ANNALES SCIENTIFIQUES DE L'É.N.S.

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Annales scientifiques de l'É.N.S. 4e série, tome 29, nº 2 (1996), p. 149-183

<http://www.numdam.org/item?id=ASENS_1996_4_29_2_149_0>

Ann. scient. Éc. Norm. Sup.,
4e série, t. 29, 1996, p. 149 à 183.

A SEMI-CLASSICAL PICTURE OF QUANTUM SCATTERING

BY FRANCIS NIER

ABSTRACT. – This article is devoted to some singularly perturbed semi-classical asymptotics. It corresponds to a critical case where standard semi-classical techniques do not apply any more. We show how the limiting evolution keeps trace of quantum effects and provides a picture of quantum scattering very close to physical intuition.

1. Introduction

This paper is concerned with the asymptotics as $h \to 0$ for Schrödinger equations of the form

$$(1.1) \qquad ih\partial_t u^h = \left[-\frac{h^2}{2}\Delta + U\left(\frac{x}{h}\right) + V(x)\right]u^h,$$

in general dimension d. The case $U \equiv 0$ is nothing but the well-known semi-classical asymptotics. In a former article [26], we established the relationship between the case $V \equiv 0$ and quantum scattering. Indeed setting $t' = \frac{t}{h}$ and $x' = \frac{x}{h}$ makes the asymptotics $h \to 0$ equivalent to $t' \to \infty$ and $x' \to \infty$ with $|x'| \sim t'$, which is the standard situation of quantum scattering. The general case combines the semi-classical analysis for the hamiltonian $-\frac{h^2}{2}\Delta_x + V(x)$ and its geometrical background, with the spectral properties of $-\frac{1}{2}\Delta_{x'} + U(x')$. The matching between the two asymptotics $h \to 0$ for $-\frac{h^2}{2}\Delta_x + V(x)$, describing the evolution on a macroscopic scale, and $|x'| \to \infty$ for $-\frac{1}{2}\Delta_{x'} + U(x')$, associated with the quantum or microscopic scale, is performed after a second microlocalization around the origin $x = 0$. In the sequel we do not distinguish any more the two scales by notations and x denotes the generic position variable in both cases.

Indeed we consider a more general equation than (1.1) with a potential of the form

$$(1.2) \qquad \sum_{j\in\mathbb{N}} U_j\left(\frac{x - x_j}{h}\right) + V(x),$$

where $x_0 = 0$ and $x_j \neq 0$ for $j \neq 0$. Adding the potential $\sum_{j\neq 0} U_j(\frac{x-x_j}{h})$ makes no difficulty in the analysis and is motivated by applications. We assume that U_j, $j \in \mathbb{N}$, and V satisfy

HYPOTHESIS 1.1

a) The potentials $U_j(x)$ *are uniformly bounded in* $S(\langle x\rangle^{-\mu}, \frac{dx^2}{\langle x\rangle^2})$ with $\mu > 1$.

b) The points $x_j, j \in \mathbb{N}$*, are spread so that* $\sum_{j\in\mathbb{N}} \langle x_j\rangle^{-\mu} < \infty$.

c) The potential $V(x)$ *belongs to* $S(1, dx^2)$ *and (for convenience)* $V(0) = 0$.

We followed Hörmander's notations in [20]-Chap XVIII. Let us remark that these assumptions yield the boundedness of the total potential and the essential self adjointness of the total hamiltonian for a fixed $h > 0$. The first assumption is nothing but the short-range condition for the potentials $U_j(x)$. According to [10] [22], it ensures the existence of the wave-operators

$$W_{\pm,j} = \lim_{t\to\mp\infty} e^{it(-\frac{1}{2}\Delta+U_j(x))}e^{-it(-\frac{1}{2}\Delta)},$$

and the asymptotic completeness $\mathrm{Ran}\ W_{+,j} = \mathrm{Ran}\ W_{-,j}$. The wave operators $W_{\pm,j}$ are unitary from $L^2(\mathbb{R}^d)$ onto $\mathrm{Ran}\ W_{\pm,j}$ and the scattering matrix is defined by $S_j = W_{+,j}^* W_{-,j}$. By conjugating with the Fourier transform we also define $\hat{S}_j = FS_jF^{-1}$.

The crucial point in the study of the asymptotics of (1.1) or even with potential (1.2) is the understanding of what happens close to $x = 0$. The asymptotics around the points x_j, $j \neq 0$, actually follows from the case $j = 0$ by translational invariance and by possibly changing the energy origin. We often drop the index $_0$ and write simply U, W_+, W_-, S and $\hat{S}$ instead of U_0, $W_{+,0}$, $W_{-,0}$, S_0 and $\hat{S}_0$ while we set

$$\Sigma(x,h) = \sum_{j\neq 0} U_j\left(x - \frac{x_j}{h}\right).$$

The interesting initial data are the one which concentrate at $x = 0$ and for which the solution of (1.1) eventually leaves $x = 0$. Thus we consider the following initial value problem

$$\begin{cases} ih\partial_t u^h = \left[-\frac{h^2}{2}\Delta + U\left(\frac{x}{h}\right) + \Sigma\left(\frac{x}{h}, h\right) + V(x)\right]u^h, \\ u^h(t=0) = \frac{1}{h^{d/2}}u_0\left(\frac{x}{h}\right), \end{cases} \tag{1.3}$$

where we forget the bound states of $-\frac{1}{2}\Delta + U(x)$ by taking $u_0 \in \mathrm{Ran}\ W_+ = \mathrm{Ran}\ W_-$. By inserting a Fourier transform we write

$$u_0 = W_+F^{-1}\psi_+ = W_-F^{-1}\psi_-, \qquad \psi_\pm \in L^2(\mathbb{R}^d), \tag{1.4}$$

which implies $\psi_+ = FW_+^*W_-F^{-1}\psi_- = \hat{S}\psi_-$.

