extended in an obvious way to functions in $L^2_{\rm loc}(\Omega; \mathcal{H})$, and it is easy to see (e.g., as in [Ma2] Section 2.9) that the latter property still holds with operator-valued functions $\chi \in C_0^\infty(\mathcal{N}; \mathcal{L}(\mathcal{H}))$, or even more generally, $\chi \in C_0^\infty(\mathcal{N}; \mathcal{L}(\mathcal{H}; \mathcal{H}'))$ where $\mathcal{H}'$ is an arbitrary Hilbert-space.

We first prove,

Lemma 9.1 *Let $\mathcal{W} : L^2(I\!R^n; \mathcal{H}) \to L^2(I\!R^n)$ be the operator given in Theorem 7.1. Then, for any $j \in \{0, 1, \dots, r\}$, any $\varphi \in L^2(I\!R^n; \mathcal{H})$ and $v \in L^2(I\!R^n)$, such that $\Vert\varphi\Vert = \Vert v\Vert = 1$, one has,*

$$FS(\mathcal{W}\varphi) \cap T^*\Omega_j = FS(U_j\Pi_g\varphi) \cap T^*\Omega_j;$$
$$FS(U_j\mathcal{W}^*v) \cap T^*\Omega_j = FS(v) \cap T^*\Omega_j.$$

Proof Since $\mathcal{W}\mathcal{W}^* = 1$ and $\mathcal{W}^*\mathcal{W} = \Pi_g$, it is enough to prove the two inclusions $FS(\mathcal{W}\varphi) \cap T^*\Omega_j \subset FS(U_j\Pi_g\varphi) \cap T^*\Omega_j$ and $FS(U_j\mathcal{W}^*v) \cap T^*\Omega_j \subset FS(v) \cap T^*\Omega_j$.

Therefore, let $(x_0, \xi_0) \in T^*\Omega_j$, and assume first that $(x_0, \xi_0) \notin FS(U_j\Pi_g\varphi)$. In particular, this implies that, if $\mathcal{N} \subset\subset T^*\Omega_j$ is a small enough neighborhood of (x_0, ξ_0), then $\Vert{\rm Op}_h(\chi_1)U_j\Pi_g\varphi\Vert = \mathcal{O}(h^\infty)$ for all $\chi_1 \in C_0^\infty(\mathcal{N}; \mathcal{L}(\mathcal{H}; I\!\!\!C))$. Then, taking $\chi \in C_0^\infty(\mathcal{N})$ and $\psi_j \in C_0^\infty(\Omega_j)$ such that $\psi_j(x) = 1$ near $\pi_x(\,{\rm Supp}\,\chi)$ and $\chi(x_0, \xi_0) = 1$, we write,

$$\begin{aligned} {\rm Op}_h(\chi)\mathcal{W}\varphi &= {\rm Op}_h(\chi)\mathcal{W}\Pi_g\varphi = {\rm Op}_h(\chi)\mathcal{W}\psi_j^2\Pi_g\varphi + \mathcal{O}(h^\infty) \\ &= {\rm Op}_h(\chi)\mathcal{W}U_j^{-1}\psi_j U_j\psi_j\Pi_g\varphi + \mathcal{O}(h^\infty), \end{aligned}$$

and since ${\rm Op}_h(\chi)\mathcal{W}U_j^{-1}\psi_j$ is an h-admissible operator from $L^2(I\!R^n; \mathcal{H})$ to $L^2(I\!R^n)$, with symbol supported in $\mathcal{N}$ (that is, modulo $\mathcal{O}(h^\infty)$ in $C_b^\infty(I\!R^n; \mathcal{L}(\mathcal{H}; I\!\!\!C)))$, we obtain $\Vert{\rm Op}_h(\chi)\mathcal{W}\varphi\Vert = \mathcal{O}(h^\infty)$, and thus $(x_0, \xi_0) \notin FS(\mathcal{W}\varphi)$.

Now, assume that $(x_0, \xi_0) \notin FS(v)$. Since $U_j \psi_j \mathcal{W}^*$ is an h-admissible operator, we obtain in the same way that $\|\mathrm{Op}_h(\chi) U_j \psi_j \mathcal{W}^* v\| = \mathcal{O}(h^\infty)$, and thus $(x_0, \xi_0) \notin FS(U_j \mathcal{W}^* v)$. •

Without loss of generality, we can assume $T_{\Omega'}(\varphi_0) < +\infty$. By Theorem 8.1, we have,

$$e^{-itP/h}\varphi_0 = \mathcal{W}^* e^{-itA/h} \mathcal{W}\varphi_0 + \mathcal{O}\left(h^\infty\right),$$

uniformly for $t \in [0, T_{\Omega'}(\varphi_0)]$, where $\mathcal{W}$ and A are given in Theorem 7.1. Thus, by Lemma 9.1, we immediately obtain,

$$FS(U_j e^{-itP/h}\varphi_0) \cap T^*\Omega_j = FS(e^{-itA/h}\mathcal{W}\varphi_0) \cap T^*\Omega_j.$$

On the other hand, since A is an h-admissible operator on $L^2(I\!R^n)$, a well-known result of propagation (see, e.g., [Ma2] Section 4.6, Exercise 12) tells us,

$$FS(e^{-itA/h}\mathcal{W}\varphi_0) = \exp tH_{a_0}(FS(\mathcal{W}\varphi_0)).$$

Therefore, applying Lemma 9.1 again, we obtain,

$$FS(U_j e^{-itP/h}\varphi_0) \cap T^*\Omega_j = T^*\Omega_j \cap \exp tH_{a_0}\left(\cup_{k=0}^r FS(U_k \Pi_g \varphi_0) \cap T^*\Omega_k\right). \tag{9.1}$$

By assumption, we also have,

$$\cup_{k=0}^r FS(U_k \Pi_g \varphi_0) = \cup_{k=1}^r FS(U_k \varphi_0) \subset K_0 \times I\!R^n. \tag{9.2}$$

In order to conclude, we need the following result:

Lemma 9.2 *For any $f \in C_0^\infty(I\!R)$, $\psi \in C_0^\infty(I\!R^n)$, $\chi_j \in C_0^\infty(\Omega_j)$, $\varepsilon > 0$, and $\rho \in C_b^\infty(I\!R)$ with $\operatorname{Supp} \rho \subset [C_f - \gamma + \varepsilon, +\infty)$ (where C_f is as in Corollary 2.6), one has,*

$$\|\rho(\chi_j \boldsymbol{\omega} \chi_j)\psi f(U_j \chi_j \tilde{P} U_j^{-1} \chi_j)\| = \mathcal{O}(h^\infty).$$

Proof We set $\boldsymbol{\omega}_j := \chi_j \boldsymbol{\omega} \chi_j$ and $\tilde{P}_j := U_j \chi_j \tilde{P} U_j^{-1} \chi_j$. Using Assumptions (H1), (H2), (H4) and Proposition 3.2, we see that $\tilde{P}_j \geq (1 - Ch)\boldsymbol{\omega}_j + \gamma - Ch$ for some constant $C > 0$ independent of h. As a consequence, we have,

$$\rho(\boldsymbol{\omega}_j)\tilde{P}_j \rho(\boldsymbol{\omega}_j) \geq \rho(\boldsymbol{\omega}_j)((1 - Ch)\boldsymbol{\omega}_j + \gamma - Ch)\rho(\boldsymbol{\omega}_j) \geq (C_f + \varepsilon - C'h)\rho(\boldsymbol{\omega}_j)^2,$$

with $C' = C + CC_f$. Therefore, we can write,

$$\|\rho(\boldsymbol{\omega}_j)\psi f(\tilde{P}_j)u\|^2 \leq \frac{1}{C_f + \varepsilon - C'h}\langle \tilde{P}_j \rho(\boldsymbol{\omega}_j)\psi f(\tilde{P}_j)u, \rho(\boldsymbol{\omega}_j)\psi f(\tilde{P}_j)u\rangle,$$

for any $u \in L^2(I\!R^n; \mathcal{H})$, and thus,

$$\begin{aligned} \|\rho(\boldsymbol{\omega}_j)\psi f(\tilde{P}_j)\| &\leq \frac{1}{C_f + \varepsilon - C'h}\|\tilde{P}_j \rho(\boldsymbol{\omega}_j)\psi f(\tilde{P}_j)\| \\ &\leq \frac{1}{C_f + \varepsilon - C'h}\left(\|\rho(\boldsymbol{\omega}_j)\psi \tilde{P}_j f(\tilde{P}_j)\| + \|[\tilde{P}_j, \rho(\boldsymbol{\omega}_j)\psi] f(\tilde{P}_j)\|\right). \end{aligned} \tag{9.3}$$

Now, on the one hand, since Supp f is included in $[-C_f, C_f]$, we have,

$$\begin{aligned}\frac{1}{C_f+\varepsilon-C'h}\|\rho(\boldsymbol{\omega}_j)\psi\tilde{P}_jf(\tilde{P}_j)\| &= \frac{1}{C_f+\varepsilon-C'h}\|\tilde{P}_jf(\tilde{P}_j)\psi\rho(\boldsymbol{\omega}_j)\| \\ &\leq \frac{C_f}{C_f+\varepsilon-C'h}\|f(\tilde{P}_j)\psi\rho(\boldsymbol{\omega}_j)\|. \quad (9.4)\end{aligned}$$

On the other hand, since $\tilde{P}_j$ and $\boldsymbol{\omega}_j$ are both differential operators with respect to x with smooth (operator-valued) coefficients, and $\rho(\boldsymbol{\omega}_j)\psi$ is a scalar operator, by standard symbolic calculus, we have,

$$[\tilde{P}_j, \rho(\boldsymbol{\omega}_j)\psi]f(\tilde{P}_j) = \mathcal{O}(h)\rho_1(\boldsymbol{\omega}_j)\psi_1 f(\tilde{P}_j) + \mathcal{O}(h^\infty), \quad (9.5)$$

where $\rho_1 \in C_b^\infty(I\!R)$ and $\psi_1 \in C_0^\infty(I\!R^n)$ are arbitrary functions verifying $\rho_1\rho = \rho$ and $\psi_1\psi = \psi$. Inserting (9.4)-(9.5) into (9.3), we obtain,

$$\|\rho(\boldsymbol{\omega}_j)\psi f(\tilde{P}_j)\| = \mathcal{O}(h\|\rho_1(\boldsymbol{\omega}_j)\psi_1 f(\tilde{P}_j)\|) + \mathcal{O}(h^\infty).$$

Iterating the procedure, we clearly obtain the lemma. •

Now, using, e.g., (8.4), we know that $e^{-itP/h}\varphi_0 = f(\tilde{P})e^{-itP/h}\varphi_0 + \mathcal{O}(h^\infty)$. Moreover, if $\chi_j, \psi_j \in C_0^\infty(\Omega_j)$ are such that $\chi_j = 1$ near Supp ψ_j, by Lemma 4.11, we have,

$$U_j\psi_j f(\tilde{P}) = U_j\psi_j f(\tilde{P})\chi_j^2 + \mathcal{O}(h^\infty) = U_j\psi_j f(\tilde{P})U_j^{-1}\chi_j U_j\chi_j + \mathcal{O}(h^\infty),$$

and therefore,

$$U_j\psi_j e^{-itP/h}\varphi_0 = U_j\psi_j f(\tilde{P})U_j^{-1}\chi_j U_j\chi_j e^{-itP/h}\varphi_0 + \mathcal{O}(h^\infty).$$

Then, using lemma 15.1, we obtain,

$$U_j\psi_j e^{-itP/h}\varphi_0 = \psi_j f(\tilde{P}_j)U_j\chi_j e^{-itP/h}\varphi_0 + \mathcal{O}(h^\infty),$$

with $\tilde{P}_j = U_j\chi_j\tilde{P}U_j^{-1}\chi_j$. Therefore, using Lemma 9.2, this gives,

$$\|\rho(\chi_j\boldsymbol{\omega}\chi_j)U_j\psi_j e^{-itP/h}\varphi_0\| = \mathcal{O}(h^\infty),$$

and thus, by Lemma 15.2,

$$\|\rho(\boldsymbol{\omega})U_j\psi_j e^{-itP/h}\varphi_0\| = \mathcal{O}(h^\infty). \quad (9.6)$$

Since the principal symbol of $\rho(\boldsymbol{\omega})$ is $\rho(\omega)$, we deduce from (9.2), (9.6), and standard results on FS, that,

$$\cup_{k=0}^r FS(U_k\Pi_g\varphi_0) \subset K(f) := \{(x,\xi)\,;\, x\in K_0\,,\, \omega(x,\xi) \leq C_f - \gamma\},$$

and thus, by (9.1),

$$FS(U_j e^{-itP/h}\varphi_0) \cap T^*\Omega_j \subset \exp tH_{a_0}\,(K(f)) \cap T^*\Omega_j, \quad (9.7)$$

for all $t \geq 0$.

Then, for any $j \in \{0, 1, \ldots, r\}$, $\psi_j, \tilde{\psi}_j \in C_0^\infty(\Omega_j)$ with $\tilde{\psi}_j \psi_j = \psi_j$, and any $\alpha \in C_0^\infty(I\!R^n)$, we write,

$$U_j \psi_j e^{-itP/h} \varphi_0 = \alpha(hD_x) \tilde{\psi}_j(x) U_j \psi_j e^{-itP/h} \varphi_0 + (1 - \alpha(hD_x)) U_j \psi_j e^{-itP/h} \varphi_0,$$

and therefore, if $\alpha(\xi) = 1$ in a sufficiently large compact set,

$$U_j \psi_j e^{-itP/h} \varphi_0 = \alpha(hD_x) \tilde{\psi}_j(x) U_j \psi_j e^{-itP/h} \varphi_0 + \mathcal{O}(h^\infty).$$

Finally, if $\text{Supp}\ \tilde{\psi}_j \cap \pi_x \left(\exp tH_{a_0} \left(K(f)\right)\right) = \emptyset$ (or, more generally, $\text{Supp}\ \tilde{\psi}_j \cap \pi_x \left(\cup_{k=0}^r \exp tH_{a_0}(FS(U_k \Pi_g \varphi_0))\right) = \emptyset$), then, (9.1) and (9.7) tell us,

$$\|\alpha(hD_x) \tilde{\psi}_j(x) U_j \psi_j e^{-itP/h} \varphi_0\| = \mathcal{O}(h^\infty),$$

and thus, by the unitarity of U_j,

$$\|\psi_j e^{-itP/h} \varphi_0\| = \|U_j \psi_j e^{-itP/h} \varphi_0\| = \mathcal{O}(h^\infty),$$

uniformly for $t \in [0, T_{\Omega'}(\varphi_0)]$. Since we also know that $\|e^{-itP/h} \varphi_0\|_{K^c} = \mathcal{O}(h^\infty)$ for some compact set $K \subset I\!R^n$ (by definition of $T_{\Omega'}(\varphi_0)$), this proves that we can actually take for K any compact neighborhood of $\pi_x \left(\exp tH_{a_0} \left(K(f)\right)\right)$. Thus, if $T_{\Omega'}(\varphi_0) < \sup\{T > 0\,;\, \pi_x(\cup_{t\in[0,T]} \exp tH_{a_0}(K(f))) \subset \Omega'\}$, clearly (e.g., by using Theorem 14.1), one can find $T > T_{\Omega'}(\varphi_0)$ and $K_T \subset\subset \Omega'$, such that $\sup_{t\in[0,T]} \|e^{-itP/h} \varphi_0\|_{K_T^c} = \mathcal{O}(h^\infty)$. This is in contradiction with the definition of $T_{\Omega'}(\varphi_0)$, and therefore, necessarily,

$$T_{\Omega'}(\varphi_0) \geq \sup\{T > 0\,;\, \pi_x(\cup_{t\in[0,T]} \exp tH_{a_0}(K(f))) \subset \Omega'\}.$$

This proves Corollary 2.6, and also Remark 2.8 since, in the last argument, one can replace $K(f)$ by $\cup_{k=0}^r \exp tH_{a_0}(FS(U_k \Pi_g \varphi_0))$ everywhere. •

10 Computing the Effective Hamiltonian

Now that we know the existence of an effective Hamiltonian describing the evolution of those states φ_0 that verify (2.4), the problem remains of computing its symbol up to any arbitrary power of h (in Theorem 2.1, only the principal symbol of A is given). Because of the conditions of localization (2.4), it is clear that such an effective Hamiltonian is not unique (for instance, the three operators A, $Af(A)$ or $\mathcal{W} f(\tilde{P}) \mathcal{W}^* A \mathcal{W} f(\tilde{P}) \mathcal{W}^*$ could indifferently be taken). However, its symbol is certainly uniquely determined in the relevant region of the phase space where $\tilde{\varphi}(t) := \mathcal{W} e^{-itP/h} \varphi_0$ lives (that is, on $FS(\tilde{\varphi}(t))$ in the sense of the previous section, and for $t \in [0, T_{\Omega'}(\varphi_0))$). Therefore, as long as we deal with h-admissible operators (that is, with operators that do not move the Frequency Set), or even with *twisted* h-admissible operators (that become standard h-admissible operators once conjugated with $\mathcal{W}$ or Z_L) it is enough, for computing the symbol A in this region, to start by performing formal computations on the operators themselves (instead of immediately using the twisted symbolic calculus, that appears to be a little bit too heavy at the beginning).

In this section, we describe a rather easy way to perform these computations, and we give a simple expression of the effective Hamiltonian up to $\mathcal{O}(h^4)$. Moreover, as an example, we also compute its symbol, up to $\mathcal{O}(h^3)$, in the case $L = 1$. Let us inform the reader that the results of this section are not used in the rest of the paper (except for Theorem 12.3), and thus can be skipped without problem at a first reading.

We start from the definition of A given in Section 7 (in particular (7.8)):

$$A = \mathcal{W}\tilde{P}\mathcal{W}^* = Z_L\mathcal{V}\tilde{P}\mathcal{V}^* Z_L^*.$$

Since Z_L is rather explicit, the problem mainly consists in determining the expansion of $\mathcal{V}$. Setting,

$$\Delta := h^{-1}(\Pi_g - \tilde{\Pi}_0),$$

and using that $\Pi_g^2 - \Pi_g = \tilde{\Pi}_0^2 - \tilde{\Pi}_0 = 0$, we immediately obtain,

$$\Pi_g\Delta + \Delta\Pi_g = \Delta + h\Delta^2. \tag{10.1}$$

Thus, we deduce from (7.6),

$$\begin{aligned}\mathcal{V} &= ((\Pi_g - h\Delta)\Pi_g + (1 - \Pi_g + h\Delta)(1 - \Pi_g))(1 - h^2\Delta^2)^{-\frac{1}{2}} \\ &= (1 + h[\Pi_g, \Delta] - h^2\Delta^2)(1 - h^2\Delta^2)^{-\frac{1}{2}}.\end{aligned}$$

Then, using the (convergent) series expansion,

$$(1 - h^2\Delta^2)^{-\frac{1}{2}} = 1 + \sum_{k=1}^{\infty} \nu_k h^{2k}\Delta^{2k},$$

with,

$$\nu_k = \frac{1}{2}(\frac{1}{2} + 1)(\frac{1}{2} + 2)\dots(\frac{1}{2} + k - 1)\frac{1}{k!} = \frac{(2k-1)!}{2^{2k-1}k!(k-1)!},$$

we obtain,

$$\mathcal{V} = 1 - ih\mathcal{V}_1 + h^2\mathcal{V}_2,$$

where the two selfadjoint operators $\mathcal{V}_1$ and $\mathcal{V}_2$ are given by,

$$\begin{aligned}\mathcal{V}_1 &= i[\Pi_g, \Delta](1 + \sum_{k=1}^{\infty} \nu_k h^{2k}\Delta^{2k}); \\ \mathcal{V}_2 &= -\frac{1}{2}\Delta^2 + \sum_{k=1}^{\infty}(\nu_{k+1} - \nu_k)h^{2k}\Delta^{2(k+1)},\end{aligned}$$

that is, observing that $\nu_k - \nu_{k+1} = \nu_k/(2k+2)$,

$$\begin{aligned}\mathcal{V}_1 &= i[\Pi_g, \Delta]F_1(\Delta^2); \\ \mathcal{V}_2 &= F_2(\Delta^2),\end{aligned}$$

with, (setting also $\nu_0 := 1$),

$$\begin{aligned} F_1(s) &= \sum_{k=0}^{\infty} \nu_k h^{2k} s^k; \\ F_2(s) &= -\sum_{k=0}^{\infty} \frac{\nu_k}{2(k+1)} h^{2k} s^{k+1}. \end{aligned}$$

As a consequence,

$$\mathcal{V}^* = 1 + ih\mathcal{V}_1 + h^2\mathcal{V}_2,$$

and therefore,

$$\mathcal{V}\tilde{P}\mathcal{V}^* = \tilde{P} + ih[\tilde{P}, \mathcal{V}_1] + h^2(\mathcal{V}_1\tilde{P}\mathcal{V}_1 + \mathcal{V}_2\tilde{P} + \tilde{P}\mathcal{V}_2) + ih^3(\mathcal{V}_2\tilde{P}\mathcal{V}_1 - \mathcal{V}_1\tilde{P}\mathcal{V}_2) + h^4\mathcal{V}_2\tilde{P}\mathcal{V}_2,$$

that is,

$$A = Z_L(\tilde{P} + ih[\tilde{P}, \mathcal{V}_1] + h^2(\mathcal{V}_1\tilde{P}\mathcal{V}_1 + \mathcal{V}_2\tilde{P} + \tilde{P}\mathcal{V}_2) + ih^3(\mathcal{V}_2\tilde{P}\mathcal{V}_1 - \mathcal{V}_1\tilde{P}\mathcal{V}_2) + h^4\mathcal{V}_2\tilde{P}\mathcal{V}_2)Z_L^*. \tag{10.2}$$

From now on, we work modulo $\mathcal{O}(h^5)$ error-terms, and, as we observed at the beginning of this section, if we restrict our attention to the relevant region of the phase space, then formal computations are sufficient and Π_g can be replaced by the formal series $\tilde{\Pi} := \sum_{k\geq 0} h^k\tilde{\Pi}_k$ constructed in Section 6. In particular, $\tilde{P}$ formally commutes with $\tilde{\Pi}$ and thus, since $[\tilde{P}, \tilde{\Pi}_0] = -ihS_0$ (see Section 6),

$$[\tilde{P}, [\tilde{\Pi}, \Delta]] = -h^{-1}[\tilde{P}, [\tilde{\Pi}, \tilde{\Pi}_0]] = -h^{-1}[\tilde{\Pi}, [\tilde{P}, \tilde{\Pi}_0]] = i[\tilde{\Pi}, S_0], \tag{10.3}$$

where, from now on, Δ stands for $h^{-1}(\tilde{\Pi} - \tilde{\Pi}_0) = \sum_{k\geq 1} h^k\tilde{\Pi}_k$.

Moreover, from the identities $[\tilde{P}, \tilde{\Pi}] = 0$, $\tilde{\Pi} = \tilde{\Pi}_0 + h\Delta$, we deduce,

$$[\tilde{P}, \Delta] = -h^{-1}[\tilde{P}, \tilde{\Pi}_0] = iS_0,$$

and therefore,

$$\begin{aligned} [\tilde{P}, \mathcal{V}_1] &= [S_0, \tilde{\Pi}]F_1(\Delta^2) + i[\tilde{\Pi}, \Delta][\tilde{P}, F_1(\Delta^2)]; \\ [\tilde{P}, F_1(\Delta^2)] &= i\sum_{k=1}^{\infty} \nu_k h^{2k} \sum_{j=0}^{2k-1} \Delta^j S_0 \Delta^{2k-1-j}. \end{aligned}$$

Since $\nu_0 = 1$ and $\nu_1 = 1/2$, this gives,

$$[\tilde{P}, \mathcal{V}_1] = [S_0, \tilde{\Pi}](1 + \frac{h^2}{2}\Delta^2) - \frac{h^2}{2}[\tilde{\Pi}, \Delta](S_0\Delta + \Delta S_0) + \mathcal{O}(h^4) \tag{10.4}$$

Moreover, (10.1) implies $\tilde{\Pi}\Delta\tilde{\Pi} = h\Delta^2\tilde{\Pi} = h\tilde{\Pi}\Delta^2$, and thus, in particular, Δ^2 commutes with $\tilde{\Pi}$. As a consequence, we can write,

$$\begin{aligned} \mathcal{V}_1\tilde{P}\mathcal{V}_1 &= F_1(\Delta^2)[\tilde{\Pi}, \Delta]\tilde{P}[\Delta, \tilde{\Pi}]F_1(\Delta^2) \\ &= [\tilde{\Pi}, \Delta]\tilde{P}[\Delta, \tilde{\Pi}] + h^2 \operatorname{Re} \Delta^2[\tilde{\Pi}, \Delta]\tilde{P}[\Delta, \tilde{\Pi}] + \mathcal{O}(h^4), \end{aligned}$$

and, still using (10.1), we have,

$$\begin{aligned}
[\tilde\Pi,\Delta]\tilde P[\Delta,\tilde\Pi] &= \tilde\Pi\Delta\tilde P\Delta\tilde\Pi + \Delta\tilde\Pi\tilde P\tilde\Pi\Delta - \tilde\Pi\Delta\tilde P\tilde\Pi\Delta - \Delta\tilde\Pi\tilde P\Delta\tilde\Pi\\
&= (\tilde\Pi\Delta+\Delta\tilde\Pi)\tilde P(\Delta\tilde\Pi+\tilde\Pi\Delta) - 2\tilde\Pi\Delta\tilde P\tilde\Pi\Delta - 2\Delta\tilde\Pi\tilde P\Delta\tilde\Pi\\
&= (\Delta+h\Delta^2)\tilde P(\Delta+h\Delta^2) - 2h\tilde\Pi\Delta^2\tilde P\Delta - 2h\Delta\tilde P\Delta^2\tilde\Pi\\
&= \Delta\tilde P\Delta + h(1-2\tilde\Pi)\Delta^2\tilde P\Delta + h\Delta\tilde P\Delta^2(1-2\tilde\Pi)\\
&= \frac12(\Delta^2P+P\Delta^2) + \frac i2[\Delta,S_0] + 2h\,\mathrm{Re}\,\Delta^2(1-2\tilde\Pi)\tilde P\Delta.
\end{aligned}$$

Therefore,

$$\mathcal V_1\tilde P\mathcal V_1 = \mathrm{Re}\,\Delta^2P + \frac i2[\Delta,S_0] + 2h\,\mathrm{Re}\,\Delta^2(1-2\tilde\Pi)\tilde P\Delta + h^2\,\mathrm{Re}\,\Delta^2(\,\mathrm{Re}\,\Delta^2P + \frac i2[\Delta,S_0]) + \mathcal O(h^3).$$

and, since $\mathcal V_2 = -\frac12\Delta^2 - \frac18 h^2\Delta^4 + \mathcal O(h^4)$, we obtain,

$$\begin{aligned}
\mathcal V_1\tilde P\mathcal V_1 + \mathcal V_2\tilde P + \tilde P\mathcal V_2 &= \frac i2[\Delta,S_0] + 2h\,\mathrm{Re}\,\Delta^2(1-2\tilde\Pi)\tilde P\Delta\\
&\quad + h^2\left(\mathrm{Re}\,\Delta^2(\,\mathrm{Re}\,\Delta^2P + \frac i2[\Delta,S_0]) - \frac14\,\mathrm{Re}\,\Delta^4\tilde P\right) + \mathcal O(h^3)\\
&= \frac i2[\Delta,S_0] + 2h\,\mathrm{Re}\,\Delta^2(1-2\tilde\Pi)\tilde P\Delta\\
&\quad + \frac12 h^2\left(\mathrm{Re}\,(i\Delta^2[\Delta,S_0]) + \Delta^2\tilde P\Delta^2 + \frac14\,\mathrm{Re}\,\Delta^4\tilde P\right) + \mathcal O(h^3)
\end{aligned}$$

Finally, since, obviously, Δ^2 also commutes with Δ, thus with $[\tilde\Pi,\Delta]$, too, we see that $\mathcal V_1$ and $\mathcal V_2$ commute together, and therefore,

$$\begin{aligned}
\mathcal V_2\tilde P\mathcal V_1 - \mathcal V_1\tilde P\mathcal V_2 &= [\tilde P,\mathcal V_1]\mathcal V_2 - [\tilde P,\mathcal V_2]\mathcal V_1\\
&= -\frac12[S_0,\tilde\Pi]\Delta^2 + \frac i2[\tilde P,\Delta^2][\tilde\Pi,\Delta] + \mathcal O(h^2)\\
&= -\frac12[S_0,\tilde\Pi]\Delta^2 - \frac12(S_0\Delta+\Delta S_0)[\tilde\Pi,\Delta] + \mathcal O(h^2).
\end{aligned}$$

Summing up, we have found,

$$\mathcal V\tilde P\mathcal V^* = B_0 + hB_1 + h^2B_2 + h^3B_3 + h^4B_4 + \mathcal O(h^5),$$

with,

$$\begin{aligned}
B_0 &= \tilde P\\
B_1 &= i[S_0,\tilde\Pi]\\
B_2 &= \frac i2[\Delta,S_0]\\
B_3 &= -\,\mathrm{Re}\,i[\tilde\Pi,\Delta](S_0\Delta+\Delta S_0) + 2\,\mathrm{Re}\,\Delta^2(1-2\tilde\Pi)\tilde P\Delta\\
B_4 &= \frac12\left(\mathrm{Re}\,(i\Delta^2[\Delta,S_0]) + \Delta^2\tilde P\Delta^2 + \frac14\,\mathrm{Re}\,\Delta^4\tilde P\right)
\end{aligned}$$

Then, writing $\tilde{\Pi} = \sum_{k=0}^{3} h^k \tilde{\Pi}_k + \mathcal{O}(h^4)$ and $\Delta = \sum_{k=1}^{3} h^{k-1}\tilde{\Pi}_k + \mathcal{O}(h^3)$, we obtain,

$$\mathcal{V}\tilde{P}\mathcal{V}^* = C_0 + hC_1 + h^2C_2 + h^3C_3 + h^4C_4 + \mathcal{O}(h^5),$$

with,

$$\begin{aligned}
C_0 &= \tilde{P} \\
C_1 &= i[S_0, \tilde{\Pi}_0] \\
C_2 &= \frac{i}{2}[S_0, \tilde{\Pi}_1] \\
C_3 &= \frac{i}{2}[S_0, \tilde{\Pi}_2] - \text{ Re } i[\tilde{\Pi}_0, \tilde{\Pi}_1](S_0\tilde{\Pi}_1 + \tilde{\Pi}_1 S_0) + 2 \text{ Re } \tilde{\Pi}_1^2(1 - 2\tilde{\Pi}_0)\tilde{P}\tilde{\Pi}_1 \\
C_4 &= \frac{i}{2}[S_0, \tilde{\Pi}_3] - \text{ Re } i[\tilde{\Pi}_0, \tilde{\Pi}_2](S_0\tilde{\Pi}_1 + \tilde{\Pi}_1 S_0) - \text{ Re } i[\tilde{\Pi}_0, \tilde{\Pi}_1](S_0\tilde{\Pi}_2 + \tilde{\Pi}_2 S_0) \\
&\quad +2 \text{ Re } (\tilde{\Pi}_1\tilde{\Pi}_2 + \tilde{\Pi}_2\tilde{\Pi}_1)(1 - 2\tilde{\Pi}_0)\tilde{P}\tilde{\Pi}_1 - 4 \text{ Re } \tilde{\Pi}_1^3\tilde{P}\tilde{\Pi}_1 + 2 \text{ Re } \tilde{\Pi}_1^2(1 - 2\tilde{\Pi}_0)\tilde{P}\tilde{\Pi}_2 \\
&\quad +\frac{1}{2}\left(\text{ Re } (i\tilde{\Pi}_1^2[\tilde{\Pi}_1, S_0]) + \tilde{\Pi}_1^2\tilde{P}\tilde{\Pi}_1^2 + \frac{1}{4} \text{ Re } \tilde{\Pi}_1^4\tilde{P}\right)
\end{aligned}$$

Now, due to (6.7)-(6.8), we observe that $\tilde{\Pi}_0 S_0 \tilde{\Pi}_0 = \tilde{\Pi}_0^\perp S_0 \tilde{\Pi}_0^\perp = \tilde{\Pi}_0\tilde{\Pi}_1\tilde{\Pi}_0 = \tilde{\Pi}_0^\perp\tilde{\Pi}_1\tilde{\Pi}_0^\perp = 0$. As a consequence,

$$\tilde{\Pi}_0 C_1 \tilde{\Pi}_0 = i\tilde{\Pi}_0[S_0, \tilde{\Pi}_0]\tilde{\Pi}_0 = 0,$$

and,

$$\tilde{\Pi}_0[\tilde{\Pi}_0, \tilde{\Pi}_1](S_0\tilde{\Pi}_1 + \tilde{\Pi}_1 S_0)\tilde{\Pi}_0 = \tilde{\Pi}_0[\tilde{\Pi}_0, \tilde{\Pi}_1]\tilde{\Pi}_0(S_0\tilde{\Pi}_1 + \tilde{\Pi}_1 S_0)\tilde{\Pi}_0 = 0;$$

$$\begin{aligned}
\tilde{\Pi}_0\tilde{\Pi}_1^2(1 - 2\tilde{\Pi}_0)\tilde{P}\tilde{\Pi}_1\tilde{\Pi}_0 &= \tilde{\Pi}_0\tilde{\Pi}_1^2\tilde{\Pi}_0^\perp\tilde{P}\tilde{\Pi}_1\tilde{\Pi}_0 + \tilde{\Pi}_0\tilde{\Pi}_1^2(1 - 2\tilde{\Pi}_0)[\tilde{P}, \tilde{\Pi}_0^\perp]\tilde{\Pi}_1\tilde{\Pi}_0 \\
&= ih\tilde{\Pi}_0\tilde{\Pi}_1^2(1 - 2\tilde{\Pi}_0)S_0\tilde{\Pi}_1\tilde{\Pi}_0 \\
&= -ih\tilde{\Pi}_0\tilde{\Pi}_1^2 S_0\tilde{\Pi}_1\tilde{\Pi}_0.
\end{aligned}$$

(In the last two steps we have used that $\tilde{\Pi}_0\tilde{\Pi}_1^2\tilde{\Pi}_0^\perp = \tilde{\Pi}_0^\perp S_0\tilde{\Pi}_1\tilde{\Pi}_0 = 0$.) Since we also have $Z_L = Z_L\tilde{\Pi}_0$ and $Z_L^* = \tilde{\Pi}_0 Z_L^*$, we deduce,

$$\begin{aligned}
&Z_L C_1 Z_L^* = 0; \\
&Z_L C_3 Z_L^* = \frac{i}{2} Z_L[S_0, \tilde{\Pi}_2]Z_L^* + 2h \text{ Im } \tilde{\Pi}_0\tilde{\Pi}_1^2 S_0\tilde{\Pi}_1\tilde{\Pi}_0. \qquad (10.5)
\end{aligned}$$

In particular, since $A = Z_L\mathcal{V}\tilde{P}\mathcal{V}^* Z_L^*$, we have proved,

Proposition 10.1 *The effective Hamiltonian A verifies,*

$$A = A_0 + h^2A_2 + h^3A_3 + \mathcal{O}(h^4), \qquad (10.6)$$

with,

$$\begin{aligned}
A_0 &= Z_L\tilde{P}Z_L^* \\
A_2 &= \frac{i}{2}Z_L[S_0, \tilde{\Pi}_1]Z_L^* \\
A_3 &= \frac{i}{2}Z_L[S_0, \tilde{\Pi}_2]Z_L^*.
\end{aligned}$$

It is interesting to observe that, at this level, the absence of a term in h (that is, an extra-term of the form hA_1) is completely general and, in particular, is not related to any particular form of $\boldsymbol{\omega}$ (however, some term in h may be hidden in A_0, as we shall see in the sequels).

Here, we have stopped the computation of A at the third power of h, but it is clear from the expression of C_4 and (10.5) that the coefficient of h^4 can be written down, too (but has a more complicated form). Of course, pushing forward the series and spending more time in the calculation would permit to also obtain the next terms.

From that point, in order to have an even more explicit expression of A (in particular to compute its symbol), one must use the expressions of $\tilde{\Pi}_1$ and $\tilde{\Pi}_2$ obtained in Section 6. Let us do it in the case $L = 1$. In that case, setting $\lambda(x) := \lambda_{L'+1}(x)$, one has $\tilde{\Pi}_0(z - \tilde{Q}(x))^{-1} = (z - \lambda(x))^{-1}\tilde{\Pi}_0$, and thus,

$$\tilde{\Pi}_0^{\perp}\tilde{\Pi}_1\tilde{\Pi}_0 = -\frac{1}{2\pi}\oint_{\gamma(x)} \frac{(z - \tilde{Q}(x))^{-1}\tilde{\Pi}_0^{\perp}(x)S_0\tilde{\Pi}_0(x)}{z - \lambda(x)}dz = -iR'(\lambda(x))S_0,$$

where $R'(x,z) := \tilde{\Pi}_0^{\perp}(x)(z - \tilde{Q}(x))^{-1}\tilde{\Pi}_0^{\perp}(x)$ is the so-called *reduced resolvent* of $\tilde{Q}(x)$.

As a consequence,

$$\tilde{\Pi}_0[S_0, \tilde{\Pi}_1]\tilde{\Pi}_0 = S_0\tilde{\Pi}_0^{\perp}\tilde{\Pi}_1\tilde{\Pi}_0 - \tilde{\Pi}_0\tilde{\Pi}_1\tilde{\Pi}_0^{\perp}S_0 = -2iS_0R'(x,\lambda(x))S_0,$$

that leads to,

$$A_2 = Z_1S_0R'(x,\lambda(x))S_0Z_1^*.$$

In the same way,

$$\tilde{\Pi}_0^{\perp}\tilde{\Pi}_2\tilde{\Pi}_0 = -iR'(x,\lambda(x))S_1\tilde{\Pi}_0,$$

and therefore,

$$A_3 = \text{ Re } Z_1S_0R'(x,\lambda(x))S_1Z_1^*.$$

Now, we can start to use the twisted symbolic calculus introduced in Section 4. We denote by $s_0 = (s_0^j)_{0\le j\le r}$ and $\pi_0 = (\pi_0^j)_{0\le j\le r}$ the (twisted) symbols of S_0 and $\tilde{\Pi}_0$ respectively. We also set $\tilde{\omega} = (\tilde{\omega}_j)_{0\le j\le r}$, where,

$$\tilde{\omega}_j(x,\xi) := \omega(x,\xi) + h\sum_{|\beta|\le m-1}\omega_{\beta,j}(x)\xi^\beta, \quad ((x.\xi) \in T^*\Omega_j),$$

is the symbol of the operator introduced in (2.3) (we remind that we work with the standard quantization of symbols, as described in Section 13). From (6.4)-(6.6) and the considerations of Section 4 (and since $\pi_0^j = \pi_0^j(x)$ does not depend on ξ), it s easy to see that,

$$s_0^j = \partial_\xi\tilde{\omega}_j\partial_x\pi_0^j + i\sum_{|\beta|\le m-1}[\omega_{\beta,j}(x), \pi_0^j(x)]\xi^\beta - \frac{ih}{2}\sum_{|\alpha|=2}(\partial_\xi^\alpha\omega)(\partial_x^\alpha\pi_0^j) + \mathcal{O}(h^2)$$

Also setting $\tilde{Q}_j(x) := U_j(x)\tilde{Q}(x)U_j(x)^{-1}$, the symbol $\rho = (\rho_j)_{0\leq j\leq r}$ of $R'(x,\lambda(x))$ is simply given by,

$$\rho_j(x) = (1-\pi_0^j(x))(\lambda(x)-\tilde{Q}_j(x))^{-1}(1-\pi_0^j(x)),$$

and thus, the symbol $\sigma_2 = (\sigma_2^j)_{0\leq j\leq r}$ of $S_0R'(x,\lambda(x))S_0$ verifies,

$$\sigma_2^j(x,\xi) = s_0^j(x,\xi)\rho_j(x)s_0^j(x,\xi) + \frac{h}{i}\partial_\xi s_0^j(x,\xi)\partial_x(\rho_j(x)s_0^j(x,\xi)) + \mathcal{O}(h^2).$$

From (6.8)-(6.10), we also obtain,

$$\begin{aligned}\tilde{\Pi}_1 &= i[S_0, R'(x,\lambda(x))]\\ S_1 &= \frac{i}{h}[\boldsymbol{\omega}+\zeta W, \tilde{\Pi}_1].\end{aligned}$$

Therefore, since ω and ζW are scalar operators, the respective symbols $\pi_1 = (\pi_1^j)_{0\leq j\leq r}$ and $s_1 = (s_1^j)_{0\leq j\leq r}$ of $\tilde{\Pi}_1$ and S_1, verify,

$$\begin{aligned}\pi_1^j(x,\xi) &= i[s_0^j(x,\xi),\rho_j(x)] + \mathcal{O}(h) = i\partial_\xi\omega(x,\xi)[\partial_x\pi_0^j(x),\rho_j(x)] + \mathcal{O}(h)\\ s_1^j &= \{\omega+\zeta W,\pi_1^j\} + \mathcal{O}(h) = \partial_\xi\omega\cdot\partial_x\pi_1^j - \partial_\xi\pi_1^j\cdot\partial_x(\omega+\zeta W) + \mathcal{O}(h),\end{aligned}$$

and thus,

$$s_1^j = i\sum_{k,\ell=1}^n \Big((\partial_{\xi_k}\omega)\partial_{x_k}(\partial_{\xi_\ell}\omega[\partial_{x_\ell}\pi_0^j,\rho_j]) - (\partial_{\xi_k}\partial_{\xi_\ell}\omega)[\partial_{x_\ell}\pi_0^j,\rho_j]\partial_{x_k}(\omega+\zeta W)\Big) + \mathcal{O}(h). \tag{10.7}$$

This permits to compute the symbol $\sigma_3 = (\sigma_3^j)_{0\leq j\leq r}$ of $\operatorname{Re} S_0R'(x,\lambda(x))S_1$, through the formula,

$$\sigma_3^j(x,\xi) = \frac{1}{2}\partial_\xi\omega\cdot\Big((\partial_x\pi_0^j)\rho_j s_1^j + s_1^j\rho_j(\partial_x\pi_0^j)\Big) + \mathcal{O}(h). \tag{10.8}$$

Observe that one also has,

$$\partial_x\pi_0^j(x) = \langle\cdot,\nabla_x u_j(x)\rangle_{\mathcal{H}}u_j(x) + \langle\cdot,u_j(x)\rangle_{\mathcal{H}}\nabla_x u_j(x),$$

where $\langle\cdot,u\rangle_{\mathcal{H}}$ stands for the operator $w\mapsto\langle w,u\rangle_{\mathcal{H}}$, and $u_j =: U_j(x)u_{L'+1}(x)$ is the normalized eigenfunction of $\tilde{Q}_j(x)$ associated with $\lambda(x)$.

Finally, we use the following elementary remark: let B is a twisted h-admissible (or PDO) operator on $L^2(\mathbb{R}^n;\mathcal{H})$, with symbol $b = (b_j)_{0\leq j\leq r}$, and let $u(x), v(x)\in\mathcal{H}$ such that, for all $j = 0,\dots,r$, $u_j(x) := U_j(x)u(x)$ and $v_j(x) := U_j(x)v(x)$ are in $C^\infty(\Omega_j;\mathcal{H})$. Denote by $\mathcal{Z}_u$, $\mathcal{Z}_v$ the operators $L^2(\mathbb{R}^n;\mathcal{H})\to L^2(\mathbb{R}^n)$ defined by ,

$$\mathcal{Z}_u w := \langle w,u\rangle_{\mathcal{H}}\ ;\ \mathcal{Z}_v w := \langle w,v\rangle_{\mathcal{H}}.$$

Then, the symbol $\check{b}$ of the (standard) h-admissible operator $\mathcal{Z}_v B\mathcal{Z}_u^*$ verifies,

$$\forall\,(x,\xi)\in T^*\Omega_j,\;\; \check{b}(x,\xi)=\langle b_j(x,\xi)\sharp u_j(x), v_j(x)\rangle_{\mathcal{H}},$$

where the operation $\sharp$ is defined in an obvious way, by substituting the usual product with the action of an operator (here, the various derivatives of $b_j(x,\xi)$) on a function (here, the various derivatives of $u_j(x)$).

We can clearly apply this remark to compute the symbol of A_2 and A_3, but also that of A_0, since we have,

$$A_0=Z_1\tilde{P}Z_1^*=\mathcal{Z}_u\tilde{P}\mathcal{Z}_u^*=\mathcal{Z}_{Q_0u}Q_0^{-1}\tilde{P}\mathcal{Z}_u^*,$$

with $u:=\tilde{u}_{L'+1}$ (defined in Section 3), and, by Proposition 5.5, we know that $Q_0^{-1}\tilde{P}$ is a twisted PDO.

Combining all the previous computations, using that $\tilde{Q}_j(x)u_j(x)=\lambda(x)u_j(x)$ for all $j=0,\dots,r$ and $x\in\Omega_j$, and gathering (as far as possible) the terms with same homogeneity in h, we finally arrive to the following result (leaving some details to the reader):

Proposition 10.2 *In the case* $\mathrm{Rank}\,\Pi_0(x)=1$*, the effective Hamiltonian* A *verifies (10.6) with,*

$$\begin{aligned}A_0 &= Z_1\tilde{P}Z_1^*;\\ A_2 &= \frac{1}{h^2}Z_1[\tilde{P},\tilde{\Pi}_0]R'(x,\lambda(x))[\tilde{\Pi}_0,\tilde{P}]Z_1^*; \qquad (10.9)\\ A_3 &= \frac{1}{h^3}\,\mathrm{Re}\;Z_1[\tilde{P},\tilde{\Pi}_0]R'(x,\lambda(x))[[[\tilde{P},\tilde{\Pi}_0],R'(x,\lambda(x))],\boldsymbol{\omega}+\zeta W]Z_1^*,\end{aligned}$$

where $\lambda(x)$ *is the (only) eigenvalue of* $\tilde{Q}(x)\tilde{\Pi}_0$*, and* $R'(x,\lambda(x))=\tilde{\Pi}_0^\perp(x)(\lambda(x)-\tilde{Q}(x))^{-1}\tilde{\Pi}_0^\perp(x)$ *is the reduced resolvent of* $\tilde{Q}(x)$*.*

Moreover, the symbol $a(x,\xi;h)$ *of* A *verifies,*

$$a(x,\xi;h)=a_0(x,\xi)+ha_1(x,\xi)+h^2a_2(x,\xi)+\mathcal{O}(h^3),$$

with, for any $(x,\xi)\in T^*\Omega_j$ *(*$j=0,\dots,r$ *arbitrary),*

$$\begin{aligned}a_0(x,\xi) &= \omega(x,\xi;h)+\lambda(x)+\zeta(x)W(x);\\ a_1(x,\xi) &= \sum_{|\beta|\le m-1}\langle\omega_{\beta,j}(x)u_j(x),u_j(x)\rangle\xi^\beta - i\langle\nabla_\xi\omega(x,\xi)\nabla_x u_j(x),u_j(x)\rangle;\\ a_2(x,\xi) &= \sum_{k,\ell=1}^n(\partial_{\xi_k}\omega)(\partial_{\xi_\ell}\omega)\langle\rho_j(x)\partial_{x_k}u_j,\partial_{x_\ell}u_j\rangle-\frac12\sum_{|\alpha|=2}(\partial_\xi^\alpha\omega)\langle\partial_x^\alpha u_j,u_j\rangle\\ &\quad -i\sum_{|\beta|\le m-1}\langle\omega_{\beta,j}(x)\nabla_x u_j(x),u_j(x)\rangle\cdot\nabla_\xi(\xi^\beta)\\ &\quad -2\,\mathrm{Im}\sum_{|\beta|\le m-1}\nabla_\xi\omega(x,\xi)\langle\omega_{\beta,j}(x)\rho_j(x)\nabla_x u_j(x),u_j(x)\rangle\xi^\beta\\ &\quad +\sum_{|\beta|,|\gamma|\le m-1}\langle\omega_{\beta,j}(x)\rho_j(x)u_j(x),\omega_{\beta,j}(x)u_j(x)\rangle\xi^{\beta+\gamma}.\end{aligned}$$

Remark 10.3 *Although some of these terms may seem to depend on the choice of j verifying $(x,\xi)\in T^*\Omega_j$, actually we know that this cannot be the case. In fact, the independency with respect to j is due to the compatibility conditions (4.9) satisfied by the symbols of twisted pseudodifferential operators.*

Remark 10.4 *Actually, it results from the previous computations that (10.9) is still valid in the (slightly) more general case where L is arbitrary and $\lambda_{L'+1}(x)=\ldots=\lambda_{L'+L}(x)$ for all $x\in\Omega$.*

Remark 10.5 *Using (10.7)-(10.8), one can find an expression for the h^3-term of the symbol of A, too. We leave it as an exercise to the reader.*

11 Propagation of Wave-Packets

In this section, we assume $L=1$ and we make the following additional assumption on the coefficients c_α of $\boldsymbol{\omega}$:

$$c_\alpha(x;h)\sim\sum_{k=0}^{\infty}h^k c_{\alpha,k}(x), \tag{11.1}$$

with $c_{\alpha,k}$ independent of h. Then, in a similar spirit as in [Ha6], we investigate the evolution of an initial state of the form,

$$\varphi_0(x)=(\pi h)^{-n/4}f(P)\Pi_g(e^{ix\xi_0/h-(x-x_0)^2/2h}u_{L'+1}(x)), \tag{11.2}$$

where $(x_0,\xi_0)\in T^*\Omega$ is fixed, $f,g\in C_0^\infty(I\!\!R)$ are such that $f=1$ near $a_0(x_0,\xi_0)$ (here, $a_0(x,\xi)$ is the same as in Corollary 2.6), $g=1$ near $\operatorname{Supp} f$, and Π_g is constructed as in Section 6, starting from the operator $\tilde P$ constructed in Section 3 with $K\ni x_0$. In particular, since $e^{-(x-x_0)^2/2h}$ is exponentially small for x outside any neighborhood of x_0, by Lemma 8.2, we have,

$$\varphi_0(x)=(\pi h)^{-n/4}f(\tilde P)\Pi_g(e^{ix\xi_0/h-(x-x_0)^2/2h}\tilde u_{L'+1}(x))+\mathcal{O}(h^\infty),$$

in $L^2(I\!\!R^n;\mathcal{H})$. Moreover, due to the properties of Π_g, and the fact that the coherent state $\phi_0:=(\pi h)^{-n/4}e^{ix\xi_0/h-(x-x_0)^2/2h}$ is normalized in $L^2(I\!\!R^n)$, we also obtain,

$$\varphi_0(x)=(\pi h)^{-n/4}f(\tilde P)e^{ix\xi_0/h-(x-x_0)^2/2h}\tilde u_{L'+1}(x)+\mathcal{O}(h),$$

and thus, in particular, $\|\varphi_0\|=1+\mathcal{O}(h)$. Actually, we even have the following better result:

Proposition 11.1 *The function φ_0 admits, in $L^2(I\!\!R^n;\mathcal{H})$, an asymptotic expansion of the form,*

$$\varphi_0(x)\sim(\pi h)^{-n/4}e^{ix\xi_0/h-(x-x_0)^2/2h}\sum_{k=0}^{\infty}h^k v_k(x)+\mathcal{O}(h^\infty), \tag{11.3}$$

with $v_k \in L^\infty(\mathbb{R}^n;\mathcal{H})$ $(k \geq 0)$, *and* $v_0(x) = \tilde{u}_{L'+1}(x) + \mathcal{O}(|x-x_0|)$ *in* $\mathcal{H}$, *uniformly with respect to* $x \in \mathbb{R}^n$. *Moreover, for any* $j \in \{0,1,\dots,r\}$ *and any* $\chi_j \in C_d^\infty(\Omega_j)$, *the function* $U_j\chi_j\varphi_0$ *admits, in* $C_d^\infty(\Omega_j;\mathcal{H})$, *an asymptotic expansion of the form,*

$$U_j(x)\chi_j(x)\varphi_0(x) \sim (\pi h)^{-n/4} e^{ix\xi_0/h-(x-x_0)^2/2h} \sum_{k=0}^{\infty} h^k \chi_j(x) v_{j,k}(x) + \mathcal{O}(h^\infty), \tag{11.4}$$

with $v_{j,k} \in C^\infty(\Omega_j;\mathcal{H})$, $v_{j,0}(x) = U_j(x)\tilde{u}_{L'+1}(x) + \mathcal{O}(|x-x_0|)$.

Proof For $j = 0,1,\dots,r$, let $\chi_j \in C_d^\infty(\Omega_j)$, such that $\sum \chi_j = 1$, and let $\tilde{\chi}_j \in C_d^\infty(\Omega_j)$, such that $\tilde{\chi}_j = 1$ near $\operatorname{Supp}\chi_j$. Then, since $f(\tilde{P})$ and Π_g are twisted h-admissible operators, have,

$$\begin{aligned}
\varphi_0 &= \sum_j \chi_j \varphi_0 \\
&= \sum_j U_j^{-1}\tilde{\chi}_j U_j \chi_j f(\tilde{P}) \tilde{\chi}_j^2 \Pi_g \tilde{\chi}_j^2 (\phi_0(x)\tilde{u}_{L'+1}(x)) + \mathcal{O}(h^\infty) \\
&= \sum_j U_j^{-1}\tilde{\chi}_j U_j \chi_j f(\tilde{P}) U_j^{-1}\tilde{\chi}_j U_j \tilde{\chi}_j \Pi_g \tilde{\chi}_j^2 (\phi_0(x)\tilde{u}_{L'+1}(x)) + \mathcal{O}(h^\infty),
\end{aligned}$$

and thus, by Lemma 15.1, and setting $\tilde{P}_j := U_j\tilde{\chi}_j\tilde{P}U_j^{-1}\tilde{\chi}_j$, $\Pi_{g,j} := U_j\tilde{\chi}_j\Pi_g U_j^{-1}\tilde{\chi}_j$, and $u_{L'+1,j}(x) := U_j(x)\tilde{\chi}_j(x)\tilde{u}_{L'+1}(x)$ ($\in C_d^\infty(\Omega_j;\mathcal{H})$), we obtain,

$$\varphi_0 = \sum_{j=0}^{r} U_j^{-1}\chi_j f(\tilde{P}_j)\Pi_{g,j}(\phi_0(x)u_{L'+1,j}(x)) + \mathcal{O}(h^\infty). \tag{11.5}$$

Now, using the results of Sections 4 and 6, we see that $f(\tilde{P}_j)\Pi_{g,j}$ is an h-admissible operator on $L^2(\mathbb{R}^n;\mathcal{H})$, with symbol b_j verifying,

$$\begin{aligned}
&b_j(x,\xi;h) \sim \sum_{k=0}^{\infty} h^k b_{j,k}(x,\xi); \\
&b_{j,0}(x,\xi) = f(\tilde{\chi}_j(x)^2(\omega_0(x,\xi) + \tilde{Q}_j(x) + W(x)))\tilde{\chi}_j(x)^2\tilde{\Pi}_{0,j}(x),
\end{aligned}$$

where $\omega_0(x,\xi) := \sum_{|\alpha|\leq m} c_{\alpha,0}(x)\xi^\alpha$, $\tilde{Q}_j(x) = U_j(x)\tilde{Q}(x)U_j(x)^{-1}$, and $\tilde{\Pi}_{0,j}(x) = U_j(x)\tilde{\Pi}_0(x)U_j(x)^{-1}$. Moreover, we have,

$$\operatorname{Op}_h(b_j)(\phi_0 u_{L'+1,j})(x;h) = \frac{1}{(2\pi h)^n}\int e^{i(x-y)\xi/h+iy\xi_0/h}\rho(x,y,\xi;h)\,dy\,d\xi,$$

with,

$$\rho(x,y,\xi;h) = (\pi h)^{-n/4}e^{-(y-x_0)^2/2h}b_j(x,\xi;h)u_{L'+1,j}(y),$$

and it is easy to check that, for any $\alpha,\beta \in \mathbb{N}^n$, one has,

$$\|(hD_y)^\alpha (hD_\xi)^\beta \rho(x,y,\xi;h)\|_{\mathcal{H}} = \mathcal{O}(h^{|\alpha|/2+|\beta|}),$$

uniformly for $(x, y, \xi) \in I\!R^{3n}$ and $h > 0$ small enough. As a consequence, we can perform a standard stationary phase expansion in the previous (oscillatory) integral (see, e.g., [DiSj1, Ma2]), and since the unique critical point is given by $y = x$ and $\xi = \xi_0$, we obtain,

$$\mathrm{Op}_h(b_j)(\phi_0 v_j)(x; h) = e^{ix\xi_0/h} w_j(x; h) + \mathcal{O}(h^\infty),$$

with,

$$w_j(x; h) \sim \sum_{k=0}^{\infty} \frac{h^k}{i^k k!} (\nabla_y \cdot \nabla_\xi)^k \rho(x, y, \xi; h) \Big|_{\substack{y=x \\ \xi=\xi_0}} .$$

Therefore, since $e^{(y-x_0)^2/2h} \nabla_y e^{-(y-x_0)^2/2h} = \nabla_y - \frac{y-x_0}{h}$, and, for any $k \in I\!N$, $|y - x_0|^k e^{-(y-x_0)^2/2h} = \mathcal{O}(h^{k/2})$, we also obtain,

$$\mathrm{Op}_h(b_j)(\phi_0 u_{L'+1,j})(x; h) = (\pi h)^{-n/4} e^{ix\xi_0/h - (x-x_0)^2/2h} \tilde{w}_j(x; h),$$

with,

$$\tilde{w}_j(x, h) = \sum_{k=0}^{N} \frac{h^k}{i^k k!} ((\nabla_y - h^{-1}(y - x_0)) \cdot \nabla_\xi)^k b_j(x, \xi; h) u_{L'+1,j}(y) \Big|_{\substack{y=x \\ \xi=\xi_0}} + \mathcal{O}(h^{N/2}), \tag{11.6}$$

for any $N \geq 0$. Then, taking a ressummation of the formal series in $(x - x_0)$ obtained for each degree of homogeneity in h in (11.6), we obtain an asymptotic expansion of $\tilde{w}_j$, of the form,

$$\tilde{w}_j(x, h) \sim \sum_{k=0}^{\infty} h^k \tilde{w}_{j,k}(x).$$

(Alternatively – and equivalently – one could have used instead the stationary phase theorem with complex-valued phase function [MeSj1] Theorem 2.3, with the phase $(x - y)\xi + y\xi_0 + i(y - x_0)^2/2$.) In particular, the first coefficient $\tilde{w}_{j,0}(x)$ is obtained as a resummation of the formal series $\sum_{k\geq 0} \frac{i^k}{k!}((y - x_0)) \cdot \nabla_\xi)^k b_j(x, \xi; h) u_{L'+1,j}(y) \Big|_{\substack{y=x \\ \xi=\xi_0}}$, and thus,

$$\begin{aligned}
\tilde{w}_{j,0}(x)(x) &= b_j(x, \xi_0; h) u_{L'+1,j}(x) + \mathcal{O}(|x - x_0|) \\
&= f(\tilde{X}_j(x)^2(\omega_0(x, \xi_0) + \tilde{Q}_j(x) + W(x))) \tilde{X}_j(x)^2 u_{L'+1,j}(x) \\
&\qquad + \mathcal{O}(|x - x_0|) \\
&= f(\tilde{X}_j(x)^2(\omega_0(x, \xi_0) + \lambda_{L'+1}(x) + W(x))) \tilde{X}_j(x)^2 u_{L'+1,j}(x) \\
&\qquad + \mathcal{O}(|x - x_0|) \\
&= f(\tilde{X}_j(x)^2(a_0(x_0, \xi_0))\tilde{X}_j(x)^2 u_{L'+1,j}(x) + \mathcal{O}(|x - x_0|).
\end{aligned}$$

Going back to (11.5), this gives an asymptotic expansion for φ_0 of the form (11.3), with,

$$v_0(x) = \sum_{j=0}^{r} U_j(x)^{-1} \chi_j(x) f(\tilde{X}_j(x)^2 a_0(x_0, \xi_0)) u_{L'+1,j}(x) + \mathcal{O}(|x - x_0|)$$

$$\begin{aligned} &= \sum_{j=0}^{r} U_j(x)^{-1}\chi_j(x) f(a_0(x_0,\xi_0)) u_{L'+1,j}(x) + \mathcal{O}(|x-x_0|) \\ &= \sum_{j=0}^{r} U_j(x)^{-1}\chi_j(x) u_{L'+1,j}(x) + \mathcal{O}(|x-x_0|) \\ &= \tilde{u}_{L'+1}(x) + \mathcal{O}(|x-x_0|). \end{aligned}$$

The asymptotic expansion (11.4) is obtained exactly in the same way. •

As a consequence, we also obtain,

Proposition 11.2 *For any $j \in \{0, 1, \dots, r\}$, one has,*

$$FS(U_j\varphi_0) = \{(x_0, \xi_0)\} \cap T^*\Omega_j.$$

Proof For $\chi_j \in C_d^\infty(\Omega_j)$ fixed, we denote by $w_j(x; h)$ a resummation of the formal series $\sum_{k\geq 0} h^k U_j(x)\chi_j(x) v_{j,k}(x)$ in $C_d^\infty(\Omega_j; \mathcal{H})$, where the $v_{j,k}$'s are those in (11.4). Then, defining,

$$\begin{aligned} A = A(x, hD_x) &:= (hD_x - \xi_0)^2 + (x - x_0)^2 \\ &= (hD_x - \xi_0 + i(x - x_0)) \cdot (hD_x - \xi_0 - i(x - x_0)) + nh, \end{aligned}$$

a straightforward computation gives,

$$A(U_j\varphi_0) = A(\phi_0(x) w_j(x; h)) + \mathcal{O}(h^\infty) = h\phi_0(x) B w_j(x; h) + \mathcal{O}(h^\infty)$$

with $Bw_j(x; h) := 2i(x - x_0) \cdot \partial_x w_j - ih\partial_x^2 w_j + nw_j$, and thus, by an iteration,

$$A^N(\phi_0(x) w_j(x; h)) = h^N \phi_0(x) B^N w_j + \mathcal{O}(h^\infty),$$

for any $N \geq 1$. In particular, due to the form of B, and since $\|(x - x_0)^\alpha \phi_0\| = \mathcal{O}(1)$ for any $\alpha \in \mathbb{N}^n$ (actually, $\mathcal{O}(h^{|\alpha|/2})$), we obtain,

$$\|A^N(U_j\varphi_0)\|_{L^2(\Omega_j', \mathcal{H})} = \mathcal{O}(h^N),$$

for any $\Omega_j' \subset\subset \Omega_j$. Now, if $(x_1, \xi_1) \in T^*\Omega_j$ is different from (x_0, ξ_0), then A^N is elliptic at (x_1, ξ_1) and thus, given any $\chi \in C_0^\infty(T^*\Omega_j)$ with $\chi(x_1, \xi_1) = 1$, the standard construction of a microlocal parametrix (see, e.g., [DiSj1]) gives an uniformly bounded operator A_N' , such that,

$$A_N' \circ A^N = \chi(x, hD_x) + \mathcal{O}(h^\infty).$$

As a consequence, we obtain,

$$\|\chi(x, hD_x)(U_j\varphi_0)\|_{L^2(\Omega_j', \mathcal{H})} = \mathcal{O}(h^N),$$

for all $N \geq 1$. Therefore $(x_1, \xi_1) \notin FS(\phi_0(x) v_j(x))$, and thus, we have proved,

$$FS(U_j\varphi_0) \subset \{(x_0, \xi_0)\} \cap T^*\Omega_j.$$

This means that $FS(U_j\varphi_0)$ consists in at most one point. Conversely, if $x_0 \in \Omega_j$ and $FS(U_j\varphi_0) = \emptyset$, by the ellipticity of A^N as $|\xi| \to \infty$, we would have (see, e.g., [Ma2] Prop. 2.9.7),

$$\|U_j\varphi_0\|_{\Omega_j'} = \mathcal{O}(h^\infty),$$

for any $\Omega_j' \subset\subset \Omega_j$. But this contradicts the fact that $\|U_j\varphi_0\|_{\Omega_j'} = \|\varphi_0\|_{\Omega_j'} = 1 + \mathcal{O}(h)$ if $x_0 \in \Omega_j'$. •

Now, applying Theorem 2.1 and Corollary 2.6 (or rather Remark 2.8), we obtain,

$$e^{itP/h}\varphi_0 = \mathcal{W}^* e^{-itA/h}\mathcal{W}\varphi_0 + \mathcal{O}(\langle t\rangle h^\infty), \tag{11.7}$$

uniformly for $t \in [0, T_{\Omega'}(x_0,\xi_0))$,where $\Omega' \subset\subset \Omega$ is the same as the one used to define $\tilde{P}$ in Section 3, and

$$T_{\Omega'}(x_0,\xi_0) := \sup\{T > 0\,;\, \pi_x(\cup_{t\in[0,T]} \exp tH_{a_0}(x_0,\xi_0)) \subset \Omega'\}. \tag{11.8}$$

Moreover, by Lemma 9.1 and Proposition 11.2, we see that,

$$FS(\mathcal{W}\varphi_0) = \{(x_0,\xi_0)\}. \tag{11.9}$$

Assuming, e.g., that $x_0 \in \Omega_1$, and taking $\chi_1 \in C_0^\infty(\Omega_1)$ such that $\chi_1 = 1$ in a neighborhood of x_0, we also have,

$$\mathcal{W}\varphi_0 = \mathcal{W}\chi_1^2\varphi_0 + \mathcal{O}(h^\infty) = \mathcal{W}U_1^{-1}\chi_1 U_1\chi_1\varphi_0 + \mathcal{O}(h^\infty),$$

and therefore, using (11.4), (7.7), and the fact that $\mathcal{W}U_1^{-1}\chi_1$ is an h-admissible operator from $L^2(I\!R^n;\mathcal{H})$ to $L^2(I\!R^n)$ (see Theorem 7.1), we obtain as before (by a stationary phase expansion),

$$\mathcal{W}\varphi_0(x;h) \sim (\pi h)^{-n/4} e^{ix\xi_0/h-(x-x_0)^2/2h} \sum_{k=0}^{\infty} h^k w_k(x) + \mathcal{O}(h^\infty), \tag{11.10}$$

with $w_k \in C_b^\infty(I\!R^n)$, $w_0(x) = \langle \tilde{u}_{L'+1}(x), \tilde{u}_{L'+1}(x)\rangle + \mathcal{O}(|x-x_0|) = 1 + \mathcal{O}(|x-x_0|)$, and where the asymptotic expansion takes place in $C_b^\infty(I\!R^n)$.

This means that $\mathcal{W}\varphi_0$ is a coherent state in $L^2(I\!R^n)$, centered at (x_0,ξ_0), and from this point we can apply all the standard (and less standard) results of semiclassical analysis for scalar operators, in order to compute $e^{-itA/h}\mathcal{W}\varphi_0$ (see, e.g., [CoRo, Ha1, Ro1, Ro2] and references therein). In particular, we learn from [CoRo] Theorem 3.1 (see also [Ro2]), that, for any $N \geq 1$,

$$e^{-itA/h}\mathcal{W}\varphi_0 = e^{i\delta_t/h} \sum_{k=0}^{3(N-1)} c_k(t;h)\Phi_{k,t} + \mathcal{O}(e^{NC_0 t}h^{N/2}), \tag{11.11}$$

where $\Phi_{k,t}$ is a (generalized) coherent state centered at $(x_t,\xi_t) := \exp tH_{a_0}(x_0,\xi_0)$, $\delta_t := \int_0^t (\dot{x}_s\xi_s - a_0(x_s,\xi_s))ds + (x_0\xi_0 - x_t\xi_t)/2$, $C_0 > 0$ is a constant, the coefficients $c_k(t;h)$'s are of the form,

$$c_k(t;h) = \sum_{\ell=0}^{N_k} h^\ell c_{k,\ell}(t), \tag{11.12}$$

with $c_{k,\ell}$ universal polynomial with respect to $(\partial^\gamma a_0(x_t,\xi_t))_{|\gamma|\leq M_k}$, and where the estimate is uniform with respect to (t,h) such that $0\leq t<T_{\Omega'}(x_0,\xi_0)$ and he^{C_0t} remains bounded ($h>0$ small enough). In particular, (11.11) supplies an asymptotic expansion of $e^{-itA/h}\mathcal{W}\varphi_0$ if one restricts to the values of t such that $0\leq t<<\ln\frac{1}{h}$.

Now, applying $\mathcal{W}^*$ to (11.11), and observing that $\mathcal{W}^*\Phi_{k,t}=\mathcal{V}^*(\Phi_{k,t}\tilde{u}_{L'+1})=U_j^{-1}\mathcal{V}_j^*(\Phi_{k,t}u_{L'+1,j})$, where $j=j(t)$ is chosen in such a way that $\exp tH_{a_0}(x_0,\xi_0)\in\Omega_j$, and where $\mathcal{V}_j^*:=U_j\mathcal{V}^*U_j^{-1}$ is an h-admissible operator on $L^2(\Omega_j;\mathcal{H})$ (that is, becomes an h-admissible operator on $L^2(I\!R^n;\mathcal{H})$ once sandwiched by cutoff functions supported in Ω_j), we deduce from (11.7),

Theorem 11.3 *Let φ_0 be as in (11.2), and let $T_{\Omega'}(x_0,\xi_0)$ defined in (11.8). Then, there exists $C>0$ such that, for any $N\geq 1$, one has,*

$$e^{-itP/h}\varphi_0=e^{i\delta_t/h}\sum_{k=0}^{3(N-1)}c_k(t;h)\Phi_{k,t}U_{j(t)}^{-1}\tilde{v}_{k,j(t)}(x)+\mathcal{O}(h^{N/4}),$$

where $\Phi_{k,t}$ is a coherent state centered at $(x_t,\xi_t):=\exp tH_{a_0}(x_0,\xi_0)$, $j(t)\in\{1,\dots,r\}$ is such that $\exp tH_{a_0}(x_0,\xi_0)\in\Omega_{j(t)}$, $\tilde{v}_{k,j(t)}\in C^\infty(\Omega_{j(t)};\mathcal{H})$, $c_k(t;h)$ is as in (11.12), $\delta_t:=\int_0^t(\dot{x}_s\xi_s-a_0(x_s,\xi_s))ds+(x_0\xi_0-x_t\xi_t)/2$, and where the estimate is uniform with respect to (t,h) such that $h>0$ is small enough and $t\in[0,\min(T_{\Omega'}(x_0,\xi_0),C^{-1}\ln\frac{1}{h}))$.

Remark 11.4 *Actually, the coherent state $\Phi_{k,t}$ is of the form,*

$$\Phi_{k,t}=c_k(t)f_k(x,\sqrt{h})h^{-n/4}e^{ix\xi_t/h-q_t(x-x_t)/h},$$

where $c_k(t)$ is a normalizing factor, f_k is polynomial in 2 variables, and q_t is a t-dependent quadratic form with positive-definite real part, that can be explicitly computed by using a classical evolution involving the Hessian of a_0 at (x_t,ξ_t) (see [CoRo]). More precisely, one has $q_t(x)=-i\langle\Gamma_t x,x\rangle/2$ with $\Gamma_t=(C_t+iD_t)(A_t+iB_t)^{-1}$, where the $2n\times 2n$ matrix,

$$F_t=\begin{pmatrix}A_t & B_t\\ C_t & D_t\end{pmatrix}$$

is, by definition, the solution of the classical problem,

$$\dot{F}_t=J\mathrm{Hess}\,a_0(x_t,\xi_t)F_t\quad;\quad F(0)=I_{2n}.$$

Here, $J:=\begin{pmatrix}0 & I_n\\ -I_n & 0\end{pmatrix}$, and $\mathrm{Hess}\,a_0$ stands for the Hessian of a_0. (We are grateful to M. Combescure and D. Robert for having explained to us this construction and the main result of [CoRo].)

Remark 11.5 *As in [CoRo], one can also consider more general initial states, of the form,*

$$\varphi_0(x)=e^{i(\xi_0\cdot x-x_0\cdot hD_x)/h}f\left(\frac{x}{\sqrt{h}}\right),$$

where $f \in \mathcal{S}(I\!R^n)$ (we refer to [CoRo] Theorem 3.5 for more details). In the same way, a similar result can also be obtained for oscillating initial states of the form,

$$\varphi_0(x) = f(x)e^{iS(x)/h},$$

where $f \in C_0^\infty(I\!R^n)$ and $S \in C^\infty(I\!R^n; I\!R)$ (see [CoRo] Remark 3.9).

Remark 11.6 *In principle, all the terms of the asymptotic series can be computed explicitly by an inductive procedure (although, in practical, this task may result harder than expected since the simplifications are sometimes quite tricky). Indeed, all our constructions mainly rely on symbolic pseudodifferential calculus, that provides very explicit inductive formulas.*

12 Application to Polyatomic Molecules

In this section, we apply all the previous results to the particular case of a polyatomic molecule with Coulomb-type interactions, imbedded in an electromagnetic field. Denoting by $x = (x_1, \dots, x_n) \in I\!R^{3n}$ the position of the n nuclei, and by $y = (y_1, \dots, y_p) \in I\!R^{3p}$ the position of the p electrons, the corresponding Hamiltonian takes the form,

$$H = \sum_{j=1}^{n} \frac{1}{2M_j}(D_{x_j} - A(x_j))^2 + \sum_{k=1}^{p} \frac{1}{2m_k}(D_{y_k} - A(y_k))^2 + V(x,y), \qquad (12.1)$$

where the magnetic potential A is assumed to be in $C_b^\infty(I\!R^3)$, and where the electric potential V can be written as,

$$V(x,y) = V_{\rm nu}(x) + V_{\rm el}(y) + V_{\text{el-nu}}(x,y) + V_{\rm ext}(x,y) = V_{\rm int}(x,y) + V_{\rm ext}(x,y). \qquad (12.2)$$

Here, $V_{\rm nu}$ (resp. $V_{\rm el}$, resp. $V_{\text{el-nu}}$) stands for sum of the nucleus-nucleus (resp. electron-electron, resp. electron-nucleus) interactions, and $V_{\rm ext}$ stands for the external electric potential. Actually, our techniques can be applied to a slightly more general form of Hamiltonian (also allowing, somehow, a strong action of the magnetic field upon the nuclei), namely,

$$H = \sum_{j=1}^{n} \frac{1}{2M_j}(D_{x_j} - a_jA_j(x))^2 + \sum_{k=1}^{p} \frac{1}{2m_k}(D_{y_k} - B_k(x,y))^2 + V(x,y), \qquad (12.3)$$

where $A_1, \dots, A_n$ (respectively $B_1, \dots, B_p$) are assumed to be in $C_b^\infty(I\!R^n; I\!R)$ (respectively $C_b^\infty(I\!R^{n+p}; I\!R)$), the a_j's are extra parameters, and V is as in (12.2) with,

$$V_{\rm nu}(x) = \sum_{1 \le j < j' \le n} \frac{\alpha_{j,j'}}{|x_j - x_{j'}|} \quad ; \quad V_{\rm el}(y) = \sum_{1 \le k < k' \le p} \frac{\beta_{k,k'}}{|y_k - y_{k'}|} \ ;$$

$$V_{\text{el-nu}}(x,y) = \sum_{\substack{1 \le j \le n \\ 1 \le k \le p}} \frac{-\gamma_{j,k}}{|x_j - y_k|} \quad ; \quad V_{ext} \in C_b^\infty(I\!R^{n+p}; I\!R), \qquad (12.4)$$

$\alpha_{j,j'}, \beta_{k,k'}, \gamma_{j,k} > 0$ constant. In fact, as in [KMSW], more general forms can be allowed for the interaction potentials, e.g., by replacing any function of the type $|z_j - z'_k|^{-1}$ (where the letters z and z' stand for x or y indifferently) by some $V_{j,k}(z_j - z'_k)$, where $V_{j,k}$ is assumed to be Δ-compact on $L^2(I\!\!R^3)$ and to verify some estimates on its derivatives (see [KMSW] Section 2). In the same way, one could also have admitted singularities of the same kind for the exterior potentials. However, here we keep the form (12.4) since it is more concrete and corresponds to the usual physical situation.

Then, we consider the Born-Oppenheimer limit in the following sense: We set,

$$M_j = h^{-2}b_j \, ; \, a_j = h^{-1}c_j + d_j, \tag{12.5}$$

and we consider the limit $h \to 0_+$ for some fix $b_j, m_k > 0$, $c_j, d_j \in I\!\!R$. By scaling the time variable, too, the quantum evolution of the molecule is described by the Schrödinger equation,

$$ih\frac{\partial \varphi}{\partial t} = P(h)\varphi,$$

where,

$$P(h) := \sum_{j=1}^{n} \frac{1}{2b_j}(hD_{x_j} - (c_j + hd_j)A_j(x))^2 + \sum_{k=1}^{p} \frac{1}{2m_k}(D_{y_k} - B_k(x,y))^2 + V(x,y). \tag{12.6}$$

In particular, we see that $P(h)$ satisfies to Assumptions (H1) and (H2), with,

$$\boldsymbol{\omega} = \sum_{j=1}^{n} \frac{1}{2b_j}(hD_{x_j} - (c_j + hd_j)A_j(x))^2,$$

$$\omega(x,\xi;h) = \sum_{j=1}^{n} \frac{1}{2b_j}\left[(\xi_j - (c_j + hd_j)A_j(x))^2 + ih(c_j + hd_j)(\partial_{x_j}A_j)(x)\right],$$

$$Q(x) = \sum_{k=1}^{p} \frac{1}{2m_k}(D_{y_k} - B_k(x,y))^2 + V_{\text{el}}(y) + V_{\text{el-nu}}(x,y) + V_{\text{ext}}(x,y),$$

$$W(x) = V_{\text{nu}}(x).$$

Now, following the terminology of [KMSW], we denote by

$$\mathcal{C} := \bigcup_{\substack{1 \le j,k \le n \\ j \ne k}} \{x = (x_1, \dots, x_n) \in I\!\!R^{3n} \, ; \, x_j = x_k\}$$

the so-called *collision set* of nuclei, and we make on $Q(x)$ the following gap condition:

$(H3')$ There exists a contractible bounded open set $\Omega \subset I\!\!R^{3n}$ such that $\overline{\Omega} \cap \mathcal{C} = \emptyset$, and, for all $x \in \overline{\Omega}$, the $L' + L$ first values $\lambda_1(x), \dots, \lambda_{L'+L}(x)$, given by the Mini-Max principle for $Q(x)$ on $L^2(I\!\!R^{3p})$, are discrete eigenvalues of $Q(x)$, and verify,

$$\inf_{x \in \Omega} \text{dist} \, (\sigma(Q(x)) \backslash \{\lambda_{L'+1}(x), \dots, \lambda_{L'+L}(x)\}, \{\lambda_{L'+1}(x), \dots, \lambda_{L'+L}(x)\}) > 0.$$

As it is well known (see [CoSe]), under these assumptions the spectral projections $\Pi_0^-(x)$ and $\Pi_0(x)$ of $Q(x)$, corresponding to $\{\lambda_1(x),\dots,\lambda_{L'}(x)\}$ and $\{\lambda_{L'+1}(x),\dots,\lambda_{L'+L}(x)\}$ respectively, are twice differentiable with respect to $x\in\Omega$. In particular, the whole assumption (H3) is indeed satisfied in that case (and even with a slightly larger open subset of $I\!R^{3n}$).

Now, in order to be able to apply the results of the previous sections to this molecular Hamiltonian, it remains to construct a family $(\Omega_j, U_j(x))_{1\le j\le r}$ that verifies Assumption (H4). We do it by following [KMSW].

More precisely, for any fixed $x_0=(x_1^0,\dots,x_n^0)\in I\!R^{3n}\backslash\mathcal{C}$, we choose n functions $f_1,\dots,f_n\in C_0^\infty(I\!R^3;I\!R)$, such that,

$$f_j(x_k^0)=\delta_{j,k}\ \ (1\le j,k\le n),$$

and, for $x\in I\!R^{3n}$, $s\in I\!R^3$, and $y=(y_1,\dots,y_p)\in I\!R^{3p}$, we set,

$$\begin{aligned}
F_{x_0}(x,s) &:= s+\sum_{k=1}^n (x_k-x_k^0)f_k(s)\in I\!R^3,\\
G_{x_0}(x,y) &:= (F_{x_0}(x,y_1),\dots,F_{x_0}(x,y_p))\in I\!R^{3p}.
\end{aligned}$$

Then, by the implicit function theorem, for x in a sufficiently small neighborhood Ω_{x_0} of x_0, the application $y\mapsto G_{x_0}(x,y)$ is a diffeomorphism of $I\!R^{3p}$, and we have,

$$\begin{aligned}
&x_k=F_{x_0}(x,x_k^0),\\
&G_{x_0}(x,y)=y \text{ for } |y| \text{ large enough.}
\end{aligned}$$

Now, for $v\in L^2(I\!R^{3p})$ and $x\in\Omega_{x_0}$, we define,

$$U_{x_0}(x)v(y):=|\det d_yG_{x_0}(x,y)|^{\frac12}v(G_{x_0}(x,y))|,$$

and we see that $U_{x_0}(x)$ is a unitary operator on $L^2(I\!R^{3p})$ that preserves both $\mathcal{D}_Q=H^2(I\!R^{3p})$ and $C_0^\infty(I\!R^{3p})$. Moreover, denoting by U_{x_0} the operator on $L^2(\Omega_{x_0}\times I\!R^{3p})$ induced by $U_{x_0}(x)$, we have the following identities:

$$\begin{aligned}
&U_{x_0}hD_xU_{x_0}^{-1}=hD_x+hJ_1(x,y)D_y+hJ_2(x,y),\\
&U_{x_0}D_yU_{x_0}^{-1}=J_3(x,y)D_y+J_4(x,y),\\
&U_{x_0}\frac{1}{|y_k-y_k'|}U_{x_0}^{-1}=\frac{1}{|F_{x_0}(x,y_k)-F_{x_0}(x,y_k'),|}\\
&U_{x_0}\frac{1}{|x_j-y_k|}U_{x_0}^{-1}=\frac{1}{|F_{x_0}(x,x_j^0)-F_{x_0}(x,y_k)|},
\end{aligned}\tag{12.7}$$

where the (matrix or operator-valued) functions J_ν's $(1\le\nu\le4)$ are all smooth on $\Omega_{x_0}\times I\!R^{3p}$. Indeed, denoting by $\tilde G_{x_0}(x,\cdot)$ the inverse diffeomorphism of $G_{x_0}(x,\cdot)$, one finds,

$$J_1(x,y)\ \ =\ \ ({}^td_x\tilde G_{x_0})(x,y'=G_{x_0}(x,y)),$$

$$
\begin{aligned}
J_2(x,y) &= |\det d_y G_{x_0}(x,y)|^{\frac12} D_x \left(|\det d_{y'} \tilde{G}_{x_0}(x,y')|^{\frac12} \right) \Big|_{y'=G_{x_0}(x,y))} , \\
J_3(x,y) &= ({}^t d_{y'} \tilde{G}_{x_0})(x, y' = G_{x_0}(x,y)), \\
J_4(x,y) &= |\det d_y G_{x_0}(x,y)|^{\frac12} D_{y'} \left(|\det d_{y'} \tilde{G}_{x_0}(x,y')|^{\frac12} \right) \Big|_{y'=G_{x_0}(x,y))} .
\end{aligned}
$$

The key-point in (12.7) is that the (x-dependent) singularity at $y_k = x_j$ has been replaced by the (fix) singularity at $y_k = x_j^0$. Then, as in [KMSW], one can easily deduce that the map $x \mapsto U_{x_0} Q(x) U_{x_0}^{-1}$ is in $C^\infty(\Omega_{x_0}; \mathcal{L}(H^2(I\!R^{3p}), L^2(I\!R^{3p}))$. Moreover, so is the map $x \mapsto U_{x_0} \Delta_y U_{x_0}^{-1}$, and we also see that $U_{x_0} \boldsymbol{\omega} U_{x_0}^{-1}$ can be written as in (2.3) (with Ω_{x_0} instead of Ω_j, $m = 2$, and $Q_0 = -\Delta_y + C_0$, $C_0 > 0$ large enough). Indeed, with the notations of (12.7), and setting $\mathcal{J}(x) = (\mathcal{J}_1(x), \dots, \mathcal{J}_n(x)) := J_1(x,y) D_y + J_2(x,y)$, we have,

$$
\begin{aligned}
U_{x_0} \boldsymbol{\omega} U_{x_0}^{-1} &= \sum_{k=1}^n \frac{1}{2b_k} (hD_{x_k} + h\mathcal{J}_k(x) - (c_k + hd_k) A_k(x))^2 \\
&= \boldsymbol{\omega} + h \sum_{k=1}^n \frac{1}{b_k} \mathcal{J}_k (hD_{x_k} - c_k A_k) \qquad (12.8) \\
&\quad + h^2 \sum_{k=1}^n \frac{1}{2b_k} (\mathcal{J}_k^2 - i(\nabla_x \mathcal{J}_k) - 2 d_k A_k \mathcal{J}_k).
\end{aligned}
$$

To complete the argument, we just observe that the previous construction can be made around any point x_0 of $\overline{\Omega}$, and since this set is compact, we can cover it by a finite family $\tilde{\Omega}_1, \dots, \tilde{\Omega}_r$ of open sets such that each one corresponds to some Ω_{x_0} as before. Denoting also $U_1(x), \dots, U_r(x)$ the corresponding operators $U_{x_0}(x)$, and setting $\Omega_j = \tilde{\Omega}_j \cap \Omega$, we can conclude that the family $(\Omega_j, U_j(x))_{1 \le j \le r}$ verifies (H4) with $\mathcal{H}_\infty = C_0^\infty(I\!R^{3p})$. As a consequence, we can apply to this model all the results of the previous sections, and thus, we have proved,

Theorem 12.1 *Let $P(h)$ be as in (12.6) with V given by (12.2) and (12.4), $A_1, \dots, A_n \in C_b^\infty(I\!R^n; I\!R)$, and $B_1, \dots, B_p \in C_b^\infty(I\!R^{n+p}; I\!R)$. Assume also (H3'). Then, the conclusions of Theorem 2.1 are valid for $P = P(h)$.*

We also observe that, in this case, we have,

$$
\omega(x,\xi;h) = \omega_0(x,\xi) + h\omega_1(x,\xi) + h^2\omega_2(x),
$$

with,

$$
\begin{aligned}
\omega_0(x,\xi) &= \sum_{k=1}^n \frac{1}{2b_k} (\xi_k - c_k A_k(x))^2 \\
\omega_1(x,\xi) &= \sum_{k=1}^n \frac{1}{2b_k} \left[2 d_k A_k(x) (c_k A_k(x) - \xi_k) + i c_k (\partial_{x_k} A_k)(x) \right] \qquad (12.9) \\
\omega_2(x) &= \sum_{k=1}^n \frac{1}{2b_k} \left[d_k^2 A_k(x)^2 + i d_k (\partial_{x_k} A_k)(x) \right].
\end{aligned}
$$

In particular, the conditions (2.6) and (11.1) are satisfied, and thus, we also have,

Theorem 12.2 *Let $P(h)$ be as in (12.6) with V given by (12.2) and (12.4), $A_1, \dots, A_n \in C_b^\infty(I\!R^n; I\!R)$, and $B_1, \dots, B_p \in C_b^\infty(I\!R^{n+p}; I\!R)$. Assume also (H3') and $L = 1$. Then, the conclusions of Corollary 2.6 and Theorem 11.3 are valid for $P = P(h)$.*

Moreover, concerning the symbol of the effective Hamiltonian, in that case we have,

Theorem 12.3 *Let $P(h)$ be as in (12.6) with V given by (12.2) and (12.4), $A_1, \dots, A_n \in C_b^\infty(I\!R^n; I\!R)$, and $B_1, \dots, B_p \in C_b^\infty(I\!R^{n+p}; I\!R)$. Assume also (H3') and $L = 1$. Then, the symbol $a(x, \xi; h)$ of the effective Hamiltonian verifies,*

$$a(x, \xi; h) = a_0(x, \xi) + ha_1(x, \xi) + h^2 a_2(x, \xi) + \mathcal{O}(h^3),$$

with, for $(x, \xi) \in T^*(\Omega)$,

$$\begin{aligned}
a_0(x, \xi) &= \omega_0(x, \xi) + \lambda_{L'+1}(x) + W(x); \\
a_1(x, \xi) &= \omega_1(x, \xi) - i\nabla_\xi \omega_0(x, \xi)\langle \nabla_x u(x), u(x)\rangle \\
a_2(x, \xi) &= \sum_{k=1}^n \frac{1}{2b_k}\langle (D_{x_k} - d_k A_k(x))^2 u(x), u(x)\rangle \\
&\quad + \sum_{k,\ell=1}^n \frac{1}{b_k b_\ell}(\xi_k - c_k A_k)(\xi_\ell - c_\ell A_\ell)\langle R'(x, \lambda(x))\nabla_{x_k} u, \nabla_{x_\ell} u\rangle,
\end{aligned}$$

where ω_0 and ω_1 are defined in (12.9).

Proof A possible proof may consist in using Proposition 10.2. Then, observing (with the notations of (12.8)) that, by definition,

$$\mathcal{J} = U_{x_0} D_x U_{x_0}^{-1} - D_x, \tag{12.10}$$

and, exploiting the fact that the $(L' + 1)$-th normalized eigenstate $u(x)$ of $Q(x)$ is a twice differentiable function of x with values in $L^2(I\!R^{2p})$ (see , e.g., [CoSe], but this is also an easy consequence of (12.10) and the fact that $x \mapsto U_{x_0}(x)u(x)$ is smooth), and setting $v(x) = U_{x_0}(x)u(x)$, one can write,

$$\langle \mathcal{J} v, v\rangle_{\mathcal{H}} = \langle D_x u, u\rangle_{\mathcal{H}} - \langle D_x v, v\rangle_{\mathcal{H}}.$$

As a consequence, one also finds,

$$\sum_{k=1}^n \frac{1}{b_k}(\xi_k - c_k A_k)\langle \mathcal{J}_k v, v\rangle_{\mathcal{H}} - i\langle \nabla_\xi \omega_0 \nabla_x v, v\rangle_{\mathcal{H}} = -i\langle \nabla_\xi \omega_0 \nabla_x u, u\rangle_{\mathcal{H}}.$$

where ω_ℓ $(0 \le \ell \le 2)$ are defined in (12.9), and this permits to make appear many cancellations in the expression of $a(x, \xi; h)$ given in Proposition 10.2, leading to the required formulas.

However, there is a much simpler way to prove it, using directly the expressions (10.9) given in Proposition 10.2 for the operator A. Indeed, since in our case $x \mapsto u(x)$ is twice differentiable, for all $w \in L^2(I\!R^{n+p})$, we can write,

$$[D_x, \tilde{\Pi}_0]w = -i\langle w, \nabla_x u(x)\rangle u(x) - i\langle w, u(x)\rangle \nabla_x u(x),$$

and, for all $w \in C^1(I\!R^{3n}; L^2(I\!R^{3p}))$,

$$\begin{aligned}
[D_x^2, \tilde{\Pi}_0]w &= [D_x, \tilde{\Pi}_0] \cdot D_x w + D_x \cdot [D_x, \tilde{\Pi}_0]w \\
&= -2i\langle D_x w, \nabla_x u(x)\rangle u(x) - 2i\langle D_x w, u(x)\rangle \cdot \nabla_x u(x) \\
&\quad -\langle w, \nabla_x u(x)\rangle \cdot \nabla_x u(x) - \langle w, u(x)\rangle \nabla_x \cdot \nabla_x u(x).
\end{aligned}$$

This permits to write explicitly the operator $[\tilde{\Pi}_0, \tilde{P}] = [\tilde{\Pi}_0, \boldsymbol{\omega}]$ as,

$$\begin{aligned}
[\tilde{\Pi}_0, \tilde{P}]w &= ih \sum_{k=1}^{n} \frac{1}{b_k} \langle (hD_{x_k} - (c_k + hd_k)A_k)w, \nabla_{x_k} u(x)\rangle u(x) \\
&\quad + ih \sum_{k=1}^{n} \frac{1}{b_k} \langle (hD_{x_k} - (c_k + hd_k)A_k)w, u(x)\rangle \cdot \nabla_{x_k} u(x) \\
&\quad + h^2 \sum_{k=1}^{n} \frac{1}{2b_k} \left(\langle w, \nabla_{x_k} u(x)\rangle \cdot \nabla_{x_k} u(x) + \langle w, u(x)\rangle \nabla_{x_k}^2 u(x) \right).
\end{aligned}$$

In particular, taking $w = Z_1^* \alpha(x) = \alpha(x)u(x)$, $\alpha \in H^1(I\!R^{3n})$), and using the fact that $R'(x, \lambda(x))u(x) = 0$, one finds,

$$\begin{aligned}
R'(x, \lambda(x))[\tilde{\Pi}_0, \tilde{P}]Z_1^* \alpha &= ih \sum_{k=1}^{n} \frac{1}{b_k} \left((hD_{x_k} - c_k A_k)\alpha\right) R'(x, \lambda(x)) \nabla_{x_k} u(x) \\
&\quad + \mathcal{O}(h^2 \|\alpha\|),
\end{aligned}$$

and then,

$$\begin{aligned}
&Z_1[\tilde{P}, \tilde{\Pi}_0] R'(x, \lambda(x)) [\tilde{\Pi}_0, \tilde{P}] Z_1^* \alpha \\
&= h^2 \sum_{k,\ell=1}^{n} \frac{1}{b_k b_\ell} \left((hD_{x_k} - c_k A_k)(hD_{x_\ell} - c_\ell A_\ell)\alpha\right) \times \\
&\qquad \times \langle R'(x, \lambda(x)) \nabla_{x_k} u(x), \nabla_{x_\ell} u(x)\rangle + \mathcal{O}(h^3 \|\alpha\|),
\end{aligned}$$

This obviously permits to compute the principal symbol of the partial differential operator A_2 appearing in (10.9). The (full) symbol of $A_1 = Z_1 \tilde{P} Z_1^*$ is even easier to compute, and the result follows. •

Remark 12.4 *The smoothness with respect to x of all the coefficients appearing in $a(x, \xi; h)$ is a priori known, but can also be recovered directly by using (12.10). For instance, writing $\langle \nabla_x u(x), u(x)\rangle$ as,*

$$\langle \nabla_x u(x), u(x)\rangle = \langle \nabla_x U_{x_0} u(x), U_{x_0} u(x)\rangle + i\langle \mathcal{J}(x) U_{x_0} u(x), U_{x_0} u(x)\rangle,$$

permits to see its smoothness near x_0.

Remark 12.5 *Using the expression of A_3 appearing in (10.9), one could also compute the next term (i.e., the h^3-term) in $a(x, \xi; h)$.*

Remark 12.6 *Analogous formulas can be obtained in a very similar way in the case where L is arbitrary but $\lambda_{L'+1} = \ldots = \lambda_{L'+L}$.*

Remark 12.7 *Although we did not do it here, we can also treat the case of unbounded magnetic potential (e.g., constant magnetic field). Then, the estimates on the coefficients c_α's in Assumption (H1) are not satisfied anymore, but, since we mainly work in a compact region of the x-space, it is clear that an adaptation of our arguments lead to the same results.*

Remark 12.8 *In the case of a free molecule (or, more generally, if the external electromagnetic field is invariant under the translations of the type $(x, y) \mapsto (x_1 + \alpha, \ldots, x_n + \alpha, y_1 + \alpha, \ldots, y_p + \alpha)$ for any $\alpha \in I\!R^3$), one can factorize the quantum motion, e.g., by using the so-called* center of mass of the nuclei coordinate system *, as in [KMSW]. Then, denoting by R the position of the center of mass of the nuclei, the operator takes the form,*

$$P(h) = H_0(D_R) + P'(h) + h^2 p(D_y),$$

where $H_0(D_R)$ stands for the quantum-kinetic energy of the center of mass of the nuclei, $P'(h)$ has a form similar to that of $P(h)$ in (12.6) (but now, with $x \in I\!R^{3(n-1)}$ denoting the relative *positions of the nuclei), and $p(D_y)$ is a PDO of order 2 with respect to y, with constant coefficients (the so-called* isotopic *term). Therefore, one obtains the factorization,*

$$e^{-itP(h)/h} = e^{-itH_0(D_R)/h} e^{-it(P'(h)+h^2p(D_y))/h}, \tag{12.11}$$

and it is easy to verify that our previous constructions can be performed with $Q(x)$ replaced by $Q(x) + h^2 p(D_y)$. In particular, under the same assumptions as in Theorem 12.1, the quantum evolution under $P'(h) + h^2 p(D_y)$ of an initial state φ_0 verifying (2.4) with P replaced by $P'(h)$ (that is, a much weaker assumption) can be expressed in terms of the quantum evolution associated to a $L \times L$ matrix of h-admissible operators on $L^2(I\!R^{3(n-1)})$. In that case, (12.11) provides a way to reduce the evolution of φ_0 under $P(h)$, too.

13 Appendix A: Smooth Peudodifferential Calculus with Operator-Valued Symbol

We recall the usual definition of h-admissible operator with operator-valued symbol. In some sense, this corresponds to a simple case of the more general definitions given in [Ba, GMS]. For $m \in I\!R$ and $\mathcal{H}$ a Hilbert space, we denote by $H^m(I\!R^n; \mathcal{H})$ the standard m-th order Sobolev space on $I\!R^n$ with values in $\mathcal{H}$.

Definition 13.1 *Let $m \in I\!R$ and let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert space. An operator $A = A(h) : H^m(I\!R^n; \mathcal{H}_1) \to L^2(I\!R^n; \mathcal{H}_2)$ with $h \in (0, h_0]$ is called h-admissible (of degree m) if, for any $N \geq 1$,*

$$A(h) = \sum_{j=0}^{N} h^j \mathrm{Op}_h(a_j(x, \xi; h)) + h^N R_N(h), \tag{13.1}$$

where R_N is uniformly bounded from $H^m(I\!R^n; \mathcal{H}_1)$ to $L^2(I\!R^n; \mathcal{H}_2)$ for $h \in (0, h_0]$, and, for all $h > 0$ small enough, $a_j \in C^\infty(T^*I\!R^n; \mathcal{L}(\mathcal{H}_1; \mathcal{H}_2))$, with

$$\|\partial^\alpha a_j(x, \xi; h)\|_{\mathcal{L}(\mathcal{H}_1;\mathcal{H}_2)} \leq C_\alpha \langle \xi \rangle^m \tag{13.2}$$

for all $\alpha \in I\!N^{2n}$ and some positive constant C_α, uniformly for $(x, \xi) \in T^*I\!R^n$ and $h > 0$ small enough. In that case, the formal series,

$$a(x, \xi; h) = \sum_{j \geq 0} h^j a_j(x, \xi; h), \tag{13.3}$$

is called the symbol *of A (it can be resummed up to a remainder in $\mathcal{O}(h^\infty \langle \xi \rangle^m)$ together with all its derivatives). Moreover, in the case $m = 0$ and $\mathcal{H}_2 = \mathcal{H}_1$, A is called a (bounded) h-admissible operator on $L^2(I\!R^n; \mathcal{H}_1)$.*

Here, we have denoted by $\mathrm{Op}_h(a)$ the standard quantization of a symbol a, defined by the following formula:

$$\mathrm{Op}_h(a)u(x) := \frac{1}{(2\pi h)^n} \int e^{i(x-y)\xi/h} a\,(x, \xi)\, u(y) dy d\xi, \tag{13.4}$$

valid for any tempered distribution u, and where the integral has to be interpreted as an oscillatory one. Actually, by the Calderón-Vaillancourt Theorem (see, e.g., [GMS, DiSj1, Ma2, Ro1]), the estimate (13.2) together with the quantization formula (13.4), permit to define $\mathrm{Op}_h(a)$ as a bounded operator $H^m(I\!R^n; \mathcal{H}_1) \to L^2(I\!R^n; \mathcal{H}_2)$. Let us also observe that, very often, the formal series (13.3) are indeed identified with one of their resummations (and thus, the symbol is considered as a function, rather than a formal series). Indeed, since the various resummations (together with all their derivatives) differ by uniformly $\mathcal{O}(h^\infty \langle \xi \rangle^m)$ terms, in view of (13.1) and the Calderón-Vaillancourt Theorem, it is clear that this has no real importance.

As it is well known (see, e.g., [Ba, DiSj1, GMS, Ma2]), to such a type of quantization is associated a full and explicit symbolic calculus that permits to handle these operators in a very easy and pleasant way. In particular, we have the following results:

Proposition 13.2 (Composition) *Let A and B be two bounded h-admissible operators on $L^2(I\!R^n; \mathcal{H}_1)$, with respective symbols a and b. Then, the composition $A \circ B$ is an h-admissible operators on $L^2(I\!R^n; \mathcal{H}_1)$, too, and its symbol $a \sharp b$ is given by the formal series,*

$$a \sharp b(x, \xi; h) = \sum_{\alpha \in I\!N^n} \frac{h^{|\alpha|}}{i^{|\alpha|} \alpha!} \partial_\xi^\alpha a(x, \xi; h) \partial_x^\alpha b(x, \xi; h).$$

Remark 13.3 *There is a similar result for the composition of unbounded h-admissible operators, but it requires more conditions on the remainder $R_N(h)$ appearing in (13.1) (see [Ba, GMS]).*

Proposition 13.4 (Parametrix) *Let A be an h-admissible operator on $L^2(\mathbb{R}^n;\mathcal{H}_1)$, such that any resummation a of its symbol is elliptic, in the sense that $a(x,\xi;h)$ is invertible on $\mathcal{H}_\infty$ for any $(x,\xi;h)$, and its inverse verifies,*

$$\|a(x,\xi;h)^{-1}\|_{\mathcal{L}(\mathcal{H}_1)} = \mathcal{O}(1),$$

uniformly for $(x,\xi)\in T^*\mathbb{R}^n$ and $h>0$ small enough. Then, A is invertible on $L^2(\mathbb{R}^n;\mathcal{H}_1)$, its inverse A^{-1} is h-admissible, and its symbol b verifies,

$$b = a^{-1} + hr,$$

with $r=\sum_{j\geq 0} h^j r_j$, $\|\partial^\alpha r_j\|_{\mathcal{L}(\mathcal{H}_1)} = \mathcal{O}(1)$ uniformly.

Remark 13.5 *It is easy to see that the ellipticity of any resummation of the symbol is equivalent to the ellipticity of the function $a_0(x,\xi;h)$ appearing in (13.1) (and thus, to the ellipticity of at least one resummation).*

Remark 13.6 *Of course, the r_j's can actually be all determined recursively, by using the identity $a\sharp b = 1$ (this gives a possible choice for them, but this choice is not unique since we have allowed them to depend on h).*

Proposition 13.7 (Functional Calculus) *Let A be a self-adjoint h-admissible operator on $L^2(\mathbb{R}^n;\mathcal{H}_1)$, and let $f\in C_0^\infty(\mathbb{R})$. Then, $f(A)$ is h-admissible, and its symbol b verifies,*

$$b = f(\operatorname{Re} a) + hr,$$

where $\operatorname{Re} a := (a+a^*)/2$, and $r=\sum_{j\geq 0} h^j r_j$, $\|\partial^\alpha r_j\|_{\mathcal{L}(\mathcal{H}_1)} = \mathcal{O}(1)$ uniformly.

14 Appendix B: Propagation of the Support

Theorem 14.1 *Let P be as in (2.2) with (H1)-(H2), and let K_0 be a compact subset of $\mathbb{R}^n_x$, $f\in C_0^\infty(\mathbb{R})$ and $\varphi_0\in L^2(\mathbb{R}^n;\mathcal{H})$, such that $\|\varphi_0\|=1$, and,*

$$\|(1-f(P))\varphi_0\|_{L^2(\mathbb{R}^n;\mathcal{H})} + \|\varphi_0\|_{L^2(K_0^c;\mathcal{H})} = \mathcal{O}(h^\infty).$$

Then, for any $\varepsilon>0$, any $T>0$, and any $g\in C_0^\infty(\mathbb{R})$ such that $gf=f$, the compact set defined by,

$$K_{T,\varepsilon} := \{x\in\mathbb{R}^n\,;\ \operatorname{dist}(x,K_0)\leq \varepsilon + C_1 T\},$$

with

$$C_1 := \frac{1}{2}\|\nabla_\xi \omega(x,hD_x)g(P)\|,$$

verifies,

$$\sup_{t\in[0,T]} \|e^{-itP/h}\varphi_0\|_{L^2(K_{T,\varepsilon}^c;\mathcal{H})} = \mathcal{O}(h^\infty),$$

as $h\to 0$.

Proof First, we need the following lemma:

Lemma 14.2 *For any* $\chi \in C_b^\infty(\mathbb{R}^n)$*, such that* $\mathrm{supp}\chi \subset K_0^c$*, and for any* $g \in C_0^\infty(\mathbb{R})$*, one has,*

$$\|\chi(x)g(P)\varphi_0\| = \mathcal{O}(h^\infty).$$

Proof Consider a sequence $(\chi_j)_{j\in\mathbb{N}} \subset C_b^\infty(\mathbb{R}^n)$, $\mathrm{supp}\chi_j \subset K_0^c$ and such that

$$\chi_{j+1}\chi_j = \chi_j, \quad \chi_j\chi = \chi.$$

Then, in view of (4.8), it is sufficient to show that, for any $N \geq 0$,

$$\|\chi_j(x)(P-\lambda)^{-1}\varphi_0\| = \mathcal{O}(h^N|\,\mathrm{Im}\,\lambda|^{-(N+1)}),$$

uniformly as $h, |\,\mathrm{Im}\,\lambda| \to 0_+$.

We set $u_j = \chi_j(x)(P-\lambda)^{-1}\varphi_0$, and we observe that, for all $j \in \mathbb{N}$, one has $\|u_j\| = \mathcal{O}(|\,\mathrm{Im}\,\lambda|^{-1})$. By induction on N, let us suppose, for all $j \in \mathbb{N}$,

$$\|\chi_j(x)(P-\lambda)^{-1}\varphi_0\| = \mathcal{O}(h^N|\,\mathrm{Im}\,\lambda|^{-(N+1)}).$$

Since $\chi_{j+1} = 1$ on $\mathrm{Supp}\,\chi_j$, and P is differential in x, we have,

$$(P-\lambda)u_j = \chi_j\varphi_0 + [P,\chi_j]\chi_{j+1}(P-\lambda)^{-1}\varphi_0,$$

and thus,

$$u_j = (P-\lambda)^{-1}\chi_j\varphi_0 + (P-\lambda)^{-1}[\boldsymbol{\omega},\chi_j]u_{j+1}.$$

Now, by assumption, we have $\|\chi_j\varphi_0\| = \mathcal{O}(h^\infty)$, and therefore, $\|(P-\lambda)^{-1}\chi_j\varphi_0\| = \mathcal{O}(h^\infty|\,\mathrm{Im}\,\lambda|^{-1})$. Moreover, using (H1)-(H2), it is easy to see that the operator $|\,\mathrm{Im}\,\lambda|h^{-1}(P-\lambda)^{-1}[\boldsymbol{\omega},\chi_j]$ is uniformly bounded on $L^2(\mathbb{R}^n;\mathcal{H})$. Hence, using the induction hypothesis, we obtain,

$$\|u_j\| = \mathcal{O}(h^\infty|\,\mathrm{Im}\,\lambda|^{-1}) + \mathcal{O}(h^{N+1}|\,\mathrm{Im}\,\lambda|^{-(N+2)}) = \mathcal{O}(h^{N+1}|\,\mathrm{Im}\,\lambda|^{-(N+2)})$$

for any $j \in \mathbb{N}$, and the lemma follows. •

Now, for any $F \in C^\infty(\mathbb{R}_+ \times \mathbb{R}_x^n;\mathbb{R})$, let us compute the quantity,

$$\begin{aligned}
&\partial_t\langle F(t,x)f(P)e^{-itP/h}\varphi_0, f(P)e^{-itP/h}\varphi_0\rangle \\
&\qquad = \mathrm{Re}\,\langle(\partial_t F - ih^{-1}FP)f(P)e^{-itP/h}\varphi_0, f(P)e^{-itP/h}\varphi_0\rangle \\
&\qquad = \langle(\partial_t F - \frac{i}{2h}[F,P])f(P)e^{-itP/h}\varphi_0, f(P)e^{-itP/h}\varphi_0\rangle \\
&\qquad = \langle(\partial_t F + \frac{i}{2h}[\boldsymbol{\omega},F])f(P)e^{-itP/h}\varphi_0, f(P)e^{-itP/h}\varphi_0\rangle. \quad (14.1)
\end{aligned}$$

Then, we fix $g \in C_0^\infty(\mathbb{R})$ such that $gf = f$, and, for $j \in \mathbb{N}$, we set,

$$F_j(t,x) := \varphi_j(\,\mathrm{dist}\,(x,K_0) - C_1 t), \quad (14.2)$$

where $C_1 = \frac{1}{2}\|\nabla_\xi \omega(x, hD_x)g(P)\|$, and the φ_j's are in $C_b^\infty(I\!R; I\!R_+)$ with support in $[\varepsilon, +\infty)$, verify $\varphi_j(s) = 1$ for $s \geq \varepsilon + \frac{1}{j}$, $\varphi_{j+1} = 1$ near Supp φ_j, and are such that,

$$\varphi_j' := \phi_j^2 \geq 0 \text{ with } \phi_j \in C_b^\infty(I\!R; I\!R).$$

In particular, $F_j \in C_b^\infty(I\!R_+ \times I\!R_x^n; I\!R_+)$, and, setting $d(x) :=$ dist (x, K_0), we have,

$$\nabla_x F_j = \varphi_j'(d(x) - C_1 t)\nabla d(x), \quad \partial_t F_j = -C_1 \varphi_j'(d(x) - C_1 t).$$

Moreover, since $\boldsymbol{\omega} = \omega(x, hD_x)$ is a differential operator with respect x, of degree m, we see that,

$$\frac{i}{h}[\boldsymbol{\omega}, F_j] = \nabla_x F_j \cdot \nabla_\xi \omega(x, hD_x) + hR_j, \tag{14.3}$$

where $R_j = R_j(t, x, hD_x)$ is a differential operator of degree $m-2$ in x, with coefficients in $C_b^\infty(I\!R_+ \times I\!R_x^n)$ and supported in $\{F_{j+1} = 1\}$.

Lemma 14.3 *For any* $N \geq 1$,

$$\|R_j f(P)u\| = \mathcal{O}(\sum_{k=0}^N h^k \|F_{j+k+1} f(P)u\| + h^{N+1}\|u\|).$$

Proof We write $R_j f(P) = R_j F_{j+1} f(P) = R_j g(P) F_{j+1} f(P) + R_j [F_{j+1}, g(P)] f(P)$. Then, using (4.8) and the fact that $[P, F_{j+1}] = [\boldsymbol{\omega}, F_{j+1}]$, we obtain,

$$\begin{aligned}
&R_j[F_{j+1}, g(P)] \\
&\quad = \frac{1}{\pi}\int \overline{\partial}\tilde{g}(z) R_j (P-z)^{-1}[\boldsymbol{\omega}, F_{j+1}](P-z)^{-1} dz\, d\bar{z} \\
&\quad = \frac{1}{\pi}\int \overline{\partial}\tilde{g}(z) R_j (P-z)^{-1}[\boldsymbol{\omega}, F_{j+1}]F_{j+2}(P-z)^{-1} dz\, d\bar{z} \\
&\quad = \frac{1}{\pi}\int \overline{\partial}\tilde{g}(z) R_j (P-z)^{-1}[\boldsymbol{\omega}, F_{j+1}](P-z)^{-1}F_{j+2} dz\, d\bar{z} \\
&\qquad + \frac{1}{\pi}\int \overline{\partial}\tilde{g}(z) R_j (P-z)^{-1}[\boldsymbol{\omega}, F_{j+1}](P-z)^{-1}[\boldsymbol{\omega}, F_{j+2}](P-z)^{-1} dz\, d\bar{z},
\end{aligned}$$

and thus, by iteration,

$$\begin{aligned}
&R_j[F_{j+1}, g(P)] \\
&\quad = \sum_{k=1}^N \frac{1}{\pi}\int \overline{\partial}\tilde{g}(z) R_j (P-z)^{-1}\left(\prod_{\ell=1}^k \left([\boldsymbol{\omega}, F_{j+\ell}](P-z)^{-1}\right)\right) F_{j+k+1} dz\, d\bar{z} \\
&\qquad + \frac{1}{\pi}\int \overline{\partial}\tilde{g}(z) R_j (P-z)^{-1} \prod_{\ell=1}^{N+1} \left([\boldsymbol{\omega}, F_{j+\ell}](P-z)^{-1}\right) dz\, d\bar{z}.
\end{aligned}$$

Since $\|R_j(P-z)^{-1}\| = \mathcal{O}(1)$ and $\|[\boldsymbol{\omega}, F_{j+\ell}](P-z)^{-1}\| = \mathcal{O}(h)$, the result follows. •

As a consequence, we deduce from (14.3),

$$
\begin{aligned}
&\frac{i}{h}[\boldsymbol{\omega}, F_j]f(P)e^{-itP/h}\varphi_0 \\
&= \varphi_j'(d(x) - C_1t)\nabla d(x)\nabla_\xi \omega(x, hD_x)f(P)e^{-itP/h}\varphi_0 \\
&\qquad\qquad\qquad +\mathcal{O}(\sum_{k=0}^{N} h^{k+1}\|F_{j+k+1}f(P)e^{-itP/h}\varphi_0\| + h^{N+2}) \\
&= \phi_j(d(x) - C_1t)\nabla d(x)\nabla_\xi \omega(x, hD_x)g(P)\phi_j(d(x) - C_1t)f(P)e^{-itP/h}\varphi_0 \\
&\quad +\phi_j(d(x) - C_1t))\nabla d(x)[\phi_j(d(x) - C_1t), \nabla_\xi \omega(x, hD_x)]f(P)e^{-itP/h}\varphi_0 \\
&\quad +\phi_j(d(x) - C_1t))\nabla d(x)\nabla_\xi \omega(x, hD_x)[\phi_j(d(x) - C_1t), g(P)]f(P)e^{-itP/h}\varphi_0 \\
&\qquad\qquad\qquad +\mathcal{O}(\sum_{k=0}^{N} h^{k+1}\|F_{j+k+1}f(P)e^{-itP/h}\varphi_0\| + h^{N+2}),
\end{aligned}
$$

and thus, since ϕ_j is supported in $\{F_{j+1} = 1\}$, as in the proof of Lemma 14.3, we obtain,

$$
\begin{aligned}
&\frac{i}{h}[\boldsymbol{\omega}, F_j]f(P)e^{-itP/h}\varphi_0 \\
&= \phi_j(d(x) - C_1t)\nabla d(x)\nabla_\xi \omega(x, hD_x)g(P)\phi_j(d(x) - C_1t)f(P)e^{-itP/h}\varphi_0 \\
&\qquad\qquad\qquad +\mathcal{O}(\sum_{k=0}^{N} h^{k+1}\|F_{j+k+1}f(P)e^{-itP/h}\varphi_0\| + h^{N+2}),
\end{aligned}
$$

for any fixed $N \geq 1$.

Going back to (14.1), and using the fact that $\|\nabla d(x)\nabla_\xi \omega(x, hD_x)g(P)\| \leq C_1$, this gives,

$$
\begin{aligned}
&\partial_t \langle F_j(t,x)f(P)e^{-itP/h}\varphi_0, f(P)e^{-itP/h}\varphi_0\rangle \\
&\qquad \leq \mathcal{O}(\sum_{k=0}^{N} h^{k+1}\|F_{j+k+1}f(P)e^{-itP/h}\varphi_0\|^2 + h^{N+2}),
\end{aligned}
$$

and therefore, integrating between 0 and t, and using Lemma 14.2,

$$
\begin{aligned}
&\langle F_j(t,x)f(P)e^{-itP/h}\varphi_0, f(P)e^{-itP/h}\varphi_0\rangle \\
&\qquad = \mathcal{O}(\sum_{k=0}^{N} h^{k+1}\int_0^t \|F_{j+k+1}f(P)e^{-isP/h}\varphi_0\|^2 ds + th^{N+2}),
\end{aligned}
$$

In particular, since

$$
\|F_j(t,x)f(P)e^{-itP/h}\varphi_0\|^2 \leq \langle F_j(t,x)f(P)e^{-itP/h}\varphi_0, f(P)e^{-itP/h}\varphi_0\rangle,
$$

we have $\|F_j(t,x)f(P)e^{-itP/h}\varphi_0\|^2 = \mathcal{O}(h)$ for any $j \in I\!N$, and then, by induction, $\|F_j(t,x)f(P)e^{-itP/h}\varphi_0\|^2 = \mathcal{O}(h^N)$ for all $N \in I\!N$. Due to the definition (14.2) of F_j, this proves the theorem. •

15 Appendix C: Two Technical Lemmas

Lemma 15.1 *Let* $\psi_j, \chi_j \in C_0^\infty(\mathbb{R}^n)$*, such that* $\chi_j = 1$ *near* $\mathrm{Supp}\,\psi_j$*. Then, for any* $f \in C_0^\infty(\mathbb{R})$*, one has,*

$$U_j\psi_j f(\tilde{P})U_j^{-1}\chi_j = \psi_j f(U_j\chi_j\tilde{P}U_j^{-1}\chi_j) + \mathcal{O}(h^\infty).$$

Proof By (4.8), and taking the adjoint, it is enough to prove, for any $N \geq 1$,

$$U_j\chi_j(\tilde{P}-z)^{-1}U_j^{-1}\psi_j = (U_j\chi_j\tilde{P}U_j^{-1}\chi_j - z)^{-1}\psi_j + \mathcal{O}(h^N|\,\mathrm{Im}\,z|^{-N'}),$$

locally uniformly for $z \in \mathbb{C}$, and with some $N' = N'(N) < +\infty$. Let $v \in L^2(\mathbb{R}^n)$ and set $u := (\tilde{P}-z)^{-1}U_j^{-1}\psi_j v$. By Lemma 4.11 (and its proof), we know that,

$$u = \chi_j u + \mathcal{O}(h^N|\,\mathrm{Im}\,z|^{-N'}\|v\|), \tag{15.1}$$

for some $N' = N'(N) < +\infty$. On the other hand, we have,

$$\begin{aligned}
(U_j\chi_j\tilde{P}U_j^{-1}\chi_j - z)U_j\chi_j u &= U_j\chi_j\tilde{P}u - zU_j\chi_j u + U_j\chi_j\tilde{P}(\chi_j^2-1)u \\
&= U_j\chi_j(zu + U_j^{-1}\psi_j v) - zU_j\chi_j u + U_j\chi_j\tilde{P}(\chi_j^2-1)u \\
&= \psi_j v + U_j\chi_j\tilde{P}(\chi_j^2-1)u,
\end{aligned}$$

and thus, using (15.1),

$$\begin{aligned}
U_j\chi_j u &= (U_j\chi_j\tilde{P}U_j^{-1}\chi_j - z)^{-1}(\psi_j v + U_j\chi_j\tilde{P}(\chi_j^2-1)u) \\
&= (U_j\chi_j\tilde{P}U_j^{-1}\chi_j - z)^{-1}\psi_j v + \mathcal{O}(h^N|\,\mathrm{Im}\,z|^{-N''}\|v\|),
\end{aligned}$$

for some other $N'' = N''(N) < +\infty$. Then, the result follows. •

Lemma 15.2 *Let* $\psi, \chi \in C_0^\infty(\mathbb{R}^n)$*, such that* $\chi = 1$ *near* $\mathrm{Supp}\,\psi$*. Then, for any* $\rho \in C_0^\infty(\mathbb{R})$*, one has,*

$$\rho(\chi\boldsymbol{\omega}\chi)\psi = \rho(\boldsymbol{\omega})\psi + \mathcal{O}(h^\infty).$$

Proof The proof is very similar to (but simpler than) the one of Lemma 15.1, and we omit it. •

References

[Ba] A. Balazard-Konlein, *Calcul fonctionel pour des opérateurs h-admissibles à symbole opérateurs et applications*, PhD Thesis, Université de Nantes (1985).

[Be] M. V. Berry, *The Quantum Phase, Five Years After*, in Geometric Phases in Physics (A. Shapere and F. Wilczek, Eds), World Scientific, Singapore (1989).

[BoOp] M. Born, R. Oppenheimer, *Zur Quantentheorie der Molekeln*, Ann. Phys. **84**, 457 (1927).

[BrNo] R. Brummelhuis, J. Nourrigat, *Scattering amplitude for Dirac operators*, Comm. Partial Differential Equations 24 (1999), no. 1-2, 377–394.

[CDS] J.-M. Combes, P. Duclos, R. Seiler, *The Born-Oppenheimer approximation*, in: Rigorous atomic and molecular physics, G. Velo and A. Wightman (Eds.), 185-212, Plenum Press New-York (1981).

[CoRo] M. Combescure, D. Robert, *Semiclassical spreading of quantum wave packets and applications near unstable fixed points of the classical flow*, Asymptotic Analysis 14 (1997), 377–404.

[CoSe] J.-M. Combes, R. Seiler, *Regularity and asymptotic properties of the discrete spectrum of electronic Hamiltonians*, Int. J. Quant. Chem. **XIV**, 213-229 (1978).

[DiSj1] M.Dimassi, J.Sjöstrand , *Spectral asymptotics in the semi-classical limit*. London Mathematical Society Lecture Note Series, 268. Cambridge University Press, Cambridge, 1999.

[GMS] C. Gérard, A. Martinez, J. Sjöstrand, *A mathematical approach to the effective hamiltonian in perturbed periodic problems*, Comm. Math. Physics Vol.142, n2 (1991).

[GuSt] V. Guillemin, S. Sternberg, *Geometric Asymptotics*, Amer. Math. Soc. Survey 14 (1977)

[Ha1] G. Hagedorn, *Semiclassical quantum mechanics IV*, Ann. Inst. H. Poincaré **42** (1985), 363–374.

[Ha2] G. Hagedorn, *High order corrections to the time-independent Born-Oppenheimer approximation I: Smooth potentials*, Ann. Inst. H. Poincaré **47** (1987), 1–16.

[Ha3] G. Hagedorn, *High order corrections to the time-independent Born-Oppenheimer approximation II: Diatomic Coulomb systems*, Comm. Math. Phys. **116**, (1988), 23–44.

[Ha4] G. Hagedorn, *A time-dependent Born-Oppenheimer approximation*, Comm. Math. Phys. **77**, (1980), 1–19.

[Ha5] G. Hagedorn, *High order corrections to the time-dependent Born-Oppenheimer approximation I: Smooth potentials*, Ann. Math. **124**, 571–590 (1986). Erratum. Ann. Math, **126**, 219 (1987)

[Ha6] G. Hagedorn, *High order corrections to the time-dependent Born-Oppenheimer approximation II: Coulomb systtems*, Comm. Math. Phys. **116**, (1988), 23–44.

[HaJo] G. Hagedorn, A. Joye, *A Time-Dependent Born–Oppenheimer Approximation with Exponentially Small Error Estimates*, Comm. Math. Phys. 223 (2001), no. 3, 583–626.

[HeSj11] B. Helffer, J. Sjöstrand, *Multiple wells in the semiclassical limit I*, Comm. Part. Diff. Eq. **9** (4), 337–408 (1984)

[HeSj12] B. Helffer, J. Sjöstrand, *Semiclassical Analysis of Harper's Equation III*, Mem. Soc. Math. Fr., Nouv. Ser. 39, 124 (1989)

[Ka] T. Kato, *Perturbation Theory for Linear Operators*, 2nd ed. Classics in Mathematics, Springer-Verlag, Berlin (1980)

[KMSW] M. Klein, A. Martinez, R. Seiler, X.P. Wang, *On the Born-Oppenheimer Expansion for Polyatomic Molecules*, Commun. Math. Phys. 143, No.3, 607-639 (1992)

[Ma1] A. Martinez, *Développement asymptotiques et efffet tunnel dans l'approximation de Born-Oppenheimer*, Ann. Inst. H. Poincaré **49** (1989), 239–257.

[Ma2] A. Martinez, *An Introduction to Semiclassical and Microlocal Analysis*, Universitext. Springer-Verlag, New York, 2002.

[MaSo] A. Martinez, V. Sordoni, *A general reduction scheme for the time-dependent Born-Oppenheimer approximation*, C.R. Acad. Sci. Paris, Ser. I 334, 185-188 (2002)

[MeSj1] A. Melin, J. Sjöstrand, *Fourier integral operators with complex phase functions and parametrix for an interior boundary value problem*, Commun. Partial Differ. Equations 1, 313-400 (1976)

[Ne1] G. Nenciu *Linear Adiabatic Theory, Exponential Estimates*, Commun. Math. Phys. 152, 479-496 (1993).

[Ne2] G. Nenciu *On asymptotic perturbation theory for quantum mechanics: almost invariant subspaces and gauge invariant magnetic perturbation theory* J. Math. Phys. 43, 1273-1298 (2002).

[NeSo] G. Nenciu, V. Sordoni, *Semiclassical limit for multistate Klein-Gordon systems: almost invariant subspaces and scattering theory*, J. Math. Phys.,Vol. 45 (2004), pp.3676-3696

[PST] G. Panati, H. Spohn, S. Teufel, *Space-adiabatic perturbation theory*, Adv. Theor. Math. Phys. 7 (2003).

[Ra] A. Raphaelian, *Ion-atom scattering within a Born-Oppenheimer framework*, Dissertation Technische Universität Berlin (1986)

[Ro1] D. Robert, *Autour de l'Approximation Semi-Classique*, Birkhäuser (1987)

[Ro2] D. Robert, *Remarks on asymptotic solutions for time dependent Schrödinger equations*, in Optimal Control and Partial Differential Equations, IOS Press (2001)

[Sj1] J. Sjöstrand, *Singularités Analytiques Microlocales*, Astérisque 95 (1982)

[Sj2] J. Sjöstrand, *Projecteurs adiabatique du point de vue pseudodifferéntiel*, C. R. Acad. Sci. Paris 317, Série I, 217-220 (1993)

[So] V. Sordoni, *Reduction scheme for semiclassical operator-valued Schrödinger type equation and application to scattering*, Comm. Partial Differential Equations 28 (2003), no. 7-8, 1221–1236

[SpTe] H. Spohn, S. Teufel, *Adiabatic decoupling and time-dependent Born-Oppenheimer theory*, Comm. Math. Phys. 224 (2001), no. 1, 113–132.

[Te] S. Teufel, *Adiabatic Perturbation Theory in Quantum Dynamics*, Lecture Notes in Math. 1821, Springer-Verlag, Berlin, Heidelberg, New York (2003)