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Born-Oppenheimer Reduction of Quantum Evolution of Molecules

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1 Introduction

This paper is an announcement of [MaSo2] and we refer the interested reader to the whole paper for further details and applications.

We are interested in the quantum evolution of a molecule, 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 various particles of the molecule (electron and nuclei). 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 $\alpha \in \mathbb{R}$ constant.

In 1927, M. Born and R. Oppenheimer [BoOp] proposed a formal method for studying the spectrum of H, asymptotically as the mass of the nuclei tends to infinity. 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. In that way, the evolution of the molecule reduces to that of the nuclei imbedded in an effective electric potential created by the electrons.

Many years later, this method has been made completely rigorous (from a mathematical point of view) in the case of a diatomic molecule by Hagedorn [Ha3], and then in the general case by Klein-Martinez-Seiler-Wang [KMSW].

Concerning the general problem of evolution (1.1), however, until now no such reduction had ever been proved in the physical case of Coulomb interactions. The only rigorous results concern the non-physical case of smooth interactions, and the first ones are due to Hagedorn [Ha4, Ha5, Ha6], that provide complete asymptotic expansions, as $h := M^{-\frac{1}{2}}$ goes to 0 (M = average mass of the nuclei), of the solution of (1.1) when the initial state is a convenient perturbation of a single electronic-level state. In particular, these results provide a case where the relevant information on the initial state is directly connected with the localization in energy of the electrons and the localization in phase space of the nuclei. This fits very well with the semiclassical intuition of the problem, in concomitance with the fact that the classical flow of some effective Hamiltonian H_{eff} (depending on the nuclei variables only) is involved.

However, from a conceptual point of view, something was missing in the previous results. 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 $e^{-it\tilde{H}_{\text{eff}}/h}$, for some $\tilde{H}_{\text{eff}}$ close to H_{eff}. In that way, one would be able to use all the well developed semiclassical (microlocal) machinery on the operator $\tilde{H}_{\text{eff}}(x, hD_x)$, in order to deduce many results on its quantum evolution group $e^{-it\tilde{H}_{\text{eff}}(x,hD_x)/h}$ (e.g., a representation of it as a Fourier integral operator), and, in particular, to allow more general initial states.

The first results concerning such a reduced quantum evolution have been obtained recently (and independently) by H. Spohn and S. Teufel in [SpTe], and by the present authors in [MaSo1]. 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 $H_{\text{el}}(x)$. In [SpTe], the authors find an approximation of $e^{-itH/h}$ in terms of $e^{-itH_{\text{eff}}(x,hD_x)/h}$, 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 [MaSo1] (following a procedure of [NeSo, So], and later reproduced with further applications in [?, ?]), a whole perturbation $\tilde{H}_{\text{eff}} \sim H_{\text{eff}} + \sum_{k\geq 1} h^k H_k$ of H_{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 [MaSo1] and those of [KMSW] in order to include possible 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.

Here, we settle a systematic framework of such transformations, by introducing the notion of "twisted pseudodifferential operators". Roughly speaking, we say that an operator P on $L^2(\mathbb{R}^n_x; \mathcal{H})$ ($\mathcal{H}$ = abstract Hilbert space) is a twisted pseudodifferential operator, if each operator $U_j P U_j^{-1}$ (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 is a smooth pseudodifferential operator with operator-valued symbol (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 [MaSo1] can essentially be reproduced, and leads to the required reduction of the quantum evolution. As an application, 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).

2 Main Results

In order to simplify this presentation, here we consider the following example only (that already contains almost all the difficulties), and we refer to [MaSo2] for more general Hamiltonians (e.g., including an external electro-magnetic field, etc...).

With $h := M^{-\frac{1}{2}}$ (M = average mass of the nuclei), and after re-scaling all the variables, we are interested in investigating the asymptotic behavior, as $h \to 0_+$, of the quantum evolution group $e^{-itP/h}$ associated to the operator,

$$P = -h^2 \Delta_x + Q(x) + W(x). \tag{2.1}$$

Here, $x = (x_1, \dots, x_n) \in I\!R^{3n}$ denotes the nuclear position variables, $Q(x)$ stands for the electronic Hamiltonian, typically of the form,

$$Q(x) = -\Delta_y + \sum_{j \neq k} \frac{\alpha_{j,k}}{|y_j - y_k|} + \sum_{j,\ell} \frac{\beta_{j,\ell}}{|y_j - x_\ell|}$$

with $y = (y_1, \dots, y_p) \in I\!R^{3p}$ and $\alpha_{j,k}$, $\beta_{j,\ell}$ constants, and $W(x)$ is the potential of nuclei-nuclei interaction, tipically of the form,

$$W(x) = \sum_{\ell \neq \ell'} \frac{\gamma_{\ell,\ell'}}{|x_\ell - x_{\ell'}|},$$

with $\gamma_{\ell,\ell'} > 0$ constant.

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 $Q(x)$:

(H) There exists a contractible bounded open set $\Omega \subset I\!R^{3n}$ and $L \geq 1$ such that,
(i) $\Omega \cap \mathcal{C} = \emptyset$, where $\mathcal{C} := \{(x_1, \dots x_n)\,;\, x_\ell = x_{\ell'}$ for some $\ell \neq \ell'\}$ is the so-called collision set of nuclei;

(ii) For all $x \in \Omega$, $\lambda_1(x), \dots, \lambda_{L+L'}(x)$ are discrete eigenvalues of $Q(x)$, and one has,

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

Then, denoting by $L^2(I\!R^n)^{\oplus L}$ the space $(L^2(I\!R^n))^L$ endowed with its natural Hilbert structure, we have,

Theorem 2.1 *Assume (H) and let $\Omega' \subset\subset \Omega$ with Ω' open subset of $I\!R^{3n}$. Then, for any $g \in C_0^\infty(I\!R)$, there exists an orthogonal projection $\Pi = \Pi_g$ on $L^2(I\!R^n;\mathcal{H})$, an operator $\mathcal{W} = \mathcal{W}_g : L^2(I\!R^n;\mathcal{H}) \to L^2(I\!R^n)^{\oplus L}$, uniformly bounded with respect to h, and a selfadjoint $L \times L$ matrix A of h-admissible operators $H^2(I\!R^n) \to L^2(I\!R^n)$, with the following properties:*

- *For all $\chi \in C_0^\infty(\Omega')$,*
$$\Pi\chi = \Pi_0\chi + \mathcal{O}(h);$$
- *$\mathcal{W}\mathcal{W}^* = 1$ and $\mathcal{W}^*\mathcal{W} = \Pi$;*
- *For $x \in \Omega'$, the symbol $a(x,\xi;h)$ of A verifies,*
$$a(x,\xi;h) = \xi^2\mathbf{I}_L + \mathcal{M}(x) + W(x)\mathbf{I}_L + hr(x,\xi;h)$$
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 $\partial^\alpha r(x,\xi;h) = \mathcal{O}(\langle\xi\rangle)$ for any multi-index α and uniformly with respect to $(x,\xi) \in \Omega' \times I\!R^{3n}$ and $h > 0$ small enough;
- *For any $f \in C_0^\infty(I\!R)$ with $\text{Supp } f \subset \{g = 1\}$, and for any $\varphi_0 \in L^2(I\!R^n;\mathcal{H})$ such that $\|\varphi_0\| = 1$, and,*
$$\|\varphi_0\|_{L^2(K_0^c;\mathcal{H})} + \|(1-\Pi)\varphi_0\| + \|(1-f(P))\varphi_0\| = \mathcal{O}(h^\infty), \qquad (2.2)$$
for some $K_0 \subset\subset \Omega'$, one has,
$$e^{-itP/h}\varphi_0 = \mathcal{W}^*e^{-itA/h}\mathcal{W}\varphi_0 + \mathcal{O}\left(\langle t\rangle h^\infty\right) \qquad (2.3)$$
uniformly with respect to $h > 0$ small enough and $t \in [0, T_{\Omega'}(\varphi_0))$, where,
$$T_{\Omega'}(\varphi_0) := \sup\{T > 0;\, \exists K_T \subset\subset \Omega',\ \sup_{t\in[0,T]} \|e^{-itP/h}\varphi_0\|_{L^2(K_T^c;\mathcal{H})} = \mathcal{O}(h^\infty)\}.$$

Remark 2.2 *It can be shown that,*

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

and, when $L = 1$, a much better estimate is given Theorem 2.5 below.

Remark 2.3 *Actually, much more informations are obtained on the operators Π, $\mathcal{W}$ and A. In particular, they all admit an asymptotic expansion in powers of h, and are indeed "twisted h-admissible operator" (in the sense of the next section) that can be computed by the corresponding "twisted symbolic calculus".*

Remark 2.4 *The three terms in condition (2.2) 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.*

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:

Theorem 2.5 *Assume moreover that $L = 1$, and set,*

$$a_0(x,\xi) := \xi^2 + \lambda_{L'+1}(x) + W(x) \qquad (x \in \Omega').$$

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 $f \in C_0^\infty(I\!R)$ with $\operatorname{Supp} f \subset \{g = 1\}$, and for any $\varphi_0 \in L^2(I\!R^n; \mathcal{H})$ verifying (2.2) with $\|\varphi_0\| = 1$, one has,

$$T_{\Omega'}(\varphi_0) \geq \sup\{T > 0\,;\, \pi_x(\cup_{t\in[0,T]} \exp tH_{a_0}(K(f))) \subset \Omega'\}, \tag{2.4}$$

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

$$K(f) := \{(x,\xi)\,;\, x \in K_0,\ \xi^2 + \inf_{x'\in\Omega'} \inf \sigma(Q(x')) \leq \mathrm{Max}|\operatorname{Supp} f|\}.$$

Remark 2.6 *An even better estimate (somehow optimal) can be obtained in the case where φ_0 is a coherent state: see Section 7.*

3 Twisted Pseudodifferential Calculus

Definition 3.1 *We call "regular covering" of $I\!R^n$ any finite family $(\Omega_j)_{j=0,\cdots,r}$ of open subsets of $I\!R^n$ such that $\cup_{j=0}^r \Omega_j = I\!R^n$ and such that there exists a family of functions $\chi_j \in C_b^\infty(I\!R^n)$ (the space of smooth functions on $I\!R^n$ with uniformly bounded derivatives of all order) with $\sum_{j=0}^r \chi_j = 1$, $0 \leq \chi_j \leq 1$, and* $\operatorname{dist}(\operatorname{Supp}(\chi_j), I\!R^n \backslash \Omega_j) > 0$ *($j = 0, \cdots, r$). 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 $L^2(I\!R^n; \mathcal{H})$.*

Then, we denote by $C_d^\infty(\Omega_j)$ the space of functions $\chi \in C_b^\infty(I\!R^n)$ such that $\operatorname{dist}(\operatorname{Supp}(\chi), I\!R^n \backslash \Omega_j) > 0$.

Definition 3.2 (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 $L^2(I\!R^n; \mathcal{H})$. 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,*

$$A = \sum_{j=0}^{r} U_j^{-1}\chi_j A_j^N U_j \chi_j + \mathcal{O}(h^N), \tag{3.1}$$

where, for any $j = 0,..,r$, A_j^N *is a bounded* h*-admissible operator on* $L^2(\mathbb{R}^n;\mathcal{H})$ *(in the sense of [Ba, GMS]) 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* $L^2(\mathbb{R}^n;\mathcal{H})$.

An equivalent definition is given by the following proposition:

Proposition 3.3 *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,*

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

   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* $L^2(\mathbb{R}^n;\mathcal{H})$.

One also has at disposal a notion of (full) symbol for such operators. Indeed, one can show that, for all j, there exists an operator-valued symbol a_j, 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). Then, the symbol of A is defined as the family $\sigma(A) := (a_j)_{0\leq j\leq r}$.

We also clearly have a notion of ellipticity, and, defining the Moyal product $\sharp$ of two such symbols by the formula,

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

it can be shown that all the usual symbolic calculus can be extended to this situation (in particular: construction of parametrices for elliptic operators; functional calculus; ...). Moreover, a similar definition can be done for unbounded operators, at least in the case of *differential* operators (which is enough for our purposes).

Then, concerning our operator P under study, we first modify it outside Ω' in the following way: We choose a function $\zeta \in C_0^\infty(\Omega;[0,1])$ such that $\zeta = 1$ near Ω', and we set,

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

where $Q_0 = -\Delta_y + 1$, and $\tilde{\Pi}_0^{\pm}(x)$ are convenient extensions (smooth with respect to x outside Ω) of the spectral projections $\Pi_0^{\pm}(x)$ of $Q(x)$ associated with $\sigma(Q(x)) \cap (\lambda_{L'+L}(x), +\infty)$ and $\sigma(Q(x)) \cap (-\infty, \lambda_{L'}(x)]$ respectively. Then, we replace P by the operator,

$$\tilde{P} := -h^2\Delta_x + \tilde{Q}(x) + \zeta(x)W(x), \tag{3.2}$$

which is equal to P for x in Ω', and has smooth coefficients with respect to x outside Ω. Moreover, the local gap in the spectrum of $Q(x)$ becomes a *global* gap in that of $\tilde{Q}(x)$, and we denote by $\tilde{\Pi}_0(x)$ the corresponding extension of $\Pi_0(x)$.

Then, following [KMSW], one can construct a family $(\Omega_j, U_j(x))_{1\leq j\leq r}$ such that $\overline{\Omega} \subset \cup_{j=1}^r \Omega_j$ and $U_j(x)PU_j(x)^{-1}$ is a differential operator depending smoothly on x in Ω_j. Then, completing this family by adding some Ω_0 such that $\cup_{j=0}^r \Omega_j = I\!R^{3n}$, and by taking $U_0 = I$, we obtain a regular unitary covering $\mathcal{U}$ of $L^2(I\!R^{3n}; L^2(I\!R^{3p}))$, and we see that $(\tilde{P}+i)^{-1}$ is a $\mathcal{U}$-twisted h-admissible operator.

Let us briefly recall the construction of [KMSW]. For any fixed $x_0 = (x_1^0, \ldots, x_n^0) \in I\!R^{3n}\backslash\mathcal{C}$, we choose n functions $f_1, \ldots, f_n \in C_0^\infty(I\!R^3; I\!R)$, such that,

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

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

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

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

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

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

$$U_{x_0}(x)v(y) := |\det d_y G_{x_0}(x,y)|^{\frac{1}{2}} v(G_{x_0}(x,y))|,$$

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:

$$U_{x_0} hD_x U_{x_0}^{-1} = hD_x + hJ_1(x,y)D_y + hJ_2(x,y),$$
$$U_{x_0} D_y U_{x_0}^{-1} = J_3(x,y)D_y + J_4(x,y),$$
$$U_{x_0} \frac{1}{|y_k - y_k'|} U_{x_0}^{-1} = \frac{1}{|F_{x_0}(x,y_k) - F_{x_0}(x,y_k'),|}$$
$$U_{x_0} \frac{1}{|x_j - y_k|} U_{x_0}^{-1} = \frac{1}{|F_{x_0}(x,x_j^0) - F_{x_0}(x,y_k)|}, \tag{3.3}$$

where the (matrix or operator-valued) functions J_ν's ($1 \leq \nu \leq 4$) are all smooth on $\Omega_{x_0} \times I\!R^{3p}$. The key-point in (3.3) is that the (x-dependent) singularity at $y_k = x_j$ has been replaced by the (fix) singularity at $y_k = x_j^0$, and one can easily deduce that the map $x \mapsto U_{x_0} Q(x) U_{x_0}^{-1}$ is in $C^\infty(\Omega_{x_0}; \mathcal{L}(H^2(I\!R^{3p}), L^2(I\!R^{3p}))$. To complete the argument, one just observes that the previous construction can be made around any point x_0 of $\overline{\Omega}$, and since this set is compact, one 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.

4 Construction of a Quasi-Invariant Subspace

Here, we adopt the general strategy of [Ne1, Ne2, NeSo, So], consisting in constructing a projector close to $\tilde{\Pi}_0$, and that approximately commutes with $\tilde{P}$, up to $\mathcal{O}(h^\infty)$. It is precisely for this construction that we need the twisted pseudodifferential calculus.

Theorem 4.1 *Assume (H), and denote by $\mathcal{U} := (U_j, \Omega_j)_{j=0,\cdots,r}$ the regular unitary covering of $L^2(I\!R^{3n}; L^2(I\!R^{3p}))$ constructed at the end of the previous section. 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,*

$$\Pi_g = \tilde{\Pi}_0 + \mathcal{O}(h) \tag{4.1}$$

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

$$\tilde{P}^\ell [f(\tilde{P}), \Pi_g] = \mathcal{O}(h^\infty). \tag{4.2}$$

Moreover, Π_g is uniformly bounded as an operator: $L^2(I\!R^{3n}; L^2(I\!R^{3p})) \to L^2(I\!R^{3n}; H^2(I\!R^{3p}))$ 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,

$$\tilde{P}^\ell \mathrm{ad}_{\chi_1} \circ \cdots \circ \mathrm{ad}_{\chi_N}(\Pi_g) = \mathcal{O}(h^N). \tag{4.3}$$

Sketch of Proof: We first perform a formal construction, by essentially following a procedure taken from [Ne1] (see also [BrNo] in the case $L = 1$). Since $Q := \tilde{Q}(x) + \zeta(x) W(x)$ commutes with $\tilde{\Pi}_0$, we have,

$$[\tilde{P}, \tilde{\Pi}_0] = [-h^2 \Delta_x, \tilde{\Pi}_0].$$

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,

$$\tilde{\Pi}_0(x) = \frac{1}{2i\pi} \int_{\gamma(x)} (z - \tilde{Q}(x))^{-1} dz, \tag{4.4}$$

and we see that $Q_0 \tilde{\Pi}_0(x)$ is a $\mathcal{U}$-twisted Partial Differential Operator (in short: PDO) of degree 0. Applying the twisted symbolic calculus, we deduce,

$$[\tilde{P}, \tilde{\Pi}_0] = -ihS_0, \tag{4.5}$$

where S_0 is a twisted PDO, too, and satisfies $S_0 = \tilde{\Pi}_0 S_0 \tilde{\Pi}_0^\perp + \tilde{\Pi}_0^\perp S_0 \tilde{\Pi}_0$, where $\tilde{\Pi}_0^\perp := 1 - \tilde{\Pi}_0$. Then, we set,

$$\tilde{\Pi}_1 := -\frac{1}{2\pi}\int_{\gamma(x)} (z-\tilde{Q}(x))^{-1}\left[\tilde{\Pi}_0^\perp(x)S_0\tilde{\Pi}_0(x) - \tilde{\Pi}_0(x)S_0\tilde{\Pi}_0^\perp(x)\right](z-\tilde{Q}(x))^{-1}dz, \tag{4.6}$$

which is a $\mathcal{U}$-twisted PDO, too. Applying again the twisted symbolic calculus, we obtain,

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

where B is a twisted PDO. A direct computation also gives,

$$[\tilde{P},\tilde{\Pi}_1] = iS_0 - ihS_1, \tag{4.7}$$

where S_1 is a twisted PDO, and thus,

$$[\tilde{P},\tilde{\Pi}_0 + h\tilde{\Pi}_1] = -ih^2 S_1. \tag{4.8}$$

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 twisted PDO. This procedure can be iterated, and one finally obtain a whole formal series $\tilde{\Pi} = \sum_{k=0}^\infty h^k\tilde{\Pi}_k$, where the $\tilde{\Pi}_k$'s are twisted PDO's, and such that, formally,

$$\tilde{\Pi}^2 = \tilde{\Pi} \tag{4.9}$$

$$[\tilde{P},\tilde{\Pi}] = 0. \tag{4.10}$$

However, it appears that the degree of $\tilde{\Pi}_k$ increases with k, and that makes the re-summation of such a formal series far from being straightforward. However, follow an idea of [So], we observe that, for $g \in C_0^\infty(\mathbb{R})$, 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, and thus one can re-sum in a standard way the series $\sum_{k=0}^\infty h^k g(\tilde{P})\tilde{\Pi}_k$. Denoting by $\Pi(g)$ such a resummation, we set,

$$\tilde{\Pi}_g := \Pi(g)+\Pi(g)^* - \frac{1}{2}(g(\tilde{P}))\Pi(g)^* + \Pi(g)g(\tilde{P})) + (1-g(\tilde{P}))\tilde{\Pi}_0(1-g(\tilde{P})). \tag{4.11}$$

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,

$$\|\tilde{\Pi}_g - \tilde{\Pi}_0\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H}))} + \|\tilde{\Pi}_g^2 - \tilde{\Pi}_g\|_{\mathcal{L}(L^2(\mathbb{R}^n;\mathcal{H}))} = \mathcal{O}(h). \tag{4.12}$$

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

$$\Pi_g := \frac{1}{2i\pi}\int_{|z-1|=\frac{1}{2}} (\tilde{\Pi}_g - z)^{-1}\,dz, \tag{4.13}$$

and one can prove that it verifies all the assertions of the Theorem. •

Remark 4.2 *Our 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 $M \geq 1$.*

5 Decomposition of the Evolution for the Modified Operator

In this section we restrict our attention to the quantum evolution of $\tilde{P}$, for which a very complete result can be proved, in the same spirit as in [MaSo1].

Theorem 5.1 *Under the same assumtions as for Theorem 4.1, let $g \in C_0^\infty(\mathbb{R})$. Then, one has the following results:*
1) Let $\varphi_0 \in L^2(\mathbb{R}^n;\mathcal{H})$ verifying,

$$\varphi_0 = f(\tilde{P})\varphi_0, \tag{5.1}$$

for some $f \in C_0^\infty(\mathbb{R})$ such that Supp $f \subset \{g = 1\}$. *Then, with the projection Π_g constructed in Theorem 4.1, one has,*

$$e^{-it\tilde{P}/h}\varphi_0 = e^{-it\tilde{P}^{(1)}/h}\Pi_g\varphi_0 + e^{-it\tilde{P}^{(2)}/h}(1-\Pi_g)\varphi_0 + \mathcal{O}(|t|h^\infty\|\varphi_0\|) \tag{5.2}$$

uniformly with respect to h small enough, $t \in \mathbb{R}$ and φ_0 verifying (5.1), 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 $\varphi_0 \in L^2(\mathbb{R}^n;\mathcal{H})$ (possibly h-dependent) verifying $\|\varphi_0\| = 1$, and,

$$\varphi_0 = f(\tilde{P})\varphi_0 + \mathcal{O}(h^\infty), \tag{5.3}$$

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

$$e^{-it\tilde{P}/h}\varphi_0 = e^{-it\tilde{P}^{(1)}/h}\Pi_g\varphi_0 + e^{-it\tilde{P}^{(2)}/h}(1-\Pi_g)\varphi_0 + \mathcal{O}(\langle t\rangle h^\infty) \tag{5.4}$$

uniformly with respect to h small enough and $t \in \mathbb{R}$.
3) There exists a bounded operator $\mathcal{W} : L^2(\mathbb{R}^n;\mathcal{H}) \to L^2(\mathbb{R}^n)^{\oplus L}$ 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 $L^2(\mathbb{R}^n;\mathcal{H})$ to $L^2(\mathbb{R}^n)^{\oplus L}$;*
- *$\mathcal{W}\mathcal{W}^* = 1$ 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 $L^2(\mathbb{R}^n)^{\oplus L}$ with domain $H^m(\mathbb{R}^n)^{\oplus L}$, 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 $(x,\xi) \in T^*\mathbb{R}^n$ and $h > 0$ small enough.

In particular, $\mathcal{W}|_{\mathrm{Ran}\,\Pi_g} : \mathrm{Ran}\,\Pi_g \to L^2(\mathbb{R}^n)^{\oplus L}$ *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* $t \in \mathbb{R}$.

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

$$ih\partial_t \Pi_g \varphi = \Pi_g \tilde{P} f(\tilde{P})\varphi = \Pi_g^2 \tilde{P} f(\tilde{P})\varphi. \tag{5.5}$$

Moreover, writing $[\Pi_g, \tilde{P}]f(\tilde{P}) = [\Pi_g, \tilde{P}f(\tilde{P})] + \tilde{P}[f(\tilde{P}), \Pi_g]$, Theorem 4.1 tells us that $\|[\Pi_g, \tilde{P}]f(\tilde{P})\| = \mathcal{O}(h^\infty)$. Therefore, we obtain from (5.5),

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

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 (5.2) follows.

2) Formula (5.4) 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,

$$\mathcal{V} = \left(\tilde{\Pi}_0\Pi_g + (1-\tilde{\Pi}_0)(1-\Pi_g)\right)\left(1 - (\Pi_g - \tilde{\Pi}_0)^2\right)^{-1/2}. \tag{5.6}$$

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,

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

Then, we define $Z_L : L^2(\mathbb{R}^n; \mathcal{H}) \to L^2(\mathbb{R}^n)^{\oplus L}$ by,

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

where the $\tilde{u}_k(x)$'s generate the range of $\tilde{\Pi}_0(x)$ and are such that, for all $j \geq 0$,

$$\tilde{u}_{k,j}(x) := U_j(x)\tilde{u}_k(x) \in C^\infty(\Omega_j; H^2(\mathbb{R}^{3p}_y)).$$

Finally, we set,

$$\mathcal{W} := Z_L \circ \mathcal{V} = Z_L + \mathcal{O}(h). \tag{5.7}$$

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 $\varphi_j, \chi_j \in C_0^\infty(\Omega_j)$ such that $\chi_j = 1$ near $\operatorname{Supp}\varphi_j$, and for any $\psi \in L^2(\mathbb{R}^n; \mathcal{H})$, we have,

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

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 $L^2(\mathbb{R}^n; \mathcal{H})$ to $L^2(\mathbb{R}^n)^{\oplus L}$, 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 3.3, and thus, with an obvious extension of the notion of twisted operator, that $\mathcal{W}$ is, indeed, a twisted h-admissible operator from $L^2(\mathbb{R}^n; \mathcal{H})$ to $L^2(\mathbb{R}^n)^{\oplus L}$.)

Then, we define

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

and it remains to prove that A in a matrix of h-admissible operators (in the sense of [Ro1]). Taking a partition of unity $(\chi_j)_{j=0,\dots,r}$ on $\mathbb{R}^{3n}$ adapted to the Ω_j's, we have, and choosing $\varphi_j \in C_0^\infty(\Omega_j)$ such that $\varphi_j = 1$ in a neighborhood of $\operatorname{Supp}\chi_j$, we write,

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

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

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

where $\tilde{P}_j = U_j\tilde{P}U_j^{-1}\varphi_j$ is an h-admissible (differential) operator from $H^2(\mathbb{R}^{3n}; H^2(\mathbb{R}^{3p}))$ to $L^2(\mathbb{R}^{3(n+p)})$, while, by construction, $U_j\varphi_j\mathcal{W}^*\varphi_j$ is an h-admissible operator from $H^2(\mathbb{R}^{3n})^{\oplus L}$ to $H^2(\mathbb{R}^{3n}; H^2(\mathbb{R}^{3p}))$ and $\varphi_j\mathcal{W}U_j^{-1}\chi_j$ is an h-admissible operator from $L^2(\mathbb{R}^{3(n+p)})$ to $L^2(\mathbb{R}^{3n})^{\oplus L}$. Therefore, A is an h-admissible operator from $H^2(\mathbb{R}^{3n})^{\oplus L}$ to $L^2(\mathbb{R}^{3n})^{\oplus L}$, and, if we set,

$$\tilde{p}_j(x,\xi;h) := \xi^2 + \tilde{Q}_j(x) + \zeta(x)W(x), \quad \tilde{Q}_j(x) := U_j(x)\tilde{Q}(x)U_j(x)^{-1}$$

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 $a = (a_{k,\ell})_{1\le k,\ell\le L}$ of A, is given by,

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

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

$$a_{k,\ell}(x,\xi,h)=\sum_{j=0}^{r}\langle \chi_j(x)(\xi^2+\tilde{Q}_j(x)+\zeta(x)W(x))\tilde{u}_{k,j}(x),\tilde{u}_{\ell,j}(x)\rangle_{\mathcal{H}}+r_{k,\ell}(h)$$

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

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

this finally gives,

$$\begin{aligned}a_{k,\ell}(x,\xi,h)&=\sum_{j=0}^{r}\chi_j(x)(\xi^2\delta_{k,\ell}+m_{k,\ell}(x)+\zeta(x)W(x)\delta_{k,\ell})+r_{k,\ell}(h)\\&=(\xi^2+\zeta(x)W(x))\delta_{k,\ell}+m_{k,\ell}(x)+r_{k,\ell}(h),\end{aligned}$$

with $m_{k,\ell}(x):=\langle\tilde{Q}(x)\tilde{u}_k(x),\tilde{u}_\ell(x)\rangle$, and Theorem 5.1 follows. •

6 Proof of the Main Theorem

We give a sketch of proof of Theorem 2.1. In view of Theorem 5.1, it is enough to prove,

Theorem 6.1 *Let $\varphi_0\in L^2(\mathbb{R}^n;\mathcal{H})$ such that $\|\varphi_0\|=1$, and,*

$$\|\varphi_0\|_{L^2(K_0^c;\mathcal{H})}+\|(1-\Pi_g)\varphi_0\|+\|(1-f(P))\varphi_0\|=\mathcal{O}(h^\infty),\tag{6.1}$$

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 4.1. Then, with the notations of Theorem 5.1, we have,

$$e^{-itP/h}\varphi_0=e^{-it\tilde{P}/h}\varphi_0+\mathcal{O}\left(\langle t\rangle h^\infty\right),\tag{6.2}$$

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

Sketch of Proof : Denote by $\chi\in C_0^\infty(\Omega)$ a cutoff function such that $\chi=1$ on Ω' and $\zeta=1$ near Suppχ. Then, the twisted pseudodifferential functional calculus tells us

$$\|(f(P)-f(\tilde{P}))\chi\|_{\mathcal{L}(L^2(\mathbb{R}^{3(n+p)}))}=\mathcal{O}(h^\infty).\tag{6.3}$$

Now, by (6.1), we have,

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

and thus, by (6.3),

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

This means that (5.3) is satisfied, and thus, by Theorem 5.1, the decomposition (5.4) is true. Using (6.1) again, this gives,

$$e^{-it\tilde{P}/h}\varphi_0 = e^{-it\tilde{P}^{(1)}/h}\Pi_g\varphi_0 + \mathcal{O}(|t|h^\infty) = \mathcal{W}^* e^{-itA/h}\mathcal{W}\varphi_0 + \mathcal{O}(\langle t\rangle h^\infty), \quad (6.4)$$

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 (6.3) again, we obtain as before, $\varphi(t) = f(\tilde{P})\varphi(t) + \mathcal{O}(h^\infty)$, and thus also,

$$\varphi(t) = f(\tilde{P})\chi\varphi(t) + \mathcal{O}(h^\infty), \quad (6.5)$$

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 $f(\tilde{P})[\chi, \tilde{P}] = f(\tilde{P})[\chi, -h^2\Delta_x]$ is bounded, and $[\chi, -h^2\Delta_x]$ is a differential operator with coefficients supported in $\mathrm{Supp}\, \nabla\chi$ (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 (6.5),

$$\varphi(t) = e^{-it\tilde{P}/h}\varphi_0 + \mathcal{O}(\langle t\rangle h^\infty), \quad (6.6)$$

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

7 Application: Propagation of Wave Packets

Here, we assume $L = 1$ and, in a similar spirit as in [Ha6], we investigate the evolution of an initial state of the form,

$$\varphi_0(x) = (\pi h)^{-n/4} f(P)\Pi_g(e^{ix\xi_0/h-(x-x_0)^2/2h}u_1(x)), \quad (7.1)$$

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 Theorem 2.5), $g = 1$ near $\mathrm{Supp}\, f$, and Π_g is the projector constructed in Theorem 2.1. In particular, since $e^{-(x-x_0)^2/2h}$ is exponentially small for x outside any neighborhood of x_0, by (6.3), we have,

$$\varphi_0(x) = (\pi h)^{-n/4} f(\tilde{P})\Pi_g(e^{ix\xi_0/h-(x-x_0)^2/2h}\tilde{u}_1(x)) + \mathcal{O}(h^\infty),$$

in $L^2(\mathbb{R}^n;\mathcal{H})$. 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 $L^2(\mathbb{R}^n)$, we also obtain,

$$\varphi_0(x) = (\pi h)^{-n/4} f(\tilde{P})e^{ix\xi_0/h-(x-x_0)^2/2h}\tilde{u}_1(x) + \mathcal{O}(h),$$

and thus, in particular, $\|\varphi_0\| = 1 + \mathcal{O}(h)$. Actually, one can even show a better result, namely:

Proposition 7.1 *The function φ_0 admits, in $L^2(\mathbb{R}^n;\mathcal{H})$, an asymptotic expansion of the form,*

$$\varphi_0(x) \sim (\pi h)^{-n/4}e^{ix\xi_0/h-(x-x_0)^2/2h}\sum_{k=0}^{\infty} h^k v_k(x) + \mathcal{O}(h^\infty), \tag{7.2}$$

with $v_k \in L^\infty(\mathbb{R}^n;\mathcal{H})$ $(k \geq 0)$, and $v_0(x) = \tilde{u}_1(x) + \mathcal{O}(|x-x_0|)$ in $\mathcal{H}$, uniformly with respect to $x \in \mathbb{R}^n$.

In particular, defining the Frequency Set of a (here, $L^2(\mathbb{R}^{3p})$-valued) function of x in a way similar to that of [GuSt], one also has,

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

for $j = 1,\dots,r$.

Now, applying Theorem 2.5, we obtain,

$$e^{itP/h}\varphi_0 = \mathcal{W}^* e^{-itA/h}\mathcal{W}\varphi_0 + \mathcal{O}(\langle t\rangle h^\infty), \tag{7.3}$$

uniformly for $t \in [0, T_{\Omega'}(\varphi_0))$,where $\Omega' \subset\subset \Omega$ is the same as the one used to define $\tilde{P}$. In that case, one also obtain the following better estimate on $T_{\Omega'}(\varphi_0)$:

$$T_{\Omega'}(\varphi_0) \geq \sup\{T > 0\,;\ \pi_x(\cup_{t\in[0,T]} \exp tH_{a_0}(x_0,\xi_0)) \subset \Omega'\}. \tag{7.4}$$

Moreover, by a stationary phase expansion, we see that,

$$\mathcal{W}\varphi_0(x;h) \sim (\pi h)^{-n/4}e^{ix\xi_0/h-(x-x_0)^2/2h}\sum_{k=0}^{\infty} h^k w_k(x) + \mathcal{O}(h^\infty), \tag{7.5}$$

with $w_k \in C_b^\infty(\mathbb{R}^n)$, $w_0(x) = \langle \tilde{u}_1(x), \tilde{u}_1(x)\rangle + \mathcal{O}(|x-x_0|) = 1 + \mathcal{O}(|x-x_0|)$, and where the asymptotic expansion takes place in $C_b^\infty(\mathbb{R}^n)$.

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

$$e^{-itA/h}\mathcal{W}\varphi_0 = e^{i\delta_t/h}\sum_{k=0}^{3(N-1)} c_k(t;h)\Phi_{k,t} + \mathcal{O}(e^{NC_0t}h^{N/2}), \tag{7.6}$$

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,

$$c_k(t;h) = \sum_{\ell=0}^{N_k} h^\ell c_{k,\ell}(t), \tag{7.7}$$

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 $he^{C_0 t}$ remains bounded ($h > 0$ small enough). In particular, (7.6) supplies an asymptotic expansion of $e^{-itA/h}\mathcal{W}\varphi_0$ if one restricts to the values of t such that $0 \leq t << \ln \frac{1}{h}$. Applying $\mathcal{W}^*$ to (7.6), and observing that $\mathcal{W}^*\Phi_{k,t} = \mathcal{V}^*(\Phi_{k,t}\tilde{u}_1) = U_j^{-1}\mathcal{V}_j^*(\Phi_{k,t}u_{1,j})$, 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 (7.3),

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

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 (7.7), $\delta_t := \int_0^t (\dot{x}_s \xi_s - a_0(x_s, \xi_s))ds + (x_0\xi_0 - x_t\xi_t)/2$, and where the estimate is uniform with respect to (t, h) such that $h > 0$ is small enough and $t \in [0, \min(T_{\Omega'}(x_0, \xi_0), C^{-1} \ln \frac{1}{h}))$.

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