Classical Limit of Elastic Scattering Operator of a Diatomic Molecule in the Born-Oppenheimer Approximation.

Th. Jecko[1]
Département de mathématiques
Université de Nantes
44072 Nantes cedex 03, France
e-mail : jecko@math.univ-nantes.fr

Abstract

In this paper, we use the Born-Oppenheimer approximation to study the elastic diffusion operator $S_{\alpha\alpha}$, for a two-cluster channel α of a diatomic molecule. Under a non-trapping condition on the effective potential, we compute the classical limit of $S_{\alpha\alpha}$, acting on quantum observables and microlocalized by coherent states, in terms of a classical diffusion operator. This work is a continuation of [KMW1], in a sense, where the channel wave operators were studied.

1 Introduction.

In this work, we study the two-cluster scattering operator for a diatomic molecule. Since the nuclei are much heavier than the electrons, one expects to observe a behaviour which would be close to the classical scattering of two particles. This is known as the Born-Oppenheimer approximation (cf. [BO]). Under suitable conditions, we justify this approximation for the elastic scattering operator of some two-cluster channel α. To this end, we study the classical limit (when the nuclei's masses tend to infinity) of the scattering operator $S_{\alpha\alpha}$, acting on a quantum observable and microlocalized by coherent states. We introduce the adiabatic operator S^{AD}, which approximates $S_{\alpha\alpha}$ but is of a simpler structure. Then we compute the classical limit of this adiabatic operator in terms of the classical scattering operator (defined in e.g. [RS3]).

In [KMW1] the classical limit of the cluster channel wave operators for such a channel α was derived. The present work is a continuation of [KMW1] under the same assumptions. Concerning other mathematical works on the Born-Oppenheimer approximation, we refer the reader to the references quoted in [KMSW] and [J]. For the classical limit see e.g. [W3], [RT], and [Y].

Studying a diatomic molecule with N_0 electrons, it is known from quantum mechanics that its dynamics is generated by its Hamiltonian, the following self-adjoint operator acting in

[1]present address : Fachbereich Mathematik MA 7-2, Technische Universitaet Berlin, Strasse der 17. Juni 136, D-10623 Berlin, Germany , e-mail : jecko@math.tu-berlin.de

the Hilbert space $L^2(I\!R^{3(N_0+2)})$,

$$H=-\frac{1}{2m_1}\Delta_{x_1}-\frac{1}{2m_2}\Delta_{x_2}+\sum_{j=3}^{N_0+2}(-\frac{1}{2}\Delta_{x_j})+\sum_{l<j}V_{lj}(x_l-x_j)$$

(the electronic mass and Planck's constant are set equal to unity). The respective mass of the two nuclei, m_1 and m_2, are then large compared to unity, the real-valued functions V_{lj} represent the two-body interactions between the particles. More generally, the configuration space of a single particle is assumed to be $I\!R^n$ for $n \geq 2$, so that the previous operator acts in $L^2(I\!R^{n(N_0+2)})$.

Let $a=(A_1,A_2)$ be a decomposition of $\{1,\cdots,N_0+2\}$ in two clusters, such that $j\in A_j$, for $j\in\{1,2\}$. Then each cluster contains a nucleus. Using a suitable change of variables and removing the center of mass motion, the Hamiltonian is replaced by the following operator :

$$P(h)=-h^2\Delta_x+P^a(h)+I_a(h),$$

acting on $L^2(I\!R^{n(N_0+1)})$ (see Section 2 for the precise expressions of $P^a(h)$ and $I_a(h)$). The positive number h given by (1) is the small parameter in this problem, the operator $P^a(h)$ is the sum of the Hamiltonians of each isolated cluster, and the intercluster potential $I_a(h)$ takes into account the interactions between particles of different clusters. The variable $x\in I\!R^n$ stands for the relative position of the cluster's centers of mass so that the energy of this relative motion is given by the operator $-h^2\Delta_x$. Temporarily ignoring this term, we consider the family $\{P_e(x;h), x\in I\!R^n, h\leq h_0\}$ of operators defined by

$$P_e(x;h)=P^a(h)+I_a(x;h),\ \forall x\in I\!R^n,\ \forall h\leq h_0,$$

for some h_0 small enough. The Hamiltonian $P_e(x;h)$ is the Hamiltonian of a system of N_0 electrons, which interact with one another while they are moving in an external field generated by the nuclei. This external field depends on the relative position x of the two clusters. The operator $P_e(x;h)$ is called the electronic Hamiltonian and one has :

$$P(h)=-h^2\Delta_x+P_e(h).$$

The two-body interactions appearing in these operators are functions $V\in C^\infty(I\!R^n;I\!R)$, such that, for some $\rho>1$, they obey

$$\forall\alpha\in I\!N^n,\ \exists C_\alpha>0;\ \forall x\in I\!R^n,\ |\partial_x^\alpha V(x)|\leq C_\alpha\langle x\rangle^{-\rho-|\alpha|}. \tag{D_ρ}$$

We are interested in thoses states of this system, whose evolution is asymptotically close to the free evolution of bound states in A_1 and A_2. This last evolution is generated by the operator

$$P_a(h)\equiv-h^2\Delta_x+P^a(h)$$

restricted to some proper subspace of $P^a(h)$. Using the free evolution generated by $P^a(h)$, the operator S^{AD} will be the scattering operator of an adiabatic operator P^{AD} whose construction is given as follows.

Considering the system for $h = 0$, we suppose that the bottom of the spectrum of the operator $P^a(0)$ is a simple eigenvalue E_0, that there is exactly one "curve" $x \mapsto \lambda(x;0)$, where $\lambda(x;0)$ is also a simple eigenvalue of $P_e(x;0)$ and such that it converges to E_0 as $|x| \to \infty$. Furthermore, suppose that the map, $x \mapsto \lambda(x;0)$, assuming its values in the spectrum $\sigma(P_e(x;0))$ of $P_e(x;0)$, is globally defined in $I\!R^n$. Let $\Pi_0(0)$ be the spectral projector of $P^a(0)$ associated to E_0, and, for all $x \in I\!R^n$, let $\Pi(x;0)$ be the spectral projector of $P_e(x;0)$ corresponding to $\lambda(x;0)$.

Definition 1.1 *Assume that there exists a constant e_0 such that, for all $x \in I\!R^n$, one has $\lambda(x;0) > e_0$. For a positive number δ, we set $e(x) = \lambda(x;0) + \delta$ and $E(x) = \lambda(x;0) + 2\delta$. Assume that we can find a positive number h_δ such that one has, for $h \leq h_\delta$,*

$$\sigma\Big(P_e(x;h)\Big) \cap [e(x), E(x)] = \emptyset. \tag{H_δ}$$

The gap condition (H_δ) is close to the assumption (1.8) in [KMW2]. For the same δ, we assume that there exists $R_0 > 0$ and $h_\delta > 0$ such that, for all $|x| \geq R_0$ and $h \in [0, h_\delta]$, one has :

$$\dim \mathrm{Ran}\Big(1\!\!1_{]-\infty,e(x)[}\Big(P_e(x;h)\Big)\Big) = 1 \tag{H_δ'}$$

($1\!\!1_{]-\infty,e(x)[}$ denotes the characteristic function of the interval $]-\infty, e(x)[$). Finally, the following condition is also assumed :

$$E_0 < \inf_{x \in I\!R^n} \inf\Big\{\sigma\Big(P_e(x;0)\Big) \setminus \{\lambda(x;0)\}\Big\}. \tag{H}$$

If these assumptions (H_δ), $(H_\delta)'$, and (H) are satisfied, for some $\delta > 0$, we will say that, for E_0, the **semiclassical stability assumption** *$(HS(h))$ is satisfied.*

Under this assumption on E_0, one can find $(\Gamma(x))_{x \in I\!R^n}$, a $h-$independent family of complex contours such that $\Gamma(x)$ encircles $\lambda(x;0)$ for all x and such that one has :

$$\forall x \in I\!R^n,\ \forall h \in [0; h_\delta],\ \mathrm{Dist}\Big[\Gamma(x), \sigma\Big(P_e(x;h)\Big)\Big] \geq \frac{\delta}{2}.$$

Making use of these contours, one can express the projectors $\Pi_0(0)$ and $\Pi(x;0)$ by means of the Cauchy integral formula (see section 2). For h small enough, one can also define a spectral projector $\Pi_0(h)$ (respectively $\Pi(x;h)$) of $P^a(h)$ (respectively $P_e(x;h)$) by the same Cauchy formula. Using a direct integral, we define a fibered operator $\Pi(h)$ by

$$\Pi(h) \ = \ \int_{I\!R^n}^{\oplus} \Pi(x;h)\, dx.$$

We can now introduce the adiabatic part of $P(h)$

$$P^{AD}(h) = \Pi(h)P(h)\Pi(h)$$

and the wave operators

$$\Omega_\pm^{AD}(h) = s - \lim_{t\to\pm\infty} e^{ih^{-1}tP^{AD}(h)} e^{-ih^{-1}tP_a(h)} \Pi_0(h).$$

In [KMW1], the existence and the completeness of these wave operators is proved, enabling us to define an adiabatic scattering operator S^{AD} by :

$$S^{AD}(h) = \left(\Omega_+^{AD}(h)\right)^* \Omega_-^{AD}(h).$$

Recall that a channel α with decomposition a is given by $(a, E_\alpha(h), \phi_\alpha(h))$, where $\phi_\alpha(h)$ is a normalized eigenvector of $P_a(h)$ associated to the eigenvalue $E_\alpha(h)$.

Let us consider the channel $\alpha = (a, E_0(h), \phi_0(h))$ whose energy $E_0(h)$ tends to E_0 as $h \to 0$. According to [KMW1], the wave operators $\Omega_\pm^{AD}(h)$ approximate the following channel wave operators

$$\Omega_\pm^{\alpha}(h) = s - \lim_{t\to\pm\infty} e^{ih^{-1}tP(h)} e^{-ih^{-1}tP_a(h)} \Pi_0(h)$$

in an appropriate energy band. More precisely, one has

$$\left\| \left(\Omega_\pm^{\alpha}(h) - \Omega_\pm^{AD}(h)\right) \chi(P_a(h)) \right\| = O(h)$$

under a suitable condition on the support of the cut-off function $\chi \in C_0^\infty(]E_0, +\infty[; I\!R)$ (see Theorem 4.1). Thus the operator $S^{AD}(h)$ is close to the elastic scattering operator

$$S_{\alpha\alpha}(h) = \left(\Omega_+^{\alpha}(h)\right)^* \Omega_-^{\alpha}(h),$$

which is well defined for short-range interactions (cf. [SS]).

From this fact, the study of the classical limit of the scattering operator $S^{AD}(h)$ (see Section 4) allows us to obtain the main result of the present work :

Theorem 1.2 *Assume (D_ρ), $\rho > 1$, for the potentials, and the semiclassical stability assumption $(HS(h))$ for the simple eigenvalue E_0 (cf. Definition 1.1). Let $\chi \in C_0^\infty(]E_0; +\infty[; I\!R)$ be non-trapping for the classical Hamiltonian $|\xi|^2 + \lambda(x;0)$ (cf. Definition 2.2) and such that its support satisfies :*

$$\sup(\operatorname{supp}\chi) < \inf_{x\in I\!R^n} \inf\left\{\sigma(P_e(x;0)) \setminus \{\lambda(x;0)\}\right\}.$$

Let $(x_0, \xi_0) \in I\!R^{2n}$ with $\chi(|\xi_0|^2 + E_0) = 1$. For the channel $\alpha = (a, E_0(h), \phi_0(h))$ and for all bounded symbols c, valued in $\mathcal{L}(L^2(I\!R^{nN_0}))$, we set :

$$\mathcal{S}_{c,\alpha}(h) = U_h(x_0,\xi_0)^* (S_{\alpha\alpha}(h))^* \chi(P_a(h)) \; c(x, hD) \; \chi(P_a(h)) S_{\alpha\alpha}(h) U_h(x_0,\xi_0),$$

where the coherent states operators $U_h(x_0, \xi_0)$ and the h-pseudodifferential operator $c(x, hD)$, with symbol c, are defined by (13) and (12) respectively. Denote by S_a^{cl} the classical scattering operator associated to the pair of classical Hamiltonians $(|\xi|^2, |\xi|^2 + \lambda(x;0) - E_0)$ (cf. (1)).

In $L^2(I\!R_x^n; L^2(I\!R^{nN_0}))$, the following strong limit exists and is given by :

$$s - \lim_{h\to 0} \mathcal{S}_{c,\alpha}(h) \;=\; \Pi_0(0) \; (c \circ S_a^{cl})(x_0, \xi_0) \; \Pi_0(0).$$

This work is organized as follows. In Section 2, some notation is introduced and the construction in [KMW1] of parametrices (see [IK]) for P^{AD} is recalled. Microlocal propagation estimates for this operator are obtained in Section 3. The proof of Theorem 1.2 follows directly from Theorem 4.2 in Section 4, which proves the existence and gives the value of the classical limit for the adiabatic scattering operator S^{AD}.

AKNOWLEDGEMENT.

The author expresses his deep gratitude to X.P. Wang for his constant support and his numerous advices. He also thanks the members of the mathematics department at TU Berlin for their hospitality and especially V. Bach for his help.

The author is supported by the TMR Programme of the European Commission - Network Postdoctoral training programme in partial differential equations and application in quantum mechanics.

Contents

2 Parametrices for the operator P^{AD}.

In this section, we recall the contruction in [KMW1] of parametrices (see [IK]) for P^{AD}, distinguishing incoming and outgoing regions. These parametrices will be used in the Sections 3 and 4. The potentials satisfy the condition (D_ρ), for $\rho > 1$.

First, we give the exact expression for the operators $P^a(h)$ and $I_a(x;h)$. Let us call y the dynamic variable in $I\!R^{nN_0}$. Denoting by A'_k the set of the electrons in the cluster A_k, by $|A'_k|$ its cardinal, and by $M_k = m_k + |A'_k|$ the total mass of the cluster A_k, for $k \in \{1,2\}$, the small parameter h is given by

$$h \;=\; \left(\frac{1}{2M_1} + \frac{1}{2M_2}\right)^{1/2}. \tag{1}$$

Then, one has :

$$P^a(h) \;=\; \sum_{k=1}^{2} \left[\sum_{j\in A'_k} \Big(-\frac{1}{2}\Delta_{y_j} + V_{kj}(y_j)\Big) - \frac{1}{2m_k} \sum_{l,j\in A'_k} \nabla_{y_l}\cdot\nabla_{y_j} + \frac{1}{2}\sum_{l,j\in A'_k} V_{lj}(y_l - y_j)\right]$$

and :

$$\begin{aligned} I_a(x;h) \;&=\; \sum_{l\in A'_1, j\in A'_2} V_{lj}(y_l - y_j + x + f_2 - f_1) + \sum_{l\in A'_1} V_{l2}(x - f_1 + f_2 - y_l) \\ &\quad + \sum_{j\in A'_2} V_{1j}(x - f_1 + f_2 - y_j) + V_{12}(x - f_1 + f_2), \end{aligned}$$

where $f_k = \frac{1}{M_k}\sum_{j\in A'_k} y_j$ are h-dependent, for $k \in \{1,2\}$. For $l < j$, we have set $V_{jl}(z) = V_{lj}(-z)$. Denote by P_{he} the following Hughes-Eckart term :

$$h^2 P_{he} \equiv -\sum_{k=1}^{2} \frac{1}{2m_k} \sum_{l,j\in A'_k} \nabla_{y_l}\cdot\nabla_{y_j}$$

(the scalar product of the gradients is meant here).

Let us now recall some properties of the projectors $\Pi(x;h)$ and $\Pi_0(h)$, especially in view of the fact that they admit an asymptotic expansion in increasing powers of h with coefficients in $\mathcal{L}(L^2(I\!R_y^{nN_0}))$. Under the assumptions of the introduction, one can express these projectors by the following Cauchy formula, provided δ, h_δ are small enough. Then, for $h \in [0, h_\delta]$,

$$\Pi_0(h) \;=\; \frac{1}{2i\pi}\int_{\Gamma(\infty)} (z - P^a(h))^{-1} dz,$$

where

$$\Gamma(\infty) \equiv \{z \in \mathbb{C};\ |z - E_0| = \delta/2\}.$$

For all $x \in I\!R^n$, one also has :

$$\Pi(x;h) \;=\; \frac{1}{2i\pi}\int_{\Gamma(x)} (z - P_e(x;h))^{-1} dz.$$

Note that we may always choose $\Gamma(x) = \Gamma(\infty)$ for $|x|$ large enough. Thanks to the exponential decay of the eigenfunctions of the operator $P^a(0)$, associated to the eigenvalue E_0 (cf. [A]), these projectors have the following properties :

Proposition 2.1 *([KMW1]) The functions $I\!R^n \ni x \mapsto \Pi(x;h) \in \mathcal{L}(L^2(I\!R_y^{nN_0}))$ are C^∞ and verify :*

$$\forall \alpha \in I\!N^n,\ \exists D_\alpha > 0;\ \forall x \in I\!R^n,\ \left\|\partial_x^\alpha\Big(\Pi(x;h) - \Pi_0(h)\Big)\right\| \le D_\alpha \langle x\rangle^{-\rho-|\alpha|}, \tag{2}$$

uniformly w.r.t. $h \in [0, h_\delta]$, h_δ small enough. Furthermore, for all natural numbers N, one has

$$\Pi_0(h) \;=\; \Pi_0(0) + \sum_{k=1}^{N} h^{2k}\pi_{0k} + O(h^{2(N+1)}) \tag{3}$$

with $\pi_{0k} \in \mathcal{L}(L^2(I\!R_y^{nN_0}))$, for all $k = 1,\dots,N$. Again for all N, one has, uniformly w.r.t. $x \in I\!R^n$

$$\Pi(x;h) \;=\; \Pi(x;0) + \sum_{k=1}^{N} h^{2k}\pi_k(x) + O(h^{2(N+1)}), \tag{4}$$

where the functions $I\!R^n \ni x \mapsto \pi_k(x) \in \mathcal{L}(L^2(I\!R_y^{nN_0}))$ are C^∞ and verify :

$$\forall \alpha \in I\!N^n,\ \exists D_\alpha > 0;\ \forall x \in I\!R^n,\ \|\partial_x^\alpha(\pi_k(x) - \pi_{0k})\| \le D_\alpha \langle x\rangle^{-\rho-|\alpha|}. \tag{5}$$

Furthermore, the operators π_{0k} and $\pi_k(x)$ have rank at most 1 *(multiplicity of E_0).*

Proof : For the first estimate (2), one may follow the proof of Theorem 2.2 in [KMW1]. We show now the second one (3). For $z \in \Gamma(\infty)$ and h small enough, one has

$$\begin{aligned}(z - P^a(0) - h^2 P_{he})^{-1} \;&=\; (z - P^a(0))^{-1}\Big(1 + h^2 P_{he}(z - P^a(0))^{-1}\Big)^{-1}\\ &=\; \sum_{k=0}^{\infty}(z - P^a(0))^{-1}\Big(h^2 P_{he}(z - P^a(0))^{-1}\Big)^k.\end{aligned}$$

For all k, define the following bounded operator

$$\tilde{\Pi}_{0k} \;=\; \frac{1}{2i\pi}\int_{\Gamma(\infty)}(z - P^a(0))^{-1}\Big(h^2 P_{he}(z - P^a(0))^{-1}\Big)^k dz.$$

Then, for all N, one has

$$\begin{aligned}\left\|\Big(\Pi_0(h) - \Pi_0(0) - \sum_{k=1}^{N} h^{2k}\tilde{\Pi}_{0k}\Big)\Pi_0(0)\right\| \;&=\; O(h^{2(N+1)}),\\ \left\|\Big(\Pi_0(h) - \Pi_0(0) - \sum_{k=1}^{N} h^{2k}\tilde{\Pi}_{0k}\Big)\Pi_0(h)\right\| \;&=\; O(h^{2(N+1)}).\end{aligned}$$

Using the relation

$$\Pi_0(h) - \Pi_0(0) \;=\; \Big(\Pi_0(h) - \Pi_0(0)\Big)\Pi_0(0) + \Pi_0(h)\Big(\Pi_0(h) - \Pi_0(0)\Big),$$

we obtain the asymptotic expansion of $\Pi_0(h)$, to all orders. Furthermore, the coefficients of this expansion are at most rank-one operators, because they all contain a factor $\Pi_0(0)$.

For the operator $\Pi(x;h)$, we use a slightly different argument because we do not know how to control the following quantity

$$\left\|(z-P_e(x;h))^{-1}-(z-P_e(x;0))^{-1}\right\|.$$

To avoid this difficulty, let us project first onto $\mathrm{Ran}\Pi(x;h)$ and onto $\mathrm{Ran}\Pi(x;0)$. For all x, the difference

$$\Big(\Pi(x;h) \ - \ \Pi(x;0)\Big)\Pi(x;0)$$

is given by

$$\begin{aligned}
&\frac{1}{2i\pi}\int_{\Gamma(x)}(z-P_e(x;h))^{-1}\Big(P_e(x;h)-P_e(x;0)\Big)(z-P_e(x;0))^{-1}dz\ \Pi(x;0)\\
= \ & h^2\frac{1}{2i\pi}\int_{\Gamma(x)}(z-P_e(x;h))^{-1}P_{he}(z-P_e(x;0))^{-1}dz\ \Pi(x;0)\\
&+\frac{1}{2i\pi}\int_{\Gamma(x)}(z-P_e(x;h))^{-1}\Big(I_a(x;h)-I_a(x;0)\Big)(z-P_e(x;0))^{-1}dz\ \Pi(x;0).
\end{aligned}$$

Using a Taylor expansion, we obtain, for all N,

$$\Big(I_a(x;h)-I_a(x;0)\Big)\Pi(x;0) \ = \ \sum_{k=1}^{N} h^{2k} I_{a,k}(x)\Pi(x;0)+O(h^{2(N+1)}),$$

where the terms $I_{a,k}(x)\Pi(x;0)$ are $O(\langle x\rangle^{-\rho-k})$, thanks to the stability assumption and the exponential decay of eigenfunctions (cf. [J]). For all N and uniformly w.r.t. x, it follows that

$$\Big(\Pi(x;h)-\Pi(x;0)\Big)\Pi(x;0) \ = \ \sum_{k=1}^{N} h^{2k}\tilde{\Pi}_k(x)\Pi(x;0)+O(h^{2(N+1)}). \tag{6}$$

In the same way, we also obtain the following expansion to all orders and with the same operators $\tilde{\Pi}_k$

$$\Big(\Pi(x;h)-\Pi(x;0)\Big)\Pi(x;h) \ = \ \sum_{k=1}^{N} h^{2k}\tilde{\Pi}_k(x)\Pi(x;h)+O(h^{2(N+1)}). \tag{7}$$

Writing

$$\Pi(x;h)-\Pi(x;0) \ = \ \Big(\Pi(x;h)-\Pi(x;0)\Big)\Pi(x;0)+\Pi(x;h)\Big(\Pi(x;h)-\Pi(x;0)\Big),$$

it follows from (6) and (7),

$$\Pi(x;h)-\Pi(x;0) \ = \ \sum_{k=1}^{N} h^{2k}\Big(\Pi(x;h)\tilde{\Pi}_k(x)+\tilde{\Pi}_k(x)\Pi(x;0)\Big)+O(h^{2(N+1)}). \tag{8}$$

On the right side of (8), we replace each $\Pi(x;h)$ by the expression given by (8). Then we obtain a new expansion of the difference $\Pi(x;h)-\Pi(x;0)$, where the coefficient of order h^2 does not contain $\Pi(x;h)$ anymore. Repeating this trick a finite number of times (depending on N), we arrive at the following formula which holds uniformly w.r.t. x :

$$\Pi(x;h) - \Pi(x;0) \;=\; \sum_{k=1}^{N} h^{2k}\pi_k(x) + O(h^{2(N+1)}),$$

with at most rank-one coefficients, since they all contain a factor $\Pi(x;0)$. We then have proved (4). Furthermore, these factors are C^∞ functions of x. In the Taylor expansions above, we may write the remainders as integrals $h^{2N}R_N(x;h)$. These remainders of order N, which are also regular functions of x, can be controlled by the following estimates :

$$\left\|\Big(\partial_x^\alpha R_N(x;h)\Big)\Pi(x;h)\right\| \;=\; O_{N,\alpha}(\langle x\rangle^{-\rho-|\alpha|}),$$

uniformly w.r.t. h and for all $\alpha \in I\!N^n$ (cf. [J]). Thus the last estimate (5) follows from the first one (2). □

Let us denote by $E_0(h)$ the simple eigenvalue of $P^a(h)$ which tends to E_0 as $h \to 0$, denote by $\lambda(x;0)$ the simple eigenvalue of $P_e(x;0)$ which tends to E_0 as $|x| \to \infty$ goes and denote by $\lambda(x;h)$ the simple eigenvalue of $P_e(x;h)$. Note that $\lambda(x;h)$ verifies :

$$\lambda(x;h) \to \lambda(x;0),\;\; h \to 0,$$

uniformly w.r.t. x (cf. Proposition 3.1 in [KMW1]) and :

$$\lambda(x;h) \to E_0(h),\;\; |x| \to \infty,$$

uniformly w.r.t. h, for h small. The simplicity of these eigenvalues implies that we may write :

$$\lambda(x;h) \;=\; \mathrm{Tr}\Big(\Pi(x;h)P_e(x;h)\Big),\;\; E_0(h) \;=\; \mathrm{Tr}\Big(\Pi_0(h)P^a(h)\Big),$$

where Tr stands for the trace operator in $\mathcal{L}(L^2(I\!R_y^{nN_0}))$. Along the lines of the proof of Proposition 2.1 we obtain, for all N,

$$E_0(h) \;=\; E_0 + \sum_{j=1}^{N} h^{2j}e_j + O(h^{2(N+1)}) \tag{9}$$

and

$$\lambda(x;h) \;=\; \lambda(x;0) + \sum_{j=1}^{N} h^{2j}\lambda_j(x) + O(h^{2(N+1)}) \tag{10}$$

uniformly w.r.t. x. Furthermore, the functions $I\!R^n \ni x \mapsto \lambda_j(x)$ are smooth and verify :

$$\forall\alpha \in I\!N^n,\; \exists D_\alpha > 0;\; \forall x \in I\!R^n,\; \|\partial_x^\alpha(\lambda_j(x) - e_j)\| \le D_\alpha\langle x\rangle^{-\rho-|\alpha|}. \tag{11}$$

Before recalling some results from [KMW1], we introduce some more notation. Set $\mathcal{H} = \mathcal{L}(L^2(I\!R_y^{nN_0}))$. For $\delta \ge 0$ and $m \in I\!R$, we consider the class $S_\delta^m(\mathcal{H})$ of symbols $a \in C^\infty(I\!R_{x\xi}^{2n};\mathcal{H})$ which have the property :

$$\forall\alpha,\beta \in I\!N^n,\; \exists D_{\alpha\beta} > 0;\; \forall(x,\xi) \in I\!R^{2n},\; \|\partial_x^\alpha\partial_\xi^\beta a(x,\xi)\| \le D_{\alpha\beta}\langle x\rangle^{m-\delta|\alpha|}.$$

The class $S_0^0(\mathcal{H})$ of bounded symbols is simply denoted by $S(\mathcal{H})$. A family $a(h) \in S_\delta^m(\mathcal{H})$ is called h-admissible if there exists an asymptotic expansion of the form

$$a(h) \;\sim\; \sum_j h^j a_j$$

where the coefficients $a_j \in S_\delta^{m-j\delta}(\mathcal{H})$. For a given phase function $\phi : I\!R^{2n} \longrightarrow I\!R$ and a given h-admissible family of symbols $a(h) \in S_\delta^m(\mathcal{H})$, we introduce the Fourier integral operator (FIO) defined by

$$\Big(J(\phi,a)f\Big)(x) \;=\; (2\pi h)^{-n} \int e^{ih^{-1}(\phi(x,\xi)-x'\cdot\xi)} a(x,\xi;h) f(x') dx' d\xi, \tag{12}$$

where $f \in \mathcal{S}(I\!R_x^n; L^2(I\!R_y^{nN_0}))$. As a special case, the h-pseudodifferential operator $a(x,hD;h)$, with $D = -i\partial_x$, is defined by the same formula where the phase function ϕ is given by $\phi(x,\xi) = x\cdot\xi$. For the phases $\phi_\pm$ we introduce below, we denote the corresponding FIO by $J_\pm(b)$, for a given symbol b.

Let us also define incoming (-) and outgoing (+) regions in the phase space by

$$\Psi_\pm(\epsilon,d,R) \;=\; \Big\{(x,\xi) \in I\!R^{2n};\; |x|>R,\, |\xi|^2>d,\, \pm x\cdot\xi \geq (-1+\epsilon)|x|\;|\xi|\Big\},$$

for $\epsilon, d, R > 0$, and spaces of symbols supported in these regions by

$$S_{\pm,\delta}^m(\epsilon,d,R;\mathcal{H}) \;=\; \Big\{a \in S_\delta^m(\mathcal{H});\, \operatorname{supp} a \subset \Psi_\pm(\epsilon,d,R)\Big\}.$$

Set :

$$S_{\pm,\delta}^m(\mathcal{H}) \;=\; \bigcup_{\epsilon,d,R>0} S_{\pm,\delta}^m(\epsilon,d,R;\mathcal{H}).$$

We also consider real-valued symbols, just replacing $\mathcal{H}$ by $I\!R$ in the previous definitions.

Now we introduce the coherent states operators. For $(x_0,\xi_0) \in I\!R_x^n \times I\!R_\xi^n \setminus \{0\}$, we define :

$$U_h(x_0,\xi_0) \;=\; U_h e^{ih^{-1/2}(x\cdot\xi_0 - x_0\cdot D_x)}, \tag{13}$$

where U_h is the isometry of $L^2(I\!R_x^n; L^2(I\!R_y^{nN_0}))$ given by

$$(U_h f)(x) \;=\; h^{-n/4} f(h^{-1/2}x),$$

and where $D_x = -i\partial_x$. To see how these operators act, we apply them to the h-pseudodifferential operator $b(x,hD)$ associated to a bounded symbol $b \in S(\mathcal{H})$. Then, we observe that

$$\begin{aligned} U_h^* b(x,hD) U_h &= b(h^{1/2}x, h^{1/2}D), \\ U_h(x_0,\xi_0)^* b(x,hD) U_h(x_0,\xi_0) &= b(h^{1/2}x + x_0, h^{1/2}D + \xi_0). \end{aligned} \tag{14}$$

By Φ^t (respectively Φ_0^t), we denote the Hamiltonian flow of the Hamilton function $p(x,\xi) = |\xi|^2 + \lambda(x;0) - E_0$ (respectively $p_0(x,\xi) = |\xi|^2$) and we set :

$$\forall (x,\xi) \in I\!R_x^n \times I\!R_\xi^n \setminus \{0\}, \quad \Phi^t(x,\xi) \;=\; \Big(q(t;x,\xi), p(t;x,\xi)\Big).$$

Definition 2.2 *For an energy $E \in I\!R$, we denote by $p^{-1}(E)$ the energy shell*

$$p^{-1}(E) \;\equiv\; \Big\{(x,\xi) \in I\!R^{2n};\; p(x,\xi) = E\Big\}.$$

The energy E is non-trapping for the Hamilton function $p(x,\xi) = |\xi|^2 + \lambda(x;0) - E_0$ if

$$\forall (x,\xi) \in p^{-1}(E), \qquad \lim_{t\to+\infty} \|\Phi^t(x,\xi)\| = \infty \quad \text{and} \quad \lim_{t\to-\infty} \|\Phi^t(x,\xi)\| = \infty,$$

where $\|\cdot\|$ denote the norm of $I\!R^{2n}$. An open interval J is non-trapping for the Hamilton function $p(x,\xi) = |\xi|^2 + \lambda(x;0) - E_0$ if each $E \in J$ is. A function $\chi \in C_0^\infty(I\!R; I\!R)$ is non-trapping if its support is included in a finite reunion of non-trapping open intervals.

Thanks to the short-range property (11) of the potential $\lambda(x;0) - E_0$, the classical flow satisfies the following properties.

Proposition 2.3 *We use the previous notation.*

1. *For all $\epsilon, d > 0$, there exist positive constants $C, R_0 > 0$ such that, for all $R > R_0$ and all $(x,\xi) \in \Psi_\pm(\epsilon, d, R)$, one has :*

$$|q(t;x,\xi)| \geq C^{-1}(|x| \pm t|\xi|) \quad \text{and} \quad \Phi^t(x,\xi) \in \Psi_\pm(\epsilon/2, d/2, R/C), \tag{15}$$

   for all $\pm t > 0$.

2. *Let I be a compact interval included in some non-trapping interval, w.r.t. the flow Φ^t. Let $\epsilon, d, R > 0$. For all $0 < \epsilon' < \epsilon$ and for all $R_0 > 0$, there exist $d_0, C, T > 0$ such that, for all $(x,\xi) \in \Psi_\pm(\epsilon, d, R) \cap p^{-1}(I)$,*

$$|q(t;x,\xi)| \geq C^{-1}(|x| \pm t|\xi|) \quad \text{and} \quad \Phi^t(x,\xi) \in \Psi_\pm(\epsilon', d_0, R_0), \tag{16}$$

   for all $\pm t \geq T$.

3. *For all $\epsilon, R_0 > 0$, there exist $d_0, T > 0$ such that*

$$(x,\xi) \in \Big\{(y,\eta) \in I\!R^{2n};\; |y| \leq R_0\Big\} \cap p^{-1}(I)$$

   implies that

$$\Phi^t(x,\xi) \in \Psi_\pm(2-\epsilon, d_0, R_0) \tag{17}$$

   for $\pm t > T$.

Proof : These results are probably not new but we did not find a reference in the literature where they are precisely proved. Then we propose a proof in appendix. □

Furthermore, the classical wave operators

$$\Omega^{cl}_{a,\pm}(x,\xi) \;=\; \lim_{t\to\pm\infty} \Phi^{-t} \circ \Phi_0^t(x,\xi), \;\text{ for } x \in I\!R^n,\; \xi \in I\!R^n \setminus \{0\}, \tag{18}$$

exist (cf. [RS3]).

In order to compute the classical limit of the operator S^{AD}, we need to establish suitable microlocal properties of the propagator $e^{ih^{-1}tP^{AD}(h)}$ of P^{AD}. To this end, we follow the WKB method developed in [KMW1] for the construction of parametrices (see also [IK]). Recall that the adiabatic wave operators are given by

$$\Omega_{\pm}^{AD}(h) = s - \lim_{t\to\pm\infty} e^{ih^{-1}tP^{AD}(h)} e^{-ih^{-1}tP_a(h)} \Pi_0(h).$$

The main point is the approximation, for $\pm t$ large, of the wave operators $\Omega_{\pm}^{AD}(h)$ by operators of the form

$$W_{\pm}(t;h) \;=\; e^{ih^{-1}tP^{AD}(h)} J(\phi_{\pm}, a_{\pm}(h)) e^{-ih^{-1}tP_a(h)} \Pi_0(h),$$

where $J(\phi_{\pm}, a_{\pm}(h))$ is a suitably chosen FIO. In others words, we require that

$$\Omega_{\pm}^{AD}(h) \;=\; s - \lim_{t\to\pm\infty} W_{\pm}(t;h).$$

On a formal level, we obtain

$$\Omega_{\pm}^{AD}(h) \;=\; W_{\pm}(t;h) + \int_t^{\pm\infty} \frac{dW_{\pm}}{ds}(s;h)ds.$$

Demanding that the integral is small, this suggests that we should choose the phases $\phi_{\pm}$ and the amplitudes $a_{\pm}(h)$ in such a way that they obey :

$$P^{AD}(h)\Big(e^{ih^{-1}\phi_{\pm}} a_{\pm}(h)\Big) \;=\; e^{ih^{-1}\phi_{\pm}} a_{\pm}(h)\Big(|\xi|^2 + E_0(h)\Big).$$

Trying

$$a_{\pm}(h) \;=\; \Pi(x;h)\tilde{a}_{\pm}(h)$$

as an ansatz, we see that the symbols $\tilde{a}_{\pm}(h)$ must verify :

$$e^{-ih^{-1}\phi_{\pm}}\Big(-h^2\Delta_x + [-h^2\Delta_x, \Pi(x;h)] + \lambda(x;h)\Big)\Big(e^{ih^{-1}\phi_{\pm}}\tilde{a}_{\pm}(h)\Big) \;-\; \tilde{a}_{\pm}(h)\Big(|\xi|^2 + E_0(h)\Big) \;=\; 0.$$

We expand $\tilde{a}_{\pm}(h)$ as an asymptotic sum of symbols in increasing order of powers of h :

$$\tilde{a}_{\pm}(h) \;\sim\; \sum_j h^j \tilde{a}_{j,\pm}. \tag{19}$$

Using the expansions in powers of h of $E_0(h)$, $\lambda(x;h)$ and $\Pi(x;h)$ (cf. (9), (10) and Proposition 2.1), one may rewrite the condition (19) in the following form :

$$\sum_j h^j c_j \;=\; 0.$$

Requiring that all these symbols c_j vanish, we arrive at the following so-called eikonal equation for the phases $\phi_{\pm}$:

$$|\nabla_x \phi_{\pm}(x,\xi)|^2 + \lambda(x;0) \;=\; |\xi|^2 + E_0,$$

and the following transport equations for the amplitudes $\tilde{a}_{j,\pm}$:

$$\begin{aligned}\Big(2(\nabla_x\phi_\pm)(x,\xi)\cdot\nabla_x+2(\nabla_x\phi_\pm)(x,\xi)\cdot(\nabla_x\Pi)(x;0)+(\Delta_x\phi_\pm)(x,\xi)\Big)\tilde{a}_{0,\pm}(x,\xi) &= 0,\\ \Big(2(\nabla_x\phi_\pm)(x,\xi)\cdot\nabla_x+2(\nabla_x\phi_\pm)(x,\xi)\cdot(\nabla_x\Pi)(x;0)+(\Delta_x\phi_\pm)(x,\xi)\Big)\tilde{a}_{k,\pm}(x,\xi) &= b_k(x,\xi),\end{aligned}$$

for $k\geq 1$ and where the symbol b_k only depends on the $\tilde{a}_{j,\pm}$ for $j<k$.

In [KMW1], these equations are solved in the regions $\Psi_\pm(\epsilon,d,R)$, for $\epsilon,d,R>0$ and R large enough. The phases $\phi_\pm\in C^\infty(I\!R^{2n})$ are constructed such that they satisfy the eikonal equation in the region $\Psi_\pm(\epsilon,d,R)$ and that they obey : for all $\delta_1,\delta_2>0$, with $\delta_1+\delta_2=\rho-1$, and for all $\alpha,\beta\in I\!N^n$, there exists a contant $C_{\alpha\beta}>0$ such that

$$\left|\partial_x^\alpha\partial_\xi^\beta\Big(\phi_\pm(x,\xi)-x\cdot\xi\Big)\right|\leq C_{\alpha\beta}R^{-\delta_1}\langle x\rangle^{-\delta_2-|\alpha|},\ \forall(x,\xi)\in I\!R^{2n}. \tag{20}$$

For R large enough, in particular, the maps $x\mapsto\nabla_\xi\phi_\pm(x,\xi)$ are global diffeomorphisms and we denote their inverses by $x_\pm(\cdot,\xi)$. This may be expressed in terms of the following identity :

$$x\ =\ x_\pm\Big(\nabla_\xi\phi_\pm(x,\xi),\xi\Big),\ \forall(x,\xi)\in I\!R^{2n}.$$

Likewise, for large R, the maps $\xi\mapsto\nabla_x\phi_\pm(x,\xi)$ are global diffeomorphisms and we denote their inverses by $\xi_\pm(x,\cdot)$. The analogous identity is :

$$\xi\ =\ \xi_\pm\Big(x,\nabla_x\phi_\pm(x,\xi)\Big),\ \forall(x,\xi)\in I\!R^{2n}.$$

Let us define the maps :

$$\begin{aligned}\kappa_{1,\pm}\ &:\ (x,\xi)\ \mapsto\ \Big(\nabla_\xi\phi_\pm(x,\xi),\xi\Big),\\ \kappa_{2,\pm}\ &:\ (x,\xi)\ \mapsto\ \Big(x,\nabla_x\phi_\pm(x,\xi)\Big).\end{aligned}$$

These diffeormorphismes $\kappa_{1,\pm}$, $\kappa_{2,\pm}$ and their inverses "conserve" incoming and outgoing regions in the following sense : for all $0<\epsilon_0'<\epsilon_0$, $0<d_0'<d_0$ and $0<R_0'<R_0$, we can find R large enough such that, for $\sigma=\pm1$,

$$\kappa_{1,\sigma}\Big(\Psi_\pm(\epsilon_0,d_0,R_0)\Big)\subset\Psi_\pm(\epsilon_0',d_0',R_0'),\quad \kappa_{2,\sigma}\Big(\Psi_\pm(\epsilon_0,d_0,R_0)\Big)\subset\Psi_\pm(\epsilon_0',d_0',R_0') \tag{21}$$

and

$$\kappa_{1,\sigma}^{-1}\Big(\Psi_\pm(\epsilon_0,d_0,R_0)\Big)\subset\Psi_\pm(\epsilon_0',d_0',R_0'),\quad \kappa_{2,\sigma}^{-1}\Big(\Psi_\pm(\epsilon_0,d_0,R_0)\Big)\subset\Psi_\pm(\epsilon_0',d_0',R_0'). \tag{22}$$

The Hamiltonian flow Φ^t, associated to the Hamilton function $|\xi|^2+\lambda(x;0)$, has a similar property :

$$\forall\pm t\geq 0,\ \Phi^t\Big(\Psi_\pm(2\epsilon_0,2d_0,2R_0)\Big)\subset\Psi_\pm(\epsilon_0,d_0,R_0), \tag{23}$$

for R_0 large enough (cf. (15)). The diffeomorphisms $\kappa_{1,\pm}$ and $\kappa_{2,\pm}$ also allow us to express the classical wave operators. For all (x,ξ) in the region $\Psi_\pm(2\epsilon,2d,2R)$, we have :

$$\Omega^{cl}_{a,\pm}(x,\xi)\ =\ \left(x_\pm(x,\xi),\nabla_x\phi_\pm\Big(x_\pm(x,\xi),\xi\Big)\right) \tag{24}$$

and if $(x,\xi) \in \Psi_\pm(2\epsilon, 2d, 2R) \cap \mathrm{Im}\Omega^{cl}_\pm$, in particular, we can invert this relation :

$$(\Omega^{cl}_{a,\pm})^{-1}(x,\xi) \;=\; \Big(\nabla_\xi \phi_\pm\big(x, \xi_\pm(x,\xi)\big), \xi_\pm(x,\xi)\Big). \tag{25}$$

On the other hand, the amplitudes $\tilde a_\pm(h)$ are h-admissible symbols in the class $S^0_{\pm,1}(\epsilon, d, R; \mathcal{H})$ given by

$$\tilde a_\pm(h) \sim \sum_j h^j \chi_\pm \tilde a_{j,\pm}$$

where the functions $\chi_\pm \in C^\infty(I\!\!R^{2n})$ satisfy :

$$\begin{array}{rcl} \operatorname{supp} \chi_\pm & \subset & \Psi_\pm(\epsilon, d, R), \\ \chi_\pm \equiv 1 & \text{on} & \Psi_\pm(2\epsilon, 2d, 2R). \end{array}$$

Their principal symbols verify the following relation for $(x,\xi) \in \Psi_\pm(2\epsilon, 2d, 2R)$:

$$\tilde a_{0,\pm}(x,\xi) \;=\; \Big|\det \partial_x \partial_\xi \phi_\pm(x,\xi)\Big|^{1/2}\; G_\pm(x,\xi), \tag{26}$$

for R large enough and with $G_\pm(x,\xi) \in \mathcal{L}(L^2(I\!\!R^{nN_0}_y))$. Furthermore, for all $\epsilon' > \epsilon$, $d' > d$, $R' > R$, there exists $C > 0$ such that, for $(x,\xi) \in \Psi_\pm(\epsilon', d', R')$, the operators $G_\pm(x,\xi)$ satisfy :

$$\|G_\pm(x,\xi) - I\| \le C\langle x\rangle^{1-\rho}, \tag{27}$$

where I stands for the identity operator on $L^2(I\!\!R^{nN_0}_y)$. The choice of R implies in particular their invertibility (See [KMW1] for more details about the operators $G_\pm(x,\xi)$). In order to control the error terms, let us consider the following symbols :

$$\tilde r_\pm(h) \;=\; e^{-ih^{-1}\phi_\pm}\Big(-h^2\Delta_x + [-h^2\Delta_x, \Pi(x;h)] + \lambda(x;h)\Big)\Big(e^{ih^{-1}\phi_\pm}\tilde a_\pm(h)\Big) - \tilde a_\pm(h)\Big(|\xi|^2 + E_0(h)\Big). \tag{28}$$

The family of symbols $h^{-1}\tilde r_\pm(h)$ is uniformly bounded in $S^{-1}_{\pm,1}(\epsilon, d, R; \mathcal{H})$ and verifies :

$$\forall \alpha, \beta \in I\!\!N^n,\ \|\partial_x^\alpha \partial_\xi^\beta \tilde r_\pm(x,\xi;h)\| \;=\; O_{\alpha\beta}(h^\infty \langle x\rangle^{-\infty}) \tag{29}$$

in the region $\Psi_\pm(2\epsilon, 2d, 2R)$. By $O_{\alpha\beta}(h^\infty\langle x\rangle^{-\infty})$ we mean $O_{\alpha,\beta,N}(h^N\langle x\rangle^{-N})$, for all $N \in I\!\!N$. Finally, we remark that the operator-valued symbols

$$a_\pm(x,\xi;h) \;=\; \Pi(x;h)\tilde a_\pm(x,\xi;h),\ \ r_\pm(x,\xi;h) \;=\; \Pi(x;h)\tilde r_\pm(x,\xi;h)$$

have the same properties as $\tilde a_\pm(x,\xi;h)$ and $\tilde r_\pm(x,\xi;h)$, according to Proposition 2.1.

Thanks to the phases $\phi_\pm$ and the amplitudes $a_\pm(h)$, one has :

Proposition 2.4 *([KMW1]) Choose $\epsilon, d > 0$ and let $1\!\!1_{]2d;+\infty[}$ denote the characteristic function of the interval $]2d, +\infty[$. Let $R = R(\epsilon, d)$ large enough. For the phases $\phi_\pm$ and for a symbol $b(h)$, we denote $J(\phi_\pm, b(h))$ (cf. (12)) simply by $J_\pm(b(h))$.*

1. *On the range of the operator* $1\!\!1_{]2d;+\infty[}(-h^2\Delta_x)$*, one has :*

$$\Omega_\pm^{AD}(h) \;=\; s-\lim_{t\to\pm\infty} W_\pm(t;h)$$

with :

$$W_\pm(t;h) \;=\; e^{ih^{-1}tP^{AD}(h)}\; J_\pm(a_\pm(h))\; e^{-ih^{-1}tP_a(h)}\Pi_0(h),$$

where $P_a(h)\Pi_0(h) = (-h^2\Delta_x + E_0(h))\Pi_0(h)$ *and* $J_\pm(a_\pm(h)) = J(\phi_\pm, a_\pm(h))$.

2. *Furthermore, for all functions* $f \in \mathrm{Im}1\!\!1_{]2d;+\infty[}(-h^2\Delta_x)$*, one has :*

$$\Omega_\pm^{AD}(h)f \;=\; W_\pm(\pm t;h)f + ih^{-1}\int_{\pm t}^{\pm\infty} e^{ih^{-1}sP^{AD}(h)}\; J(\phi_\pm, r_\pm(h))\; e^{-ih^{-1}sP_a(h)}\Pi_0(h)f\,ds,$$

where the functions $h^{-1}r_\pm(h)$ *are uniformly bounded in* $S^{-1}_{\pm,1}(\epsilon, d, R; \mathcal{H})$ *and have the property (29) in the region* $\Psi_\pm(2\epsilon, 2d, 2R)$.

3. *Considering a symbol*

$$b_\pm \in S_\pm\Big(4\epsilon, 4d, 4R; I\!R\Big) \cup C_0^\infty\Big(I\!R^n_x \times I\!R^n_\xi \setminus \{0\}; I\!R\Big),$$

there exists $T > 0$ *such that*

$$t > T \Longrightarrow \Big\|\Big(\Omega_\pm^{AD}(h) - W_\pm(\pm t;h)\Big)b_\pm(x,hD)\Big\| \;=\; O(h^\infty\langle t\rangle^{-\infty}).$$

Here $b_\pm(x,hD)$ *is the h-pseudodifferential operator with symbol* $b_\pm$.

Proof : see [KMW1]. □

Making use of Proposition 2.4, the action of the wave operators $\Omega_\pm^{AD}$ on quantum observables and on coherent states is studied in [KMW1] (cf. Theorems 5.3 and 5.4 in [KMW1]). In Section 4, some equivalent results are obtained for the adiabatic scattering operator S^{AD}.

3 Propagation estimates for P^{AD}.

In this section, we establish some estimates on the adiabatic propagation that we use in Section 4. The potentials still verify the condition (D_ρ) for $\rho > 1$. Our results are similar to those in [W1], [W2], and [W3], and we will essentially use the same arguments as in these references.

Except the pseudodifferential operators, the FIO we consider in this section, are constructed with the phases $\phi_\pm$, introduced in Section 2, and we denote them by $J_\pm(b)$, for a given symbol b (cf. (12)).

We first recall that one has a semiclassical control on the boundary value of the adiabatic resolvent of $R^{AD}(z;h) = (P^{AD}(h) - z)^{-1}$:

Theorem 3.1 *([KMW1]) Under assumption (D_ρ), $\rho > 0$, for the potentials and assumption $(HS(h))$ for the simple eigenvalue E_0 (cf. Definition 1.1), let $E \in]E_0; +\infty[$ be a non-trapping energy for the Hamilton function $|\xi|^2 + \lambda(x;0)$ (cf. Definition 2.2). For all $s > 1/2$, one has :*

$$\|\langle x\rangle^{-s} R^{AD}(\lambda \pm i0; h)\langle x\rangle^{-s}\| \;=\; O(h^{-1})$$

uniformly w.r.t. λ close enough to E and h small enough.

Proof : See Theorem 3.2 and Corollary 3.3 in [KMW1]. □

We also need a semiclassical Egorov Theorem (cf. [W4]) for the propagator $e^{-ih^{-1}tP^{AD}(h)}$, which essentially results from the arguments in [Ro] (see also [W4]).

Theorem 3.2 *Let $c \in S(\mathcal{H})$ be a bounded symbol. Denote by Φ^t the flow associated to the Hamilton function $|\xi|^2 + \lambda(x;0)$. Under assumption (D_ρ) with $\rho > 1$ for potentials, the operator*

$$\Pi(h)\; e^{ih^{-1}tP^{AD}(h)}\; c(x, hD)\; e^{-ih^{-1}tP^{AD}(h)}\; \Pi(h)$$

is an h-pseudoodifferential operator with bounded symbol $c(t;h) \in S(\mathcal{H})$, for all t. Furthermore, this symbol may be expanded asymptoticaly as

$$c(t;h) \sim \sum_{k=0}^{\infty} h^k c_k(t),$$

where the support of the bounded symbols $c_k(t) \in S(\mathcal{H})$ satisfy $\operatorname{supp} c_k(t) \subset \operatorname{supp}(c\circ\Phi^t)$. Finally, the principal symbol is given by $c_0(t)(x,\xi) = \Pi(x;0)(c\circ\Phi^t)(x,\xi)\Pi(x;0)$.

Proof : See [Ro]. □

Remark 3.3 *With the same proof, one obtains a similar result for the operator $P_a\Pi_0$. In fact, this is well known since $P_a(h)\Pi_0(h) = (-h^2\Delta_x + E_0(h))\Pi_0(h)$ (cf. [W4] and [Ro]).*

On the other hand, we will also use some composition properties of FIO and pseudodifferential operators (cf. [W1]), which are collected in the following proposition :

Proposition 3.4 *Let $\phi_\pm$ be the phases constructed in Section 2 and recall that we simply note a FIO $J(\phi_\pm, b)$ by $J_\pm(b)$, for a given symbol b. For all $0 < \epsilon_0' < \epsilon_0$, $0 < d_0' < d_0$ and $0 < R_0' < R_0$, one can find R large enough such that the following properties holds.*

Let $a_\pm, b_\pm \in S^0_{\pm,1}(\epsilon_0, d_0, R_0; \mathcal{H})$ h-admissible symbols. There exists h-admissible symbols $c_\pm(h), d_\pm(h), e_\pm(h), f_\pm(h) \in S^0_{\pm,1}(\epsilon_0', d_0', R_0'; \mathcal{H})$ such that

$$\begin{aligned} a_\pm(x, hD)J_\pm(b_\pm) &= J_\pm(c_\pm(h)), \\ c_{0,\pm}(x,\xi) &= a_{0,\pm}\Big(x, \nabla_x\phi_\pm(x,\xi)\Big)b_{0,\pm}(x,\xi), \end{aligned}$$

$$
\begin{aligned}
J_\pm(a_\pm)b_\pm(x,hD) &= J_\pm(d_\pm(h)),\\
d_{0,\pm}(x,\xi) &= a_{0,\pm}(x,\xi)b_{0,\pm}\Big(\nabla_\xi\phi_\pm(x,\xi),\xi\Big),
\end{aligned}
$$

$$
\begin{aligned}
J_\pm(a_\pm)J_\pm(b_\pm)^* &= e_\pm(x,hD),\\
e_{0,\pm}(x,\xi) &= a_{0,\pm}\Big(x,\xi_\pm(x,\xi)\Big)b_{0,\pm}\Big(x,\xi_\pm(x,\xi)\Big)^*\Big|\det\Big(\frac{\partial\xi_\pm}{\partial\xi}(x,\xi)\Big)\Big|,
\end{aligned}
$$

$$
\begin{aligned}
J_\pm(a_\pm)^*J_\pm(b_\pm) &= f_\pm(x,hD),\\
f_{0,\pm}(x,\xi) &= a_{0,\pm}\Big(x_\pm(x,\xi),\xi\Big)^*b_{0,\pm}\Big(x_\pm(x,\xi),\xi\Big)\Big|\det\Big(\frac{\partial x_\pm}{\partial x}(x,\xi)\Big)\Big|.
\end{aligned}
$$

We use the subscript 0 for the principal symbol. For each symbol $g_\pm(h)=c_\pm(h)$, $d_\pm(h)$, $e_\pm(h)$, $f_\pm(h)$ and for all $N\in I\!N$, we write :

$$g_\pm(h) \;=\; \sum_{j=0}^{N} h^j g_{j,\pm} + h^{N+1}\hat g_\pm(h).$$

For $G_{N,\pm}(h)=\hat g_\pm(x,hD)$ or $J_\pm(\hat g_\pm(h))$, according to the considered composition, one has, for all $k\in Z\!\!Z$,

$$\|\langle x\rangle^{N+k}G_{N,\pm}(h)\langle x\rangle^{-k}\| \;=\; O(1), \tag{1}$$

uniformly w.r.t. h.

These composition properties still hold for bounded symbols in $S(\mathcal{H})$. In this case, the remainders are :

$$\|G_{N,\pm}(h)\| \;=\; O(1),$$

uniformly w.r.t. h.

Remark 3.5 *Recall that, for bounded symbols, pseudodifferential operators and FIO are bounded operators on the weight spaces $L^2_s(I\!R^n;\mathcal{H})\equiv L^2(I\!R^n;\mathcal{H};\langle x\rangle^{2s}dx)$.*

Proof : The arguments of [W1] still hold if we replace real-valued by operator-valued symbols (cf. [Ba]). The control on supports is ensured by (21) and (22). About the bounded symbols the arguments in [Ro] apply. □

Now let us give propagation estimates uniformly w.r.t. h.

Proposition 3.6 *Let $\chi\in C_0^\infty(]E_0;+\infty[;I\!R)$ be non-trapping for the Hamilton function $|\xi|^2+\lambda(x;0)$ (cf. Definition 2.2).*

1. *Then, one has :*

$$\Big\|\langle x\rangle^{-1}\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}\langle x\rangle^{-1}\Big\| \;=\; O(\langle t\rangle^{-1}) \tag{2}$$

for all $t\in I\!R$, uniformly w.r.t. h.

2. *For all symbols $b_\pm \in S^0_{\pm,1}(I\!R)$, for all $k \in I\!N$, one has :*

$$\left\| \langle x\rangle^{-1-k} \chi\Big(P^{AD}(h)\Big) e^{-ih^{-1}tP^{AD}(h)} b_\pm(x,hD)\langle x\rangle^k \right\| \;=\; O(\langle t\rangle^{-1}), \tag{3}$$

   for all $\pm t > 0$, uniformly w.r.t. h.

3. *For $d_0, R_\pm > 0$ and $\epsilon_1, \epsilon_2 > 0$ such that $\epsilon_1 + \epsilon_2 > 2$, we consider symbols $b_{j,\pm} \in S^0_{\pm,1}(\epsilon_j, d_0, R_\pm; I\!R)$, $1 \leq j \leq 2$. For all $k \in I\!N$, one has :*

$$\left\| \langle x\rangle^{k} b_{1,\mp}(x,hD) \chi\Big(P^{AD}(h)\Big) e^{-ih^{-1}tP^{AD}(h)} b_{2,\pm}(x,hD)\langle x\rangle^k \right\| \;=\; O(\langle t\rangle^{-1}), \tag{4}$$

   for all $\pm t \geq 0$, uniformly w.r.t. h. The condition $\epsilon_1+\epsilon_2 > 2$ implies that the symbols $b_{1,\mp}$ and $b_{2,\pm}$ have disjoint supports.

Remark 3.7 *We remark that the estimates (3) and (4) in Proposition 3.6 still hold if a microlocalisation $b_\pm(x,hD)$ is replaced by a FIO $J_\pm(b_\pm(h))$. Indeed, if we have $b_\pm \in S^0_{\pm,1}(\epsilon_0, d_0, R_0; I\!R)$ then, for all $0 < \epsilon_0'' < \epsilon_0' < \epsilon_0$, $0 < d_0'' < d_0' < d_0$, and $0 < R_0'' < R_0' < R_0$, we can find a symbol $\tau_\pm \in S^0_{\pm,1}(\epsilon_0'', d_0'', R_0''; I\!R)$ with value 1 in the region $\Psi_\pm(\epsilon_0', d_0', R_0')$. Thanks to Proposition 3.4, we have :*

$$(1-\tau)(x,hD)J_\pm(b_\pm(h)) \;=\; J_\pm(\hat{b}_\pm(h))$$

where the family of symbols $h^{-N}\hat{b}_\pm(h)$ is uniformly bounded in the space $S^{-N}_{\pm,1}(\epsilon_0', d_0', R_0'; I\!R)$, for all N. From the estimates of Proposition 3.6 for $\tau(x,hD)$, we deduce the same estimates for $\tau(x,hD)J_\pm(b_\pm(h))$ thanks to Remark 3.5, and thus for $J_\pm(b_\pm(h))$.

For the same reason, these estimates (3) and (4) still hold for $\mathcal{H}$-valued symbols.

Proof : We follow the proof in [W2]. Let us first prove the first estimate (2). Using the operator $A^{AD}(h) = \Pi(h)A(h)\Pi(h)$ where

$$A(h) \;=\; \frac{x\cdot h\nabla_x + h\nabla_x \cdot x}{2i},$$

we have, according to Proposition 2.1,

$$i[P^{AD}(h), A^{AD}(h)] \;=\; 2P^{AD}(h) + \mathcal{V}^{AD}(h)$$

where the operator $\mathcal{V}^{AD}(h)$ is of the form :

$$\mathcal{V}^{AD}(h) \;=\; O(\langle x\rangle^{-\rho})\cdot h(\nabla_x\Pi)(h) + O(\langle x\rangle^{-\rho})$$

uniformly w.r.t. h and with $\rho > 1$. Pointwise in $\mathcal{S}(I\!R^n_x; L^2(I\!R^{nN_0}_y))$, we may write :

$$\begin{aligned} A^{AD}(h)e^{-ih^{-1}tP^{AD}(h)} \;&=\; e^{-ih^{-1}tP^{AD}(h)}A^{AD}(h) + 2tP^{AD}(h)e^{-ih^{-1}tP^{AD}(h)} \\ &\quad + \int_0^t e^{-ih^{-1}(t-s)P^{AD}(h)}\mathcal{V}^{AD}(h)e^{-ih^{-1}sP^{AD}(h)}ds \end{aligned}$$

and, therefore,

$$P^{AD}(h)e^{-ih^{-1}tP^{AD}(h)}$$

is given by

$$= \frac{1}{2t}\left([A^{AD}(h), e^{-ih^{-1}tP^{AD}(h)}] - \int_0^t e^{-ih^{-1}(t-s)P^{AD}(h)}\mathcal{V}^{AD}(h)e^{-ih^{-1}sP^{AD}(h)}ds\right). \quad (5)$$

For a real λ, with $|\lambda|$ large enough, one can verify that the operator $(A^{AD}(h)+i\lambda)^{-1}$ conserve $P^{AD}(h)$'s domain (cf. [J]). Using the functional calculus of Helffer and Sjöstrand (cf. [HS]), we infer that the operator

$$(A^{AD}(h)+i\lambda)\chi\Big(P^{AD}(h)\Big)(A^{AD}(h)+i\lambda)^{-1}$$

is bounded. Thanks to Theorem 3.1, the operators $\langle x\rangle^{-\mu}$ and $\langle x\rangle^{-\mu}h\nabla_x\Pi(h)$ for $\mu > 1/2$ are $P^{AD}(h)$-smooth locally on the support of χ (cf. [RS4]). Then there exists a h-independent constant C, such that

$$\begin{aligned}\int_{-\infty}^{+\infty}\|\langle x\rangle^{-\mu}\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}f\|^2dt &\leq C\|f\|^2\\ \int_{-\infty}^{+\infty}\|\langle x\rangle^{-\mu}h\nabla_x\Pi(h)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}f\|^2dt &\leq C\|f\|^2\end{aligned}$$

for all functions $f \in L^2(I\!R^n_x; L^2(I\!R^{nN_0}_y))$. It follows from (5) that, uniformly w.r.t. h,

$$\|(A^{AD}(h)+i)^{-1}\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}(A^{AD}(h)+i)^{-1}\| = O(\langle t\rangle^{-1}).$$

Now we choose a non-trapping function $\theta \in C_0^\infty(]E_0;+\infty[;I\!R)$ such that $\chi = \chi\theta$. The operator

$$\langle x\rangle^{-1}\theta\Big(P^{AD}(h)\Big)A^{AD}(h)$$

is bounded (cf. [J]). This yields the first estimate (2).

According to [W1], one has, under the conditions of Proposition 3.6, similar estimates as (3) and (4) for the free propagator, i.e., for all integers $k, l \geq 0$, one has :

$$\|\langle x\rangle^{-l-k}e^{-ih^{-1}tP_a(h)}\Pi_0(h)b_\pm(x,hD)\langle x\rangle^k\| = O(\langle t\rangle^{-l}), \quad (6)$$

and :

$$\|\langle x\rangle^k b_{1,\mp}(x,hD)e^{-ih^{-1}tP_a(h)}\Pi_0(h)b_{2,\pm}(x,hD)\langle x\rangle^k\| = O(\langle t\rangle^{-l}), \quad (7)$$

for all $\pm t > 0$, uniformly w.r.t. h.

Next we prove the second estimate (3) in Proposition 3.6. Let $b_\pm \in S^0_{\pm,1}(\epsilon_0, d_0, R_0; I\!R)$. Choose $\epsilon, d > 0$ small enough such that $3\epsilon < \epsilon_0$ and $2d < d_0$. Let

$$\epsilon_0' \in]3\epsilon;\epsilon_0[,\ d_0' \in]2d;d_0[\text{ and } R_0' \in]0;R_0[.$$

Pick R large enough such that the properties of Section 2 hold and that Proposition 3.4 applies. Thanks to the ellipticity of the principal symbol $\tilde{a}_{0,\pm}$ of

$$\tilde{a}_\pm(h) \sim \sum_j h^j\tilde{a}_{j,\pm},$$

in the region $\Psi_\pm(2\epsilon, 2d, 2R)$ (cf. (26)), there exist (cf. proof of Lemma 4.5 in [W1] and Proposition 3.4 in the present work) bounded symbols

$$\tilde{b}_\pm(h) \ \sim \ \sum_j h^j \tilde{b}_{j,\pm},$$

in $S^0_{\pm,1}(\epsilon'_0, d'_0, R'_0; \mathcal{H})$ such that, for all N, one has :

$$b_\pm(x, hD) \ = \ J_\pm\Big(\tilde{a}_\pm(N;h)\Big) J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^* + h^{N+1} R_{N,\pm}(h) \tag{8}$$

with :

$$\tilde{a}_\pm(N;h) \ = \ \sum_{j=0}^{N} h^j \tilde{a}_{j,\pm} \ \text{ and } \ \tilde{b}_\pm(N;h) \ = \ \sum_{j=0}^{N} h^j \tilde{b}_{j,\pm},$$

and where the operators $R_{N,\pm}(h)$ verify the property (1), i.e. :

$$\|\langle x\rangle^{N+k} R_{N,\pm}(h) \langle x\rangle^{-k}\| \ = \ O(1),$$

for all $k \in \mathbb{Z}$. By the definition of the symbols $\tilde{r}_\pm(h)$ (cf. (28)),

$$\Pi(h) e^{-ih^{-1}tP^{AD}(h)} J_\pm\Big(\tilde{a}_\pm(N;h)\Big) \ = \ \Pi(h) J_\pm\Big(\tilde{a}_\pm(N;h)\Big) e^{-ih^{-1}tP_a(h)} \Pi_0(h)$$

$$-ih^{-1} \int_0^t \Pi(h) e^{-ih^{-1}sP^{AD}(h)} J_\pm\Big(\tilde{r}_\pm(N;h)\Big) e^{-ih^{-1}(t-s)P_a(h)} \Pi_0(h) ds. \tag{9}$$

Using the functional calculus of Helffer and Robert (cf. [HR]), we can show that the operator $\chi(P^{AD}(h))$ is an h-pseudoodifferential operator with symbol in $S^0_1(\mathcal{H})$ (cf. [W1]). The operators $\chi(P^{AD}(h))$ and $J_\pm(\tilde{a}_\pm(N;h))$ are bounded on the weight spaces $L^2_s(\mathbb{R}^n; \mathcal{H})$, for all $s \in \mathbb{R}$. Thus, for all $k \in \mathbb{N}$, one has, according to (6) and to Remark 3.7,

$$\|\langle x\rangle^{-1-k} \chi\Big(P^{AD}(h)\Big) J_\pm\Big(\tilde{a}_\pm(N;h)\Big) e^{-ih^{-1}tP_a(h)} \Pi_0(h) J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^* \langle x\rangle^k\| \ = \ O(\langle t\rangle^{-1}),$$

for $\pm t > 0$. Thanks to the first estimate (2) in Proposition 3.6 and to the property (1), the term

$$\Big\|\langle x\rangle^{-1-k} \chi\Big(P^{AD}(h)\Big) e^{-ih^{-1}tP^{AD}(h)} R_{N,\pm}(h) \langle x\rangle^k\Big\|,$$

for all $N \geq k+1$, is less than

$$\Big\|\langle x\rangle^{-1-k} \chi\Big(P^{AD}(h)\Big) e^{-ih^{-1}tP^{AD}(h)} \langle x\rangle^{-1}\Big\| \cdot \Big\|\langle x\rangle^{N-k} R_{N,\pm}(h) \langle x\rangle^k\Big\| \ = \ O(\langle t\rangle^{-1}),$$

for $\pm t > 0$. To evaluate the integral in (9), we write :

$$\tilde{r}_\pm(N;h) \ = \ \tilde{r}_{\pm,1}(N;h) + \tilde{r}_{\pm,2}(N;h) + \tilde{r}_{\pm,3}(N;h) \tag{10}$$

where $\tilde{r}_{\pm,1}(N;h)$ is supported in $\Psi_\pm(2\epsilon, 2d, 2R)$, the second term $\tilde{r}_{\pm,2}(N;h)$ in

$$\Big\{(x,\xi) \in \mathbb{R}^{2n};\ |x| \leq 3R,\ |\xi|^2 \leq 3d\Big\},$$

and where the support of the third term $\tilde{r}_{\pm,3}(N;h)$ neither intersects $\Psi_\pm(3\epsilon, 3d, 3R)$ nor

$$\Big\{(x,\xi) \in \mathbb{R}^{2n};\ |x| \leq 2R,\ |\xi|^2 \leq 2d\Big\}.$$

In particular, the operator $h^{-1}\langle x\rangle^N J_\pm(\tilde r_{\pm,1}(N;h))\langle x\rangle$ is $O(h^N)$, thanks to (29). The symbols $h^{-1}\langle x\rangle\tilde r_{\pm,3}(N;h)$ are uniformly bounded in $S^0_{\mp,1}(2-3\epsilon,2d,2R)$. Due to the choice of ϵ and ϵ_0', we have $2-3\epsilon+\epsilon_0'>2$. The compactly supported symbols $h^{-1}\langle x\rangle\tilde r_{\pm,2}(N;h)$ are uniformly bounded.

Now we use Remark 3.7 and the property (6) to obtain :

$$\left\|h^{-1}\langle x\rangle J_\pm\Big(\tilde r_{\pm,j}(N;h)\Big)e^{-ih^{-1}tP_a(h)}\Pi_0(h)J_\pm\Big(\tilde b_\pm(N;h)\Big)^*\langle x\rangle^k\right\| \;=\; O(\langle t\rangle^{-3}), \qquad (11)$$

for $\pm t>0$, $j=1,2$ and $N\geq k+3$. Applying (7) to the symbols $h^{-1}\langle x\rangle\tilde r_{\pm,3}(N;h)$ and $\tilde b_\pm(N;h)$, we deduce the estimate (11) also for $j=3$. Thanks to the first estimate (2) in Proposition 3.6, we obtain, for $N\geq k+3$,

$$\begin{aligned}\Big\|h^{-1}\int_0^t \langle x\rangle^{-1-k}\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}sP^{AD}(h)}J_\pm\Big(\tilde r_\pm(N;h)\Big)\\ e^{-ih^{-1}(t-s)P_a(h)}\Pi_0(h)J_\pm\Big(\tilde b_\pm(N;h)\Big)^*\langle x\rangle^k\,ds\Big\|\\ \leq C\int_0^t\langle s\rangle^{-1}\langle t-s\rangle^{-3}ds \;=\; O(\langle t\rangle^{-1})\end{aligned}$$

for $\pm t>0$ (we have used $\langle s\rangle^{-1}\langle t-s\rangle^{-1}\leq c\langle t\rangle^{-1}$). This finishes the proof of the second estimate (3).

We come to prove the third estimate (4) in Proposition 3.6. We use the "factorisation" (8) for $b_{2,\pm}$ and we choose $\epsilon,d,R>0$ as before. For

$$0<\epsilon_2'<\epsilon_2 \text{ with } \epsilon_2'+\epsilon_1>2,\;\; 0<d_0'<d_0 \text{ and } R<R_\pm'<R_\pm,$$

we consider symbols $\tilde b_\pm(h)\in S^0_{\pm,1}(\epsilon_2',d_0',R_\pm';\mathcal{H})$ such that the decomposition (8) is valid for $b_{2,\pm}$.

Since the second estimate (3) in Proposition 3.6 also holds for the adjoint operator, we have, for all $k\in\mathbb{N}$,

$$\left\|\langle x\rangle^k b_{1,\mp}(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}\langle x\rangle^{-1-k}\right\| \;=\; O(\langle t\rangle^{-1}), \qquad (12)$$

for all $\pm t>0$, uniformly w.r.t. h. For $N\geq 2k+1$, this yields, due to (1),

$$\left\|\langle x\rangle^k b_{1,\mp}(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}R_{N,\pm}(h)\langle x\rangle^k\right\| \;=\; O(\langle t\rangle^{-1}),$$

for all $\pm t>0$.

Now we write (9) for $b_{2,\pm}$. Due to Proposition 3.4, we have :

$$b_{1,\mp}(x,hD)\chi\Big(P^{AD}(h)\Big)J_\pm\Big(\tilde a_\pm(N;h)\Big) \;=\; J_\pm\Big(\tilde b_{1,\mp}(N;h)\Big)+h^{N+1}A_{N,\pm}(h)$$

where the operators $A_{N,\pm}(h)$ verify (1). Choosing R larger if necessary, we may suppose (cf. Proposition 3.4) that $\tilde b_{1,\mp}(N;h)\in S^0_{\mp,1}(\epsilon_1',d_0/2,R_\mp/2)$ for some $\epsilon_1'<\epsilon_1$ with $\epsilon_1'+\epsilon_2'>2$.

For all $k \in I\!N$ and all $N \geq 2k+1$, using (1) for $A_{N,\pm}(h)$ and (6), this yields :

$$\left\| \langle x\rangle^k A_{N,\pm}(h) e^{-ih^{-1}tP_a(h)} \Pi_0(h) J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^* \langle x\rangle^k \right\| \;=\; O(\langle t\rangle^{-1}),$$

for all $\pm t > 0$. Thanks to inequality $\epsilon_1' + \epsilon_2' > 2$, we may apply (7) to $\tilde{b}_{1,\mp}(N;h)$ and $\tilde{b}_\pm(N;h)$. This gives :

$$\left\| \langle x\rangle^k J_\pm\Big(\tilde{b}_{1,\mp}(N;h)\Big) e^{-ih^{-1}tP_a(h)} \Pi_0(h) J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^* \langle x\rangle^k \right\| \;=\; O(\langle t\rangle^{-1}),$$

for all $\pm t > 0$.

We now have to evaluate the contribution of the integral in (9). We split the symbol $\tilde{r}_\pm(N;h)$ according to (10). Because of (6), we obtain, for all $k \in I\!N$ and all $N \geq 2k+5$,

$$\left\| \langle x\rangle^k J_\pm\Big(\tilde{r}_{\pm,j}(N;h)\Big) e^{-ih^{-1}tP_a(h)} \Pi_0(h) J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^* \langle x\rangle^k \right\| \;=\; O(\langle t\rangle^{-3}), \qquad (13)$$

where $\pm t > 0$ and $j = 1, 2$. Due to (7) and the choice of ϵ, Estimate (13) is still valid for $j = 3$. Thus one has, thanks to (12), for $N \geq 2k+5$,

$$\begin{aligned} &\Big\| h^{-1} \int_0^t \langle x\rangle^k b_{1,\mp}(x,hD) \chi\Big(P^{AD}(h)\Big) e^{-ih^{-1}sP^{AD}(h)} J_\pm\Big(\tilde{r}_\pm(N;h)\Big) \\ &\qquad e^{-ih^{-1}(t-s)P_a(h)} \Pi_0(h) J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^* \langle x\rangle^k \, ds \Big\| \\ &\leq C \int_0^t < s >^{-1} < t-s >^{-3} ds \;=\; O(\langle t\rangle^{-1}) \end{aligned}$$

for $\pm t > 0$ and uniformly w.r.t. h. This finishes the proof of Proposition 3.6. $\square$

Corollary 3.8 *Assume the same conditions as in Proposition 3.6.*

1. *For $N \in I\!N$, we have :*

$$\left\| \langle x\rangle^{-N} \chi\Big(P^{AD}(h)\Big) e^{-ih^{-1}tP^{AD}(h)} \langle x\rangle^{-N} \right\| \;=\; O(\langle t\rangle^{-N}), \qquad (14)$$

   for all $t \in I\!R$ and uniformly w.r.t. h.

2. *For all symbols $b_\pm \in S^0_{\pm,1}(I\!R)$ and for all $k, N \in I\!N$, we have :*

$$\left\| \langle x\rangle^{-N-k} \chi\Big(P^{AD}(h)\Big) e^{-ih^{-1}tP^{AD}(h)} b_\pm(x,hD) \langle x\rangle^k \right\| \;=\; O(\langle t\rangle^{-N}), \qquad (15)$$

   for all $\pm t > 0$ and uniformly w.r.t. h.

3. *For $d_0, R_\pm > 0$ and $\epsilon_1, \epsilon_2 > 0$ such that $\epsilon_1 + \epsilon_2 > 2$, assume that the symbols $b_{j,\pm} \in S^0_{\pm,1}(\epsilon_j, d_0, R_\pm; I\!R)$, $1 \leq j \leq 2$. Then, for all $k, N \in I\!N$, we have :*

$$\left\| \langle x\rangle^k b_{1,\mp}(x,hD) \chi\Big(P^{AD}(h)\Big) e^{-ih^{-1}tP^{AD}(h)} b_{2,\pm}(x,hD) \langle x\rangle^k \right\| \;=\; O(\langle t\rangle^{-N}), \qquad (16)$$

   for all $\pm t \geq 0$ and uniformly w.r.t. h.

Remark 3.7 is valid for the previous estimates.

Proof : The purpose is to improve the decay properties w.r.t. t. Let $\phi, \theta \in C_0^\infty(]E_0;+\infty[;I\!R)$ be two non-trapping functions such that $\chi = \chi\phi$ and $\phi = \phi\theta$. Putting

$$G_\chi^{AD}(t) \;=\; \chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)},$$

we write :

$$G_\chi^{AD}(t) \;=\; G_\chi^{AD}(t/2)\theta\Big(P^{AD}(h)\Big)G_\phi^{AD}(t/2). \tag{17}$$

Using arguments from [W1], we show that, for all $0 < \epsilon_3' < \epsilon_3$ and for all N, we can split $\theta(P^{AD}(h))$ into the following form :

$$\theta\Big(P^{AD}(h)\Big) \;=\; c_+(x,hD) + c_-(x,hD) + S_N \tag{18}$$

where the symbols $c_\pm(h) \in S^0_{\pm,1}(\mathcal{H})$ verify :

$\operatorname{supp} c_+ \subset \Big\{(x,\xi); x\cdot\xi \geq (-1+\epsilon_3')|x|\cdot|\xi|\Big\}$ and $\operatorname{supp} c_- \subset \Big\{(x,\xi); -x\cdot\xi \geq (-1+2-\epsilon_3)|x|\cdot|\xi|\Big\}$

and where the operator S_N satisfies Estimate (1). Thanks to (17), (18), and Proposition 3.6, we mimick the induction in the proof of Theorem 5.1 in [W1], and then we arrive at the claim. □

For the next section, we need upper bounds of the form $O(h^N\langle t\rangle^{-N})$. Adapting arguments from [W1], [W2] and [W3] to the present situation and using the symbols $\tilde{a}_\pm(h)$ and $\tilde{r}_\pm(h)$, we are going to prove the following proposition :

Proposition 3.9 *Let $\chi \in C_0^\infty(]E_0;+\infty[;I\!R)$ be non-trapping for the Hamilton function $|\xi|^2 + \lambda(x;0)$ (cf. Definition 2.2).*

1. *Let $d_0, R_\pm > 0$ and $\epsilon_1, \epsilon_2 > 0$ such that $\epsilon_1 + \epsilon_2 > 2$. Let $b_{j,\pm} \in S^0_{\pm,1}(\epsilon_j, d_0, R_\pm; I\!R)$, $1 \leq j \leq 2$. Then, for $R_+ + R_-$ large enough and for all $N \in I\!N$, we have :*

$$\Big\|b_{1,\mp}(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}b_{2,\pm}(x,hD)\Big\| \;=\; O(h^N\langle t\rangle^{-N}), \tag{19}$$

   for all $\pm t \geq 0$.

2. *Let $\epsilon_0, d_0, R_0 > 0$ and denote by $B(R_0)$ the set of all functions $\psi \in C_0^\infty(I\!R^{2n};I\!R)$ such that*

$$\operatorname{supp}\psi \subset \Big\{(x,\xi) \in I\!R^{2n};\ |x| \leq R_0\Big\}.$$

   Then, there exists $R_1 > 0$ such that, for all $\psi \in B(R_0)$, for all $b_\pm \in S^0_{\pm,1}(\epsilon_0, d_0, R_1; I\!R)$, and for all $N \in I\!N$, we have :

$$\Big\|\psi(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}b_\pm(x,hD)\Big\| \;=\; O(h^N\langle t\rangle^{-N}), \tag{20}$$

   for all $\pm t \geq 0$.

Remark 3.7 is valid for the previous estimates.

Proof : Again, similar estimates hold for the free operator $P_a(h)\Pi_0(h) = (-h^2\Delta_x + E_0(h))\Pi_0(h)$ and we refer to [W1] for the proofs. Precisely, we have, for all symbols $b_\pm \in S^0_{\pm,1}(I\!R)$, for all $N \in I\!N$, and for $\pm t > 0$,

$$\left\| \langle x\rangle^{-N} e^{-ih^{-1}tP_a(h)}\Pi_0(h)b_\pm(x,hD)\right\| \;=\; O(\langle t\rangle^{-N}), \tag{21}$$

uniformly w.r.t. h, and Estimates (19) and (20) in Proposition 3.9 hold if we replace $P^{AD}(h)$ by $P_a(h)\Pi_0(h)$. Under the conditions of Proposition 3.9, we then have, on one hand,

$$\left\| \psi(x,hD) e^{-ih^{-1}tP_a(h)}\Pi_0(h)b_\pm(x,hD)\right\| \;=\; O(h^N\langle t\rangle^{-N}), \tag{22}$$

for all $N \in I\!N$ and for $\pm t > 0$, and

$$\left\| b_{1,\mp}(x,hD) e^{-ih^{-1}tP_a(h)}\Pi_0(h)b_{2,\pm}(x,hD)\right\| \;=\; O(h^N\langle t\rangle^{-N}), \tag{23}$$

for all N and for all $\pm t > 0$, on the other hand.

First, we prove Estimate (20). Let $b_\pm \in S^0_{\pm,1}(\epsilon_0, d_0, R_1; I\!R)$. To this end, choose $\epsilon, d > 0$ small enough such that $3\epsilon < \epsilon_0'$ and $2d < d_0$. Let

$$\epsilon_0' \in]3\epsilon; \epsilon_0'[,\;\; d_0' \in]2d; d_0[\text{ and } R_0 > R_0' > 0.$$

Pick R large enough so that the properties of Section 2 hold and that Proposition 3.4 applies. Let $R_1 > 2R$ and $R_1' \in]2R; R_1[$. Using the ellipticity of the principal symbol $\tilde{a}_{0,\pm}$ of $\tilde{a}_\pm(h)$, in the region $\Psi_\pm(2\epsilon, 2d, 2R)$ (cf. (26)), and the proof of Proposition 3.6, we can find bounded symbols

$$\tilde{b}_\pm(h) \sim \sum_j h^j \tilde{b}_{j,\pm}$$

in $S^0_{\pm,1}(\epsilon_0', d_0', R_1'; \mathcal{H})$ such that, for all N, the "factorisation" (8) holds and where the operators $R_{N,\pm}(h)$ verify :

$$\|\langle x\rangle^N R_{N,\pm}(h)\| \;=\; O(1). \tag{24}$$

Due to the definition of symbols $\tilde{r}_\pm(h)$ (cf. (28)), we may write (9). Using the functional calculus of Helffer and Robert (cf. [HR]), the operator $\chi(P^{AD}(h))$ is seen to be an h-pseudoodifferential operator whose symbol belongs to $S^0_1(\mathcal{H})$ (cf. [W1]). According to Proposition 3.4, we then have :

$$\psi(x,hD)\chi\Big(P^{AD}(h)\Big)J_\pm\Big(\tilde{a}_\pm(N;h)\Big) \;=\; J_\pm\Big(\tilde{a}'_{N,\pm}(h)\Big) + h^{N+1}A_{N,\pm}(h)$$

where the symbols $\tilde{a}'_{N,\pm}(h)$ are supported in the compact set $\kappa^{-1}_{1,\pm}(\text{supp}\chi)$ and where the operator $A_{N,\pm}(h)$ satisfy (24). Taking R_1' (thus also R_1) large enough, this yields, thanks to (22),

$$\left\| J_\pm\Big(\tilde{a}'_{N,\pm}(h)\Big) e^{-ih^{-1}tP_a(h)}\Pi_0(h)J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^*\right\| \;=\; O(h^N\langle t\rangle^{-N}).$$

Now we consider (10) again. Recall that the operator

$$h^{-1}\langle x\rangle^N J_\pm\Big(\tilde{r}_{\pm,1}(N;h)\Big)\langle x\rangle$$

is $O(h^N)$, that the symbols $h^{-1}\langle x\rangle\tilde{r}_{\pm,3}(N;h)$ are uniformly bounded in $S^0_{\mp,1}(2-3\epsilon,2d,2R)$, with $2-3\epsilon+\epsilon_0'>2$, and that the compactly supported symbols $h^{-1}\langle x\rangle\tilde{r}_{\pm,2}(N;h)$ are uniformly bounded (cf. proof of Proposition 3.6).

Making use of Remark 3.7 and Property (21), we obtain the following estimate :

$$\left\|h^{-1}\langle x\rangle J_\pm\Big(\tilde{r}_{\pm,1}(N;h)\Big)e^{-ih^{-1}tP_a(h)}\Pi_0(h)J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^*\right\| \;=\; O(h^N\langle t\rangle^{-N}).$$

Due to (22), for R_1' large enough, it follows that

$$\left\|h^{-1}\langle x\rangle J_\pm\Big(\tilde{r}_{\pm,2}(N;h)\Big)e^{-ih^{-1}tP_a(h)}\Pi_0(h)J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^*\right\| \;=\; O(h^N\langle t\rangle^{-N}).$$

Using (23) for R_1' large enough, we obtain the estimate

$$\left\|h^{-1}\langle x\rangle J_\pm\Big(\tilde{r}_{\pm,3}(N;h)\Big)e^{-ih^{-1}tP_a(h)}\Pi_0(h)J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^*\right\| \;=\; O(h^N\langle t\rangle^{-N}).$$

Since ψ is compactly supported, we deduce from the first property (14) in Corollary 3.8, with $k=0$, the following estimate :

$$\begin{aligned}\Big\|\psi(x,hD)\chi\Big(P^{AD}(h)\Big)h^{-1}\int_0^t\Pi(h)e^{-ih^{-1}sP^{AD}(h)}\\ J_\pm\Big(\tilde{r}_\pm(N;h)\Big)e^{-ih^{-1}(t-s)P_a(h)}\Pi_0(h)J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^*ds\Big\|\\ \leq Ch^N\int_0^t\langle s\rangle^{-N}\langle t-s\rangle^{-N}ds\leq C'h^N\langle t\rangle^{-N+1}\end{aligned}\tag{25}$$

where the constant C neither depends on h nor on t (we have used $\langle s\rangle^{-2}\langle t-s\rangle^{-2}\leq\langle t\rangle^{-2}$). Thanks to (21) and to (24) for $A_{N,\pm}(h)$ on one hand, and thanks to the first estimate (14) of Corollary 3.8, for $k=0$, and to (24) on the other hand, we can write, for $N\geq 3$,

$$\left\|A_{N,\pm}(h)e^{-ih^{-1}tP_a(h)}\Pi_0(h)J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^*\right\| \;=\; O(\langle t\rangle^{-N})\tag{26}$$

and

$$\left\|\psi(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}R_{N,\pm}(h)\right\| \;=\; O(\langle t\rangle^{-N}),$$

uniformly w.r.t. h (we have used again Remark 3.7). Due to (8) and (9), these estimates imply Estimate (20) in Proposition 3.9.

Next, we prove Estimate (19). Assume that it holds if R_+ and R_- are large enough. Then we fix $R_\mp$ and choose $\tilde{R}_\mp$ and $R_\pm$ large enough such that Estimate (19) is valid (we treat the cases of upper and lower indices simultanously). For $b_{1,\mp}\in S^0_{\mp,1}(\epsilon_1,d_0,R_\mp;I\!R)$, we write $b_{1,\mp}=\tilde{b}_{1,\mp}+\psi$ with $\tilde{b}_{1,\mp}\in S^0_{\mp,1}(\epsilon_1,d_0,\tilde{R}_\mp;I\!R)$ and

$$\operatorname{supp}\psi\subset\Big\{(x,\xi)\in I\!R^{2n};\ |x|\leq\tilde{R}_\mp+1\Big\}.$$

Thus Estimate (19) holds for $\tilde{b}_{1,\mp}$ et $b_{2,\pm}$. Choosing $R_\pm$ large enough, we obtain the second estimate (20) in Proposition 3.9 for ψ and $b_{2,\pm}$. This yields the first estimate (19) for fixed $R_\mp$. So we just have to prove it for R_+ and R_- large enough.

We use the "factorisation" (8) for $b_{2,\pm}$ again. For

$$0<\epsilon_2'<\epsilon_2 \text{ with } \epsilon_2'+\epsilon_1>2,\ 0<d_0'<d_0,\ \text{and } R<R_\pm'<R_\pm,$$

we consider symbols $\tilde{b}_\pm(h)\in S^0_{\pm,1}(\epsilon_2',d_0',R_\pm';\mathcal{H})$ such that the decomposition (8) holds for $b_{2,\pm}$ and we choose ϵ,d,R as before. We shall show that

$$\left\|b_{1,\mp}(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}J_\pm\Big(\tilde{a}_\pm(N;h)\Big)J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^*\right\| \;=\; O(h^N\langle t\rangle^{-N+1}). \tag{27}$$

We write (9). First, we evaluate

$$\left\|b_{1,\mp}(x,hD)\chi\Big(P^{AD}(h)\Big)J_\pm\Big(\tilde{a}_\pm(N;h)\Big)e^{-ih^{-1}tP_a(h)}\Pi_0(h)J_\pm\Big(\tilde{b}_\pm(N;h)\Big)^*\right\|.$$

To this end, we remark that, for $0<\epsilon_1'<\epsilon_1$, the operators

$$b_{1,\mp}(x,hD)\chi\Big(P^{AD}(h)\Big)J_\pm\Big(\tilde{a}_\pm(N;h)\Big)$$

have the following form :

$$J_\pm\Big(\tilde{a}_\pm'(N;h)\Big)+h^{N+1}A_{N,\pm}'(h),$$

where $A_{N,\pm}'(h)$ satisfy (24) and where the symbols $\tilde{a}_\pm'(N;h))$ are supported in some region $\Psi_\mp(\epsilon_1',d_0',R_\mp')$, with

$$\epsilon_1'+\epsilon_2'>2,\ 0<d_0'<d_0,\quad \text{and}\quad 0<R_\mp'<R_\mp.$$

As before, the operators $A_{N,\pm}'(h)$ verify (26). Since $\epsilon_1'+\epsilon_2'>2$, (23) applies if $R_\mp'$ is chosen large enough. The contribution of these two terms is then seen to be $O(h^N\langle t\rangle^{-N})$.

To control the other term in (9), we use the decomposition (10). Again for $R_\pm'$ large enough, but now using (15) in Corollary 3.8 with $k=0$, we obtain as before Estimate (25), where ψ has been replaced by $b_{1,\pm}$. This yields Estimate (27).

Writing the second estimate (15) of Corollary 3.8, with $k=0$, and using it for the adjoint operator, we obtain :

$$\left\|b_{1,\mp}(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}\langle x\rangle^{-N}\right\| \;=\; O(\langle t\rangle^{-N})$$

for $\pm t>0$. Using (24), this leads to

$$\left\|b_{1,\mp}(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}R_{N,\pm}(h)\right\| \;=\; O(\langle t\rangle^{-N}).$$

We deduce from (8) again and (9) the first estimate (19) in Proposition 3.9 for $N-1$. □

In Proposition 3.9, the symbols $b_{1,\pm}$, $b_{2,\pm}$ and $b_\pm$ must be supported in a region where $|x|$ is large. Such a condition is not appropriate for the situation we consider in Section 4. However, we can get rid of this condition by trading it for $|t|$ large. This is precisely the purpose of the following proposition :

Proposition 3.10 *Let $\chi \in C_0^\infty(]E_0;+\infty[;I\!R)$ be non-trapping for the Hamilton function $|\xi|^2+\lambda(x;0)$ (cf. Definition 2.2).*

1. *For all functions $\psi_1,\psi_2 \in C_0^\infty(I\!R^{2n};I\!R)$, there exists $T>0$ such that, for all $|t|>T$ and for all $N \in I\!N$, we have :*
$$\left\|\psi_1(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}\psi_2(x,hD)\right\| \;=\; O(h^N\langle t\rangle^{-N}). \tag{28}$$

2. *For all functions $\psi \in C_0^\infty(I\!R^{2n};I\!R)$ and all symbols $b_\pm \in S^0_{\pm,1}(I\!R)$, there exists $T>0$ such that, for all $\pm t>T$ and all $N\in I\!N$, we have :*
$$\left\|\psi(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}b_\pm(x,hD)\right\| \;=\; O(h^N\langle t\rangle^{-N}). \tag{29}$$

3. *Let $d_0, R_\pm>0$ and $\epsilon_1,\epsilon_2>0$ such that $\epsilon_1+\epsilon_2>2$. Let $b_{j,\pm}\in S^0_{\pm,1}(\epsilon_j,d_0,R_\pm;I\!R)$, $1\le j\le 2$. There exists $T>0$ such that, for all $\pm t\ge T$ and all $N\in I\!N$, we have :*
$$\left\|b_{1,\mp}(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}tP^{AD}(h)}b_{2,\pm}(x,hD)\right\| \;=\; O(h^N\langle t\rangle^{-N}). \tag{30}$$

We point out that Remark 3.7 is valid for the previous estimates.

Proof : First we take a non-trapping function $\theta \in C_0^\infty(]E_0;+\infty[;I\!R)$ such that $\chi=\chi\theta$. Using the functional calculus of Helffer and Robert (cf. [HR]), one can show that the operator $\theta(P^{AD}(h))$ is an h-pseudoodifferential operator whose symbol is supported in the support of $\theta\circ p$, where $p(x,\xi)=|\xi|^2+\lambda(x;0)$. Then we can write :
$$\theta\Big(P^{AD}(h)\Big)\psi_2(x,hD) \;=\; b(x,hD)+V_N$$
where $b\in S_1^0(\mathcal{H})$ and where V_N satisfies :
$$\|\langle x\rangle^N V_N\| \;=\; O(h^N). \tag{31}$$
Because of Egorov's theorem (Theorem 3.2), we obtain :
$$e^{-ih^{-1}TP^{AD}(h)}\theta\Big(P^{AD}(h)\Big)\psi_2(x,hD) \;=\; b_T(x,hD)e^{-ih^{-1}TP^{AD}(h)}+e^{-ih^{-1}TP^{AD}(h)}V_N+V_{N,T}$$
where $V_{N,T}$ verifies the property (31), uniformly w.r.t. T, and where the support of the symbol b_T is contained in the support of $b\circ\Phi^{-T}$. For some $R_0>0$, the symbol b is supported in
$$\Big\{(x,\xi)\in I\!R^{2n};\;|x|\le R_0\Big\}.$$
For all $R_1>0$, there exists, thanks to (17), some $T_1>0$ such that, for all $T\ge T_1$, we have :
$$\Phi^T(\operatorname{supp} b)\subset \Psi_+(1,d_0,R_1)$$
for some $d_0>0$. This yields :
$$\operatorname{supp} b_T\subset\Psi_+(1,d_0,R_1).$$

Choosing R_1 large enough, we deduce, from (20) in Proposition 3.9, the following estimate :

$$\left\|\psi_1(x,hD)\chi\Big(P^{AD}(h)\Big)e^{-ih^{-1}(t-T_1)P^{AD}(h)}b_{T_1}(x,hD)\right\| \;=\; O(h^N\langle t\rangle^{-N}),$$

for all $t > T_1$. Since $V_{N,T}$ and V_N verify (31), their contribution is also $O(h^N\langle t\rangle^{-N})$, according to (14) in Corollary 3.8. This yields Estimate (28) for positive t. For negative t, it suffices to consider the adjoint operator.

We come now to the second estimate (29). Let $b_\pm \in S^0_{\pm,1}(\epsilon_0, d_0, R_0)$ for $\epsilon_0, d_0, R_0 > 0$. We proceed as before. We have :

$$e^{-ih^{-1}TP^{AD}(h)}\theta\Big(P^{AD}(h)\Big)b_\pm(x,hD) \;=\; b_{T,\pm}(x,hD)e^{-ih^{-1}TP^{AD}(h)}+e^{-ih^{-1}TP^{AD}(h)}V_{N,\pm}+V_{N,T,\pm}$$

where $b_{T,\pm}$ is supported in the support of $b_\pm\circ\Phi^{-T}$. For all $R_1 > 0$, we deduce from (16) that, for some $d > 0$, $b_{T,\pm} \in S^0_{\pm,1}(\epsilon_0/2, d, R_1)$, for all $\pm t > T$, provided T is large enough. Choosing R_1 large enough and using (20) in Proposition 3.9, we obtain (29).

To prove (30), we follow the same lines. We still have :

$$e^{-ih^{-1}TP^{AD}(h)}\theta\Big(P^{AD}(h)\Big)b_{2,\pm}(x,hD) \;=\; b_{T,2,\pm}(x,hD)e^{-ih^{-1}TP^{AD}(h)}+e^{-ih^{-1}TP^{AD}(h)}V_{N,\pm}+V_{N,T,\pm}$$

with the same properties as before. For all $R_1 > 0$ and $0 < \epsilon_1' < \epsilon_1$, we have, thanks to (16), $b_{T,2,\pm} \in S^0_{\pm,1}(\epsilon_1', d, R_1)$ for $\pm t > T$ and for T large enough, for some $d > 0$. Choosing ϵ in order to have $\epsilon_0 > \epsilon$ and taking R_1 large enough, we obtain, from the first estimate (19) in Proposition 3.9, the third and last estimate (30). □

4 Classical limit for the operator S^{AD}.

The goal of this section is to obtain Theorems 4.2 and 4.3 dealing with S^{AD}, corresponding to Theorems 5.3 and 5.4 in [KMW1] for cluster wave operators. Then we outline how Theorem 1.2 derives from Theorem 4.2. To this end, recall that the potentials satisfy the condition (D_ρ) for some $\rho > 1$. Using the results of Section 3, we can describe the action of S^{AD} on quantum observables and coherent states. The result is expressed in terms of the classical scattering operator S^{cl}_a which we define below.

As in Section 2, the Hamiltonian flow associated to the Hamilton function $|\xi|^2 + \lambda(x;0)$ is denoted by Φ^t and we set :

$$\forall (x,\xi) \in I\!R^n_x \times I\!R^n_\xi \setminus \{0\}, \quad \Phi^t(x,\xi) \;=\; \Big(q(t;x,\xi), p(t;x,\xi)\Big).$$

We consider now the following subset of the phase space :

$$\Psi_{nc} \equiv \Big\{(x,\xi) \in I\!R^{2n};\quad \lim_{t\to+\infty}\|\Phi^t(x,\xi)\| = \infty \quad\text{and}\quad \lim_{t\to-\infty}\|\Phi^t(x,\xi)\| = \infty\Big\}.$$

In fact, Ψ_{nc} is the set of phase space points which are non-trapping for the Hamilton function $|\xi|^2+\lambda(x;0)$, according to Definition 2.2. Since the eigenvalues $\lambda(x;0)$ are simple for all x, the function $I\!R^n \ni x \mapsto \lambda(x;0)$ have the properties of the function $I\!R^n \ni x \mapsto \Pi(x;0)$ (cf. Proposition 2.1). Thus, the classical wave operators (18) exist and are complete (cf. [RS3]). In particular, we have the following two inclusions :

$$\Psi_{nc} \ \subset \ \mathrm{Ran}\ \Omega^{cl}_{\pm}$$

so that we can define the scattering operator

$$S^{cl}_a : (\Omega^{cl}_{a,-})^{-1}(\Psi_{nc}) \longrightarrow (\Omega^{cl}_{a,+})^{-1}(\Psi_{nc}) \tag{1}$$

by

$$S^{cl}_a \ = \ (\Omega^{cl}_{a,+})^{-1}\Omega^{cl}_{a,-}.$$

As mentioned in the introduction, we have the following approximation :

Theorem 4.1 *([KMW1]) Under the assumption (D_ρ), $\rho > 1$, for the potentials and the assumption $(HS(h))$ for the simple eigenvalue E_0 (cf. Definition 1.1), let $\chi \in C_0^\infty(]E_0;+\infty[;I\!R)$ be non-trapping for the Hamilton function $|\xi|^2 + \lambda(x;0)$ (cf. Definition 2.2) and such that its support verifies :*

$$\sup(\mathrm{supp}\,\chi) < \inf_{x\in I\!R^n} \inf\Big\{\sigma(P_e(x;0)) \setminus \{\lambda(x;0)\}\Big\}$$

(these are the conditions of Theorem 1.2). Then we have :

$$\Big\|\Big(\Omega^{\alpha}_{\pm}(h) - \Omega^{AD}_{\pm}(h)\Big)\chi(P_a(h))\Big\| \ = \ O(h).$$

Theorem 1.2 then follows directly from the following main result of Section 4 :

Theorem 4.2 *Assume the assumption (D_ρ) with $\rho > 1$ for the potentials and the assumption $(HS(h))$ for the simple eigenvalue E_0 (cf. Definition 1.1). Let $\chi \in C_0^\infty(]E_0;+\infty[;I\!R)$ be non-trapping for the Hamilton function $|\xi|^2 + \lambda(x;0)$ (cf. Definition 2.2). Let $(x_0,\xi_0) \in I\!R^{2n}$ such that $\chi(|\xi_0|^2 + E_0) = 1$. For all bounded symbols $c \in S(\mathcal{H})$, we set :*

$$\mathcal{S}^{AD}_c(h) \ = \ U_h(x_0,\xi_0)^*(S^{AD}(h))^*\chi\Big(P_a(h)\Big)\ c(x,hD)\ \chi\Big(P_a(h)\Big)S^{AD}(h)U_h(x_0,\xi_0).$$

The operators $U_h(x_0,\xi_0)$ are given by (13) and the h-pseudodifferential operator $c(x,hD)$ is defined by (12).

In $L^2(I\!R^n_x;L^2(I\!R^{nN_0}_y))$, the following strong limit exists and is given by

$$s - \lim_{h\to 0} \mathcal{S}^{AD}_c(h) \ = \ \Pi_0(0)\ (c\circ S^{cl}_a)(x_0,\xi_0)\ \Pi_0(0).$$

To obtain Theorem 1.2, we just have to pick a function $\tilde\chi \in C_0^\infty(]E_0;+\infty[;I\!R)$, satisfying $\chi = \chi\tilde\chi$ and non-trapping for $|\xi|^2 + \lambda(x;0)$, to use the interwining property of the wave operators $\Omega^{\alpha}_{\pm}(h)$ and $\Omega^{AD}_{\pm}(h)$, and to apply Theorem 4.1 and Theorem 4.2.

We shall derive Theorem 4.2 from the following Theorem :

Theorem 4.3 *Under the assumptions of Theorem 4.2, for all symbols*

$$b_1, b_2 \in \Big(S^0_{+,1}(I\!\!R) \cap S^0_{-,1}(I\!\!R) \Big) \cup C_0^\infty(I\!\!R^{2n}; I\!\!R)$$

and for all bounded symbols $c \in S(\mathcal{H})$, we set :

$$C^{AD}(h) \;=\; b_1(x,hD)(S^{AD}(h))^* \chi\Big(P_a(h)\Big)\; c(x,hD)\; \chi\Big(P_a(h)\Big) S^{AD}(h) b_2(x,hD).$$

For T large enough and for all $t > T$, the operator $C^{AD}(h)$ is an admissible h-pseudodifferential operator with principal symbol given by

$$C_0^{AD}(x,\xi) \;=\; \chi^2(|\xi|^2 + E_0)\; b_1(x,\xi) b_2(x,\xi) G_t(x,\xi)\; c\Big(S_a^{cl}(x,\xi)\Big)\; G_t(x,\xi)^*,$$

where $S_a^{cl}(x,\xi) = (\Omega^{cl}_{a,+})^{-1} \circ \Omega^{cl}_{a,-}(x,\xi)$ is the classical scattering operator. Setting $(q_-, p_-) = \Omega^{cl}_{a,-}(x,\xi)$ and $(y,\eta) = S_a^{cl}(x,\xi)$, the symbols $G_t \in S^0_1(\mathcal{H})$, valued in $\mathcal{H} = \mathcal{L}(L^2(I\!\!R_y^{nN_0}))$, are given by

$$G_t(x,\xi) \;=\; \Pi_0(0)\Big(G_- \circ \kappa_{2,-}^{-1} \circ \Phi^{-t}(q_-,p_-)\Big)^*\; \Pi\Big(x_-(x - 2t\xi, \xi); 0\Big)\; \Pi\Big(q(-t; q_-, p_-); 0\Big)$$

$$\Pi\Big(q(t; q_-, p_-); 0\Big)\; G_+ \circ \kappa_{1,+}^{-1} \circ \Phi_0^t(y,\eta)\; \Pi_0(0).$$

See Section 2 for the definition of the operators $G_\pm$, $\kappa_{1,\pm}$, et $\kappa_{2,\pm}$.

Remark 4.4 *In contrast to Proposition 2.4 in [KMW1], we need here a non-trapping condition. This is not a surprise according to the definition of the classical scattering operator S_a^{cl}.*

Notice that the proof of Theorem 4.3 would be easier if we require that the observable c belongs to $S^0_{+,1}(\mathcal{H}) \cup C_0^\infty(I\!\!R^{2n}; \mathcal{H})$. Indeed, using Proposition 2.4, we may directly replace, in this case, each operator $\Omega_+^{AD}(h)$ by $W_+(t;h)$ in $C^{AD}(h)$, up to an error of order $O(h^\infty)$. In the general case, the same replacement is allowed by the propagation estimates established in Section 3.

Proof (of Theorem 4.2 admitting Theorem 4.3) : We follow the arguments in [KMW1]. Let $\tilde\chi \in C_0^\infty(]E_0; +\infty[; I\!\!R)$ satisfying $\chi = \chi\tilde\chi$. By the interwining property of the wave operators $\Omega_\pm^{AD}(h)$, we may write

$$\mathcal{S}_c^{AD}(h) \;=\; U_h(x_0,\xi_0)^* \tilde\chi\Big(P_a(h)\Big)(S^{AD}(h))^* \chi\Big(P_a(h)\Big)\; c(x,hD)\; \chi\Big(P_a(h)\Big) S^{AD}(h) \tilde\chi\Big(P_a(h)\Big) U_h(x_0,\xi_0).$$

It suffices to study the limit on the dense subset $C_0^\infty(I\!\!R_x^n; L^2(I\!\!R_y^{nN_0}))$. Let $\chi_1 \in C_0^\infty(I\!\!R^n; I\!\!R)$ be such that $\chi_1 = 1$ on the unit ball. We define $\chi_h(x) = \chi_1(h^{1/2}x)$. For $f \in C_0^\infty(I\!\!R_x^n; L^2(I\!\!R_y^{nN_0}))$, we have $(1-\chi_h)f = 0$, for h small enough. Since the functions $\mathcal{S}_c^{AD}(h)f$ are uniformly bounded w.r.t. h and since, for $g \in L^2(I\!\!R_x^n; L^2(I\!\!R_y^{nN_0}))$,

$$\lim_{h\to 0}(1-\chi_h)g \;=\; 0,$$

it follows that

$$\lim_{h\to 0}\Big(\chi_h \mathcal{S}_c^{AD}(h)\chi_h f - \mathcal{S}_c^{AD}(h)f\Big) \;=\; 0.$$

As already remarked in (14), we have :

$$U_h(x_0,\xi_0)\chi_h U_h(x_0,\xi_0)^* \;=\; \chi_1(\cdot - x_0).$$

Since the symbol $(x,\xi)\mapsto \chi_1(x-x_0)\tilde\chi(|\xi|^2+E_0(h))$ belongs to $C_0^\infty(I\!R^{2n};I\!R)$, we may apply Theorem 4.3 to the following operator :

$$\chi_1(\cdot - x_0)\tilde\chi\Big(P_a(h)\Big)(S^{AD}(h))^*\chi\Big(P_a(h)\Big)\; c(x,hD)\; \chi\Big(P_a(h)\Big)S^{AD}(h)\tilde\chi\Big(P_a(h)\Big)\chi_1(\cdot - x_0).$$

Then it is an admissible h-pseudodifferential operator with principal symbol given by

$$s_c(x,\xi) \;=\; \chi^2(|\xi|^2+E_0)\;\chi_1^2(x-x_0)\; G_t(x,\xi)^*\; c(S_a^{cl}(x,\xi))\; G_t(x,\xi),$$

for $t\geq T$ and for T large enough, since $\chi=\chi\tilde\chi$. Furthermore, we have :

$$\lim_{h\to 0}\Big(\chi_h\mathcal{S}_c^{AD}(h)\chi_h f - U_h(x_0,\xi_0)^* s_c(x,hD)U_h(x_0,\xi_0)f\Big) \;=\; 0.$$

But we also have :

$$U_h(x_0,\xi_0)^*s_c(x,hD)U_h(x_0,\xi_0) \;=\; s_c(x_0+h^{1/2}x,\xi_0+h^{1/2}D).$$

This leads then to :

$$\lim_{h\to 0}\mathcal{S}_c^{AD}(h)f \;=\; \chi^2(|\xi_0|^2+E_0)\; G_t(x_0,\xi_0)^*\; c(S_a^{cl}(x_0,\xi_0))\; G_t(x_0,\xi_0)f.$$

Since $\mathcal{S}_c^{AD}(h)f$ is t-independent, we can take the limit as $t\to+\infty$. Recall that $\chi(|\xi_0|^2+E_0)=1$. Because of the non-trapping condition and the behaviour of $x_-(x,\xi)$ when $|x|$ is getting large (see (20)), one can see that the phase space points $q(\pm t;q_-,p_-)$, $x_-(x-2t\xi,\xi)$ and $q(t;y,\eta)$ all go to infinity. The behaviour of the function $x\mapsto \Pi(x;0)$ at infinity (cf. Proposition 2.1) and those of $G_\pm(x,\xi)$ for large $|x|$ (cf. (27)) yield the claim. □

Proof (Theorem 4.3) : We consider a function $\tilde\chi\in C_0^\infty(]E_0;+\infty[;I\!R)$ such that $\chi=\chi\tilde\chi$. Due to the interwining property of wave operators, we can write :

$$\begin{aligned} C^{AD}(h) \;=\;& b_1(x,hD)\tilde\chi\Big(P_a(h)\Big)(\Omega_-^{AD}(h))^*\chi\Big(P^{AD}(h)\Big)\Omega_+^{AD}(h)\tilde\chi\Big(P_a(h)\Big)\; c(x,hD) \\ & \tilde\chi\Big(P_a(h)\Big)(\Omega_+^{AD}(h))^*\chi\Big(P^{AD}(h)\Big)\Omega_-^{AD}(h)\tilde\chi\Big(P_a(h)\Big)b_2(x,hD). \end{aligned}$$

Let $\epsilon,d,R>0$. We shall choose them precisely later. We first impose to R to be large enough such that the operators $\kappa_{1,\pm}$ and $\kappa_{2,\pm}$ are global diffeomorphisms (cf. Section 2). Since we have $b_1\in S^0_{-,1}(I\!R)$, we can find some $\epsilon>0$ small enough such that we have the decomposition $b_1=\tilde b_1+\psi$ with $\tilde b_1\in S^0_{-,1}(4\epsilon,4d,4R;I\!R)$ and such that ψ is supported in

$$\Big\{(x,\xi)\in I\!R^{2n};\ |x|\leq 4R+1,\ |\xi|\leq 4d+1\Big\}.$$

Applying successively Proposition 2.4 to $\tilde{b}_1$ and to ψ, we can find some $T>0$ large enough such that, for all $t\geq T$,

$$C^{AD}(h) \;=\; b_1(x,hD)\tilde{\chi}\big(P_a(h)\big)(W_-(-t;h))^*\chi\big(P^{AD}(h)\big)\Omega_+^{AD}(h)\tilde{\chi}\big(P_a(h)\big)c(x,hD)$$

$$\tilde{\chi}\big(P_a(h)\big)(\Omega_+^{AD}(h))^*\chi\big(P^{AD}(h)\big)W_-(-t;h)\tilde{\chi}\big(P_a(h)\big)b_2(x,hD) \;+\; O(h^\infty)$$

where the operators $W_\pm(t;h)$ are defined in Proposition 2.4. Thanks to the assumption on the symbols b_1 and b_2, we shall show that we may replace each Ω_+^{AD} by $W_+(t;h)$ in the previous expression.

We choose d small enough in order to have

$$E_0+2d<\inf \mathrm{supp}\tilde{\chi}.$$

Due to Proposition 2.4, we can write, for all functions $f\in L^2(I\!R^{n(N+1)}_{x,y})$,

$$\chi\big(P^{AD}(h)\big)\big(\Omega_+^{AD}(h)-W_+(t;h)\big)\tilde{\chi}\big(P_a(h)\big)f \tag{2}$$

$$=\; ih^{-1}\int_t^{+\infty} e^{ih^{-1}sP^{AD}(h)}\chi\big(P^{AD}(h)\big)J_+\big(r_+(h)\big)e^{-ih^{-1}sP_a(h)}\Pi_0(h)\tilde{\chi}\big(P_a(h)\big)f\,ds$$

and

$$\Big(W_-(-t;h)\Big)^* \;=\; J_-\Big(a_-(h)\Big)^*+ih^{-1}\int_0^t \Pi_0(h)e^{-ih^{-1}sP_a(h)}J_-\Big(r_-(h)\Big)^*e^{ih^{-1}sP^{AD}(h)}\,ds. \tag{3}$$

First, we prove that there exists $T>0$ such that, for all $m>0$ and for all $t+s>T$,

$$\Big\|J_+\Big(r_+(h)\Big)^*e^{ih^{-1}(t+s)P^{AD}(h)}\chi\Big(P^{AD}(h)\Big)J_-\Big(r_-(h)\Big)\langle x\rangle^m\Big\| \;=\; O(h^\infty\langle t+s\rangle^{-\infty}). \tag{4}$$

We split the symbols $r_+(h)$ and $r_-(h)$ according to (10). Thanks to (28) and Corollary 3.8, the contributions of $r_{+,1}(h)$ and $r_{-,1}(h)$ in (4) are $O(h^\infty\langle t+s\rangle^{-\infty})$. Because of (29), the contributions in (4) of $(r_{+,3}(h),r_{-,2}(h))$ and of $(r_{+,2}(h),r_{-,3}(h))$ are $O(h^\infty\langle t+s\rangle^{-\infty})$. To check those of $(r_{+,2}(h),r_{-,2}(h))$ and $(r_{+,3}(h),r_{-,3}(h))$, we use (28) and (30) respectively and we obtain the same estimate. We have proved (4).

Now, we use (6) for $k=0$ if $b_1\in S^0_{+,1}(I\!R)$ and the fact that (14) is also true for the free operator $P_a(h)\Pi_0(h)$ if $b_1\in C_0^\infty(I\!R^{2n};I\!R)$. Thanks to (4), this yields

$$\Big\|\int_0^t b_1(x,hD)\tilde{\chi}\Big(P_a(h)\Big)\Pi_0(h)e^{-ih^{-1}sP_a(h)}J_-\Big(r_-(h)\Big)^*e^{ih^{-1}(t+s)P^{AD}(h)}\chi\Big(P^{AD}(h)\Big)J_+\Big(r_+(h)\Big)\,ds\Big\|$$

$$=\; O(h^\infty\langle t\rangle^{-\infty}),$$

for $t>T$ (as in the proof of Proposition 3.6). Due to (2) and (3), this means that

$$b_1(x,hD)\tilde{\chi}\Big(P_a(h)\Big)\Big(W_-(-t;h)\Big)^*\chi\Big(P^{AD}(h)\Big)\Big(\Omega_+^{AD}(h)-W_+(t;h)\Big)\tilde{\chi}\Big(P_a(h)\Big) \tag{5}$$

$$=\; b_1(x,hD)\tilde{\chi}\Big(P_a(h)\Big)\Pi_0(h)J_-\Big(a_-(h)\Big)^*\chi\Big(P^{AD}(h)\Big)\Big(\Omega_+^{AD}(h)-W_+(t;h)\Big)\tilde{\chi}\Big(P_a(h)\Big)+O(h^\infty).$$

According to Proposition 3.4, one can write

$$b_1(x,hD)\tilde{\chi}\Big(P_a(h)\Big)\Pi_0(h)J_-\Big(a_-(h)\Big)^* \;=\; J_-\Big(\tilde{a}_-(h)\Big)^*\tilde{b}(x,hD) + J_-\Big(\tilde{r}_-(h)\Big)$$

where $\langle x\rangle^N J_\pm(\tilde{r}(N;h))$ is $O(h^N)$, for all N, the symbols $\tilde{a}_-(h)$ are uniformly bounded in $S^0(\mathcal{H})$, and :

$$\begin{array}{ll} \tilde{b}\in S^0_{+,1}(I\!R) & \text{if} \quad b_1\in S^0_{+,1}(I\!R), \\ \tilde{b}\in C_0^\infty(I\!R^{2n};I\!R) & \text{if} \quad b_1\in C_0^\infty(I\!R^{2n};I\!R). \end{array}$$

The contribution in (5) is seen to be $O(h^\infty)$. Next, we prove that, for $T>0$ large enough,

$$\left\|\tilde{b}(x,hD)e^{ih^{-1}tP^{AD}(h)}J_+\Big(r_+(h)\Big)\right\| \;=\; O(h^\infty\langle t\rangle^{-\infty}), \tag{6}$$

for $t>T$.

We split $r_+(h)$ again, according to (10). The contribution in (6) of $r_{+,1}(h)$ is $O(h^\infty\langle t\rangle^{-\infty})$ because of (28) and of (15) if $b_1\in S^0_{+,1}(I\!R)$, of (14) if $b_1\in C_0^\infty(I\!R^{2n};I\!R)$. To compute the contribution of $r_{+,2}(h)$, we use (29) if $b_1\in S^0_{+,1}(I\!R)$ and (28) if $b_1\in C_0^\infty(I\!R^{2n};I\!R)$. For $r_{+,3}(h)$, we choose ϵ small enough and use (30) if $b_1\in S^0_{+,1}(I\!R)$ and (29) if $b_1\in C_0^\infty(I\!R^{2n};I\!R)$. In each case, we obtain the same estimation for t large enough. This yields (6).

We obtain that the right side in (5) is in fact $O(h^\infty)$. Thus we can replace in C^{AD}, up to an error of $O(h^\infty)$, the first operator Ω_+^{AD} by $W_+(t;h)$, for $t>T$. The same arguments show that we can also the second operator Ω_+^{AD} by $W_+(t;h)$, for $t>T$. We then have, for $b_1,b_2\in[S^0_{+,1}(I\!R)\cap S^0_{-,1}(I\!R)]\cup C_0^\infty(I\!R^{2n};I\!R)$,

$$\begin{aligned} C^{AD}(h) \;=\; & b_1(x,hD)\tilde{\chi}\Big(P_a(h)\Big)W_-(-t;h)^*\chi\Big(P^{AD}(h)\Big)W_+(t;h)\tilde{\chi}\Big(P_a(h)\Big)\; c(x,hD) \\ & \tilde{\chi}\Big(P_a(h)\Big)W_+(t;h)^*\chi\Big(P^{AD}(h)\Big)W_-(-t;h)\tilde{\chi}\Big(P_a(h)\Big)b_2(x,hD) \;+\; O(h^\infty) \end{aligned}$$

and the first term may be written as follow :

$$\begin{gathered} b_1(x,hD)\tilde{\chi}\Big(P_a(h)\Big)\Pi_0(h)e^{-ih^{-1}tP_a(h)}J_-\Big(a_-(h)\Big)^*e^{2ih^{-1}tP^{AD}(h)}\chi\Big(P^{AD}(h)\Big)J_+\Big(a_+(h)\Big) \\ e^{-ih^{-1}tP_a(h)}\Pi_0(h)\tilde{\chi}\Big(P_a(h)\Big)\; c(x,hD)\; \tilde{\chi}\Big(P_a(h)\Big)\Pi_0(h)e^{ih^{-1}tP_a(h)} \\ J_+\Big(a_+(h)\Big)^*\chi\Big(P^{AD}(h)\Big)e^{-2ih^{-1}tP^{AD}(h)}J_-\Big(a_-(h)\Big)e^{ih^{-1}tP_a(h)}\Pi_0(h)\tilde{\chi}\Big(P_a(h)\Big)b_2(x,hD). \end{gathered}$$

Using now Theorem 3.2 and Proposition 3.4, we are sure that we are dealing with an admissible h-pseudodifferential operator. To finish the proof of Theorem 4.3, we just have to calculate its principal symbol.

First we remark that the operator

$$\Pi_0(h)\tilde{\chi}\Big(P_a(h)\Big)\; c(x,hD)\; \tilde{\chi}\Big(P_a(h)\Big)\Pi_0(h)$$

is an h-pseudodifferential operator with principal symbol $\Pi_0(0)c_{\chi,0}(x,\xi)\Pi_0(0)$ with $c_{\tilde{\chi},0}(x,\xi) = \tilde{\chi}^2(|\xi|^2 + E_0)c(x,\xi)$, due to the functional calculus of Helffer and Robert (cf. [HR]). According to Egorov's theorem (cf. Remark 3.3), the operator

$$\Pi_0(h)e^{-ih^{-1}tP_a(h)}\tilde{\chi}\Big(P_a(h)\Big)\ c(x,hD)\ \tilde{\chi}\Big(P_a(h)\Big)e^{ih^{-1}tP_a(h)}\Pi_0(h)$$

is an h-pseudodifferential operator $c_1(x,hD)$ with principal symbol $c_{1,0}(x,\xi) = \Pi_0(0)(c_{\tilde{\chi},0}\circ \Phi_0^{-t})(x,\xi)\Pi_0(0)$. Furthermore, Proposition 3.4 gives

$$J_+(a_+)c_1(x,hD) \ = \ J_+(c_2)$$

where the principal symbol of c_2 is given by

$$c_{2,0}(x,\xi) \ = \ a_{0,+}(x,\xi)c_{1,0}\Big(\nabla_\xi\phi_+(x,\xi),\xi\Big).$$

The operator $J_+(c_2)J_+(a_+)^*$ is an h-pseudodifferential operator $c_3(x,hD)$ with principal symbol

$$\begin{aligned}
c_{3,0}(x,\xi) \ &= \ c_{2,0}\Big(x,\xi_+(x,\xi)\Big)a_{0,+}\Big(x,\xi_+(x,\xi)\Big)^*\Big|\det\Big(\frac{\partial\xi_+}{\partial\xi}(x,\xi)\Big)\Big| \\
&= \ a_{0,+}\Big(x,\xi_+(x,\xi)\Big)\Pi_0(0)\ c_{\tilde{\chi},0}\circ\Phi_0^{-t}\bigg(\nabla_\xi\phi_+\Big(x,\xi_+(x,\xi)\Big),\xi_+(x,\xi)\bigg)\ \Pi_0(0) \\
&\quad \Big|\det\Big(\frac{\partial\xi_+}{\partial\xi}(x,\xi)\Big)\Big|a_{0,+}\Big(x,\xi_+(x,\xi)\Big)^*.
\end{aligned}$$

For $(x,\xi)\in\Psi_{nc}$ such that $(x,\xi_+(x,\xi))\in\Psi_+(2\epsilon,2d,2R)$, we have :

$$\begin{aligned}
c_{3,0}(x,\xi) \ &= \ \Pi(x;0)G_+\Big(x,\xi_+(x,\xi)\Big)\Pi_0(0)\ c_{\tilde{\chi},0}\circ\Phi_0^{-t}\circ(\Omega_{a,+}^{cl})^{-1}(x,\xi) \\
&\quad \Pi_0(0)G_+\Big(x,\xi_+(x,\xi)\Big)^*\Pi(x;0)
\end{aligned} \tag{7}$$

thanks to (25) and (26). Because of the properties of the phase ϕ_+ (cf. (22)), the previous relation (7) is, in fact, valid for $(x,\xi)\in\Psi_+(3\epsilon,3d,3R)\cap\Psi_{nc}$. For $j\in\{1,2\}$, we set :

$$G_{j,\pm}(x,\xi) \ = \ G_\pm\circ\kappa_{j,\pm}^{-1}(x,\xi). \tag{8}$$

Then we have, in $\Psi_+(3\epsilon,3d,3R)\cap\Psi_{nc}$,

$$\begin{aligned}
c_{3,0}(x,\xi) \ &= \ \Pi(x;0)\ G_{1,+}\circ(\Omega_{a,+}^{cl})^{-1}(x,\xi)\ \Pi_0(0)\ c_{\tilde{\chi},0}\circ\Phi_0^{-t}\circ(\Omega_{a,+}^{cl})^{-1}(x,\xi) \\
&\quad \Pi_0(0)\Big(G_{1,+}\circ(\Omega_{a,+}^{cl})^{-1}(x,\xi)\Big)^*\Pi(x;0)
\end{aligned}$$

due to (25). According to Theorem 3.2 and the functional calculus of Helffer and Robert (cf. [HR]), the operator

$$\chi\Big(P^{AD}(h)\Big)\Pi(h)e^{2ih^{-1}tP^{AD}(h)}\ c_3(x,hD)\ e^{-2ih^{-1}tP^{AD}(h)}\Pi(h)\chi\Big(P^{AD}(h)\Big)$$

is an h-pseudodifferential operator $c_4(x,hD)$ with principal symbol

$$\begin{aligned} c_{4,0}(x,\xi) &= \chi^2(|\xi|^2+\lambda(x;0))\ \Pi(x;0)\Pi\Big(q(2t;x,\xi);0\Big)\ G_{1,+}\circ(\Omega^{cl}_{a,+})^{-1}\circ\Phi^{2t}(x,\xi)\ \Pi_0(0) \\ & c_{\tilde\chi,0}\circ\Phi_0^{-t}\circ(\Omega^{cl}_{a,+})^{-1}\circ\Phi^{2t}(x,\xi) \\ & \Pi_0(0)\Big(G_{1,+}\circ(\Omega^{cl}_{a,+})^{-1}\circ\Phi^{2t}(x,\xi)\Big)^*\Pi\Big(q(2t;x,\xi);0\Big)\Pi(x;0), \end{aligned}$$

for $(x,\xi)\in\Psi_{nc}$ such that $\Phi^{2t}(x,\xi)\in\Psi_+(3\epsilon,3d,3R)$. We note that the interwining property of wave operators implies that

$$c_{\tilde\chi,0}\circ\Phi_0^{-t}\circ(\Omega^{cl}_{a,+})^{-1}\circ\Phi^{2t} \ = \ c_{\tilde\chi,0}\circ(\Omega^{cl}_{a,+})^{-1}\circ\Phi^{t}$$

and

$$G_{1,+}\circ(\Omega^{cl}_{a,+})^{-1}\circ\Phi^{2t}(x,\xi) \ = \ G_{1,+}\circ\Phi_0^{2t}\circ(\Omega^{cl}_{a,+})^{-1}(x,\xi).$$

The h-pseudodifferential operator

$$c_5(x,hD) \ = \ J_-(a_-)^*\ c_4(x,hD)\ J_-(a_-)$$

has, thanks to (24), the following principal symbol :

$$c_{5,0}(x,\xi) \ = \ a_{0,-}\Big(x_-(x,\xi),\xi\Big)^*\ c_{4,0}\circ\Omega^{cl}_{a,-}(x,\xi)\ a_{0,-}\Big(x_-(x,\xi),\xi\Big)\Big|\det\Big(\frac{\partial x_-}{\partial x}(x,\xi)\Big)\Big|$$

for $(x,\xi)\in\Psi_-(3\epsilon,3d,3R)$ and we have, according to (26),

$$c_{5,0}(x,\xi) \ = \ G_-\Big(x_-(x,\xi),\xi\Big)^*\Pi\Big(x_-(x,\xi);0\Big)\ c_{4,0}\circ\Omega^{cl}_{a,-}(x,\xi)\ \Pi\Big(x_-(x,\xi);0\Big)G_-\Big(x_-(x,\xi),\xi\Big).$$

If $(x,\xi)\in\Psi_-(4\epsilon,4d,4R)$ and $\Phi^{2t}\circ\Omega^{cl}_{a,-}(x,\xi)\in\Psi_+(3\epsilon,3d,3R)$,

$$c_{5,0}(x,\xi) \ = \ \chi^2\circ p\circ\Omega^{cl}_{a,-}(x,\xi)\ \tilde G(x,\xi)\ c_{\tilde\chi,0}\circ(\Omega^{cl}_{a,+})^{-1}\circ\Phi^t\circ\Omega^{cl}_{a,-}(x,\xi)\ \tilde G(x,\xi)^*$$

with $p(x,\xi)=|\xi|^2+\lambda(x;0)$ and

$$\tilde G(x,\xi) \ = \ \Big(G_{2,-}\circ\Omega^{cl}_{a,-}(x,\xi)\Big)^*\Pi\Big(x_-(x,\xi);0\Big)\Pi(q_-;0)\Pi\Big(q(2t;q_-,p_-);0\Big)\ G_{1,+}\circ\Phi_0^{2t}\circ S^{cl}_a(x,\xi)\ \Pi_0(0),$$

thanks to (8) and (24). But

$$c_{\tilde\chi,0}\circ(\Omega^{cl}_{a,+})^{-1}\circ\Phi^t\circ\Omega^{cl}_{a,-} = c_{\tilde\chi,0}\circ S^{cl}_a\circ\Phi_0^t,$$

due to the interwining property of the classical wave operators. Thanks to Egorov's theorem (cf. Remark 3.3) again, the operator

$$\Pi_0(h)e^{-ih^{-1}tP_a(h)}\ c_5(x,hD)\ e^{ih^{-1}tP_a(h)}\Pi_0(h)$$

is an h-pseudodifferential operator $c_6(x,hD)$ with principal symbol $c_{6,0}$. Choosing $\epsilon,d>0$ small enough, we can ensure that, for t large enough,

$$\Phi_0^{-t}\Big(\mathrm{supp}\, b_{1,\mp}\cap\mathrm{supp}\, b_{2,\pm}\Big) \ \subset \ \Psi_-(4\epsilon,4d,4R), \tag{9}$$

$$\Phi^{2t}\circ\Omega^{cl}_{a,-}(x,\xi)\circ\Phi_0^{-t}\Big(\mathrm{supp}\, b_{1,\mp}\cap\mathrm{supp}\, b_{2,\pm}\Big) \ \subset \ \Psi_+(3\epsilon,3d,3R). \tag{10}$$

Indeed, we deduce (9) from (16) and (17), since $b_1, b_2 \in S^0_{-,1}(I\!R) \cup C_0^\infty(I\!R^{2n}; I\!R)$. But we also have $b_1, b_2 \in S^0_{+,1}(I\!R) \cup C_0^\infty(I\!R^{2n}; I\!R)$. Using (21), (22), and (23), we obtain, for t large enough,

$$\Phi^t \circ \Omega^{cl}_{a,-}(x,\xi)\Big(\operatorname{supp} b_{1,\mp} \cap \operatorname{supp} b_{2,\pm}\Big) \;\subset\; \Psi_+(3\epsilon, 3d, 3R),$$

which yields (10).

Putting all together, we derive that, on the set $\operatorname{supp} b_{1,\mp} \cap \operatorname{supp} b_{2,\pm}$, the symbol $c_{6,0}$ is given by

$$\begin{aligned} c_{6,0}(x,\xi) \;&=\; \chi^2 \circ p \circ \Omega^{cl}_{a,-} \circ \Phi_0^{-t}(x,\xi)\; \Pi_0(0)\; \tilde{G} \circ \Phi_0^{-t}(x,\xi) c_{\tilde{\chi},0} \circ S^{cl}_a(x,\xi) \Big(\tilde{G} \circ \Phi_0^{-t}(x,\xi)\Big)^* \Pi_0(0) \\ &=\; G_t(x,\xi)\; c_{\tilde{\chi},0} \circ S^{cl}_a(x,\xi)\; G_t(x,\xi)^* \end{aligned}$$

with

$$\begin{aligned} G_t(x,\xi) \;=\; \Pi_0(0)\Big(G_{2,-} \circ \Phi^{-t} \circ \Omega^{cl}_{a,-}(x,\xi)\Big)^* \Pi\Big(x_-(x - 2t\xi, \xi); 0\Big) \Pi\Big(q(-t; q_-, p_-); 0\Big) \\ \Pi\Big(q(t; q_-, p_-); 0\Big)\; G_{1,+} \circ \Phi_0^t \circ S^{cl}_a(x,\xi)\; \Pi_0(0), \end{aligned}$$

because of the interwining property of the classical wave operators. To arrive at the claim, it suffices to note that $p \circ \Omega^{cl}_{a,-}(x,\xi) = |\xi|^2 + E_0$, that we can write :

$$c_{\tilde{\chi},0} \circ S^{cl}_a(x,\xi) \;=\; \tilde{\chi}^2(|\xi|^2 + E_0)\; c \circ S^{cl}_a(x,\xi),$$

due to conservation of energy, and that $\chi = \chi\tilde{\chi}$. □

Appendix

We have used some properties of the classical flow associated to a Hamilton function with short-range potential. We give here a proof of these properties.

Proof (of Proposition 2.3) : We only give the arguments for the indice $+$. One can recover the other case in a similar way. We denote the potential $\lambda(x; 0)$ simply by $V(x)$.

First, we show (15). We observe that, if we choose $C_0 > 1$ such that $2C_0^{-2} < \epsilon$, then we have, for all $t > 0$,

$$|x + 2t\xi| \;\geq\; C_0^{-1}\Big(|x| + 2t|\xi|\Big) \tag{1}$$

for all $(x,\xi) \in \Psi_+(\epsilon, d, R)$. Let $C = 4C_0$. Using the integral formula

$$q(t; x, \xi) \;=\; x + 2t\xi - 2\int_0^t \int_0^s \nabla V\Big(q(u; x, \xi)\Big)\, du ds, \tag{2}$$

we see that there exists some $t_0 > 0$, such that, for $t \in [0; t_0]$, we have :

$$\Big|q(t; x, \xi)\Big| \;\geq\; C^{-1}\Big(|x| + 2t|\xi|\Big) \tag{3}$$

for all $(x,\xi) \in \Psi_+(\epsilon, d, 1)$. Thanks to the short-range assumption (11) and to (2), we can choose some $R_0 > 0$ large enough such that

$$\Big|q(t_0;x,\xi)\Big| \;\geq\; \frac{1}{2}\Big(|x+2t_0\xi|\Big) \;\geq\; \frac{C_0^{-1}}{2}\Big(|x|+2t_0|\xi|\Big) \;\geq\; 2C^{-1}\Big(|x|+2t_0|\xi|\Big),$$

for all $(x,\xi) \in \Psi_+(\epsilon, d, R)$ and all $R > R_0$. Because of this improvement, we see that, in fact, (3) holds for all $t > 0$, for all $(x,\xi) \in \Psi_+(\epsilon, d, R)$, and all $R > R_0$. Furthermore, we clearly have, for $(x,\xi) \in \Psi_+(\epsilon, d, R)$ and $t > 0$,

$$\Big|q(t;x,\xi)\Big| \;\geq\; \frac{R}{C}\,.$$

Using now the integral formula

$$p(t;x,\xi) \;=\; \xi - \int_0^t \nabla V\Big(q(s;x,\xi)\Big)\,ds, \tag{4}$$

we can show that, for R_0 is large enough,

$$\Big|p(t;x,\xi)\Big|^2 \;\geq\; \frac{d}{2}\,,$$

for all $t > 0$, for all $(x,\xi) \in \Psi_+(\epsilon, d, R)$, and all $R > R_0$. Now, we note that the angle between $x + 2t\xi$ and ξ decrease i.e.

$$\frac{x+2t\xi}{|x+2t\xi|}\cdot\frac{\xi}{|\xi|} \;\geq\; \frac{x\cdot\xi}{|x|\,|\xi|}, \tag{5}$$

for $t > 0$ and $(x,\xi) \in \Big(I\!R^n \setminus \{0\}\Big)^2$. For R_0 large enough, we deduce from (2) (respectively (4)) that $q(t;x,\xi)$ (respectively $p(t;x,\xi)$) is approximated by $x + 2t\xi$ (respectively ξ), uniformly on $\Psi_+(\epsilon, d, R)$ and for $R > R_0$. Then (5) yields

$$q(t;x,\xi)\cdot p(t;x,\xi) \;\geq\; (-1+\epsilon/2)\,\Big|q(t;x,\xi)\Big|\,\Big|p(t;x,\xi)\Big|,$$

for all $t > 0$, for all $(x,\xi) \in \Psi_+(\epsilon, d, R)$, and all $R > R_0$. We have proved (15).

We come to prove (16). Since V is a bounded function, $|p(t;x,\xi)|$ must remain bounded, uniformly w.r.t $(x,\xi) \in p^{-1}(I)$ and t. Thus the non-trapping assumption implies that the position $q(t;x,\xi)$ must go to infinity. But we need some uniformity. Since the set

$$P(R_0) \;\equiv\; \Big\{(y,\eta) \in I\!R^{2n};\ |y| \leq R_0\Big\} \cap p^{-1}(I)$$

is compact, we have the following property : for all $R_0 > 0$, there exist $d, t_0 > 0$, such that, for all $t \geq t_0$,

$$\forall (x,\xi) \in P(R_0),\ \Big|q(t;x,\xi)\Big| \;\geq\; R_0 \;\text{ and }\; \Big|p(t;x,\xi)\Big|^2 \;\geq\; d. \tag{6}$$

Choosing R_0 large enough, (15) yields (16) on the set

$$\Big\{(y,\eta) \in I\!R^{2n};\ |y| \geq R_0\Big\} \cap \Psi_+(\epsilon, d, R).$$

Due to (6), we can find $C > 1$ and $t_0 > 0$, such that, for $t > t_0$, (3) holds on $P(R_0)$. Thus we can follow the proof of (15) to derive (16) on $P(R_0)$.

But the angle between $x + 2t\xi$ and ξ may be as small as one wants, uniformly on $P(R_0)$, as soon as t is large enough. This is precisely what (17) means. We prove it now.

Due to (6), we can find $d, R_0' > 0$ and $t_0 > 0$, such that

$$\Phi^{t_0}\Big(P(R_0)\Big) \;\subset\; P(R_0') \cap \Big\{(y,\eta) \in I\!\!R^{2n};\; |\eta|^2 \geq d\Big\} \;\equiv\; A.$$

Using (2) and (4) again, we can show that, for all $\epsilon' > 0$, there is $T > 0$ such that,

$$\hat{q}(t;x,\xi) \cdot \hat{p}(t;x,\xi) \;\geq\; \Big(\frac{x + 2t\xi}{|x + 2t\xi|} \cdot \hat{\xi}\Big)(1 - \epsilon')$$

(with $\hat{x} = x/|x|$) holds on A. But since x remain bounded in A, we have, for t large enough,

$$C^{-1} 2t|\xi| \;\leq\; |x + 2t\xi| \;\leq\; 2t|\xi|(1 - \epsilon').$$

Therefore,

$$\frac{(x + 2t\xi) \cdot \xi}{|x + 2t\xi|\,|\xi|} \;\geq\; C\,\frac{x \cdot \xi}{t|\xi|} + \frac{1}{1 - \epsilon'}$$

where the first term on the right hand side tend to 0, uniformly on A. For T large enough, we then obtain, for all $t > T$,

$$\hat{q}(t;x,\xi) \cdot \hat{p}(t;x,\xi) \;\geq\; 1 - \epsilon \;=\; -1 + 2 - \epsilon. \;\; \square$$

References

[A] S.Agmon : *Lectures on Exponential Decay of Solutions of Second-Order Elliptic Equations.* Princeton University Press, 1982.

[Ba] A.Balazard-Konlein : *Calcul fonctionnel pour des opérateurs h-admissibles à symbole opérateur et applications.* Thèse de troisième cycle, université de Nantes, 1985.

[BO] M.Born, R.Oppenheimer : *Zur Quantentheorie der Molekeln.* Annalen der Physik, 84, 457, 1927.

[HR] B.Helffer, D.Robert : *Calcul fonctionnel par la transformation de Melin et opérateurs admissibles.* J. Funct. Anal. 53 (1983), 246-268.

[HS] B.Helffer, J.Sjöstrand : *Opérateurs de Schrödinger avec champs magnétiques faibles et constants.* Exposé No. XII, Séminaire EDP, février 1989, Ecole Polytechnique.

[IK] H.Isozaki, H.Kitada : *Modified wave operators with time-dependent modifiers* J. Fac. Sci. Univ. Tokyo, 32, 77-104,1985.

[J] Th.Jecko : *Sections efficaces totales d'une molécule diatomique dans l'approximation de Born-Oppenheimer.* Thèse de doctorat, Université de Nantes, 1996.

[KMSW] M.Klein, A.Martinez, R.Seiler, X.P.Wang : *On the Born-Oppenheimer Expansion for Polyatomic Molecules.* Commun. Math. Phys. 143, 606-639, 1992.

[KMW1] M.Klein, A.Martinez, X.P.Wang : *On the Born-Oppenheimer Approximation of Wave Operators in Molecular Scattering Theory.* Commun. Math. Phys. 152, 73-95, 1993.

[KMW2] M.Klein, A.Martinez, X.P.Wang : *On the Born-Oppenheimer Aproximation of Wave Operators II : Singular Potentials.* preprint.

[RS3] M.Reed, B.Simon : *Methods of Modern Mathematical Physics, Tome III : Scattering Theory.* Academic Press 1979.

[RS4] M.Reed, B.Simon : *Methods of Modern Mathematical Physics, Tome IV : Analysis of Operators.* Academic Press.

[Ro] D.Robert : *Autour de l'approximation semi-classique.* Birkhäuser 1987.

[RT] D.Robert, H.Tamura : *Semiclassical estimates for resolvents and asymptotics for total cross-section.* Ann. IHP 46, 415-442, 1987.

[SS] I.M.Sigal, A.Soffer : *The N-particle scattering problem : asymptotic completeness for short range systems.* Ann. of Math. 126 (1987), 35-108.

[W1] X.P.Wang : *Time-Decay of Scattering Solutions and Resolvent Estimates for Semiclassical Schrödinger Operators.* J. Diff. Eq. 71, 348-396 (1988).

[W2] X.P.Wang : *Time-Decay of Scattering Solutions and Classical Trajectories.* Ann. IHP 47, 25-37,1987.

[W3] X.P.Wang : *Time-Delay Operators in the Semiclassical Limit II, Short Range Potentials.* Trans. AMS 322, 1990.

[W4] X.P.Wang : *Approximation semi-classique de l'équation d'Heisenberg.* Commun. in Math. Phys. 104, 77-86 (1986).

[Y] K.Yajima : *The quasi-classical limit of quantum scattering theory.* Comm. in Math. Phys., 69, 101-129,1979.