Next we state the main result which expresses the asymptotics as $h \to 0$ for the solution $u^h(t)$ of (1.3) in terms of semi-classical measures. The semi-classical measures associated with a bounded sequence of trace-class operators $(P^h)_{h\in(0,h_0)}$ are defined as the weak* limit-points of $h^{-d}p^h(x,\xi)$ in $\mathcal{M}_b(T^*\mathbb{R}^d) = \mathcal{C}_0(T^*\mathbb{R}^d)^*$, where $p^h(x,\xi)$ is the Wick-symbol P^h. They are characterized by

$$\mathrm{Tr}[P^h a^W(x,hD)] \overset{h'\to 0}{\to} \int_{T^*\mathbb{R}^d} a(x,\xi)d\mu(x,\xi), \qquad \forall a \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d),$$

after extracting a subsequence $(P^{h'})$ (*see* [3], [16], [17], [18], [23]). When the operators P^h are the orthogonal projections on uniformly bounded L^2-functions u^h, this writes

$$(1.5) \qquad (u^{h'}, a^W(x, h'D)u^{h'}) \overset{h'\to 0}{\to} \int_{T^*\mathbb{R}^d} a(x,\xi)d\mu(x,\xi), \qquad \forall a \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d).$$

According to [17], we call $\mathcal{M}(u^h, h)$ or $\mathcal{M}(P^h, h)$ the set of all semi-classical measures associated with a sequence (u^h) or P^h. Here and in the sequel, $\Phi_V(t)$ denotes the classical flow in the phase space $T^*\mathbb{R}^d$ associated with the hamiltonian $p_V(x,\xi) = \frac{1}{2}|\xi|^2 + V(x)$.

THEOREM 1.1. – *Assume that there exist $T_+ > 0$ and $T_- > 0$ so that*

$$(1.6) \qquad \forall t, \pm t \in (0, T_\pm), \quad \Phi_V(\pm t)[\{0\}\mathrm{supp}\ \psi_\pm] \cap (\underset{j\in\mathbb{N}}{\cup} T^*_{x_j}\mathbb{R}^d) = \emptyset.$$

Then for any $t \in (-T_-, 0) \cup (0, T_+)$, the sequence $(u^h(t))$ admits a unique semi-classical measure as $h \to 0$

$$(1.7) \qquad \mu(t) = \begin{cases} \Phi_V(t)_*\left[(2\pi)^{-d}\delta_{x=0}|\psi_-(\xi)|^2\right], & if\ t \in (-T_-, 0), \\ \Phi_V(t)_*\left[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi)|^2\right], & if\ t \in (0, T_+). \end{cases}$$

(The expression $\delta_{x=0}|\psi_-(\xi)|^2$ shortly denotes the measure $\delta_{x=0} \otimes |\psi_-(\xi)|^2 d\xi$.)

Remark 1.1. – a) The condition (1.6) only involves the properties of the classical flow $\Phi_V(t)$. If we set $(x(t), \xi(t)) = \Phi_V(t)(x_0, \xi_0)$ then the derivative of the scalar product $x(t).\xi(t)$ equals

$$(1.8) \qquad \frac{d}{dt}(x(t).\xi(t)) = |\xi(t)|^2 - x(t).\partial_x V(x(t)),$$

and $\frac{d}{dt}(x(t).\xi(t))\big|_{t=0} > 0$ when $x_0 = 0$ $\xi_0 \neq 0$. As a consequence and since $|x(t)|$ is estimated by $Ct|\xi_0|$ for small t, the assumption is satisfied for some $T_+ > 0$ and $T_- > 0$ when ψ_+ or equivalently ψ_- is compactly supported in $\mathbb{R}^d \setminus \{0\}$. If we forget the U_j and the corresponding positions x_j, for $j \neq 0$, the validity of (1.6) for any $\psi_+, \psi_- \in L^2(\mathbb{R}^d)$, essentially depends on the global shape of the potential V. As an example, it is valid when $V(x) < 0$ for $x \neq 0$. In such a case, the result can be extended for general $\psi_+, \psi_- \in L^2(\mathbb{R}^d)$ by a simple density argument.

b) There is a complete symmetry between $t > 0$ and $t < 0$ and we will focus on the case $t > 0$.

The outline of the article is as follows : In Section 2, we specify our notations and point out some aspects of the problem. Semi-classical propagation far away from the quantum potentials U_j is treated in Section 3. Meanwhile, we separate the incoming and outgoing flows close to $x = 0$ by 2-microlocal cut-offs and make use of 2-microlocal measures presented in the Appendix. The problem then amounts to some quantum propagation estimate to which the next three sections are devoted. Some canonical transformations which intertwins the classical hamiltonians $p_V(x,\xi) = \frac{1}{2}|\xi|^2 + V(x)$ and $p_0(x,\xi) = \frac{1}{2}|\xi|^2$ and the corresponding semi-classical Fourier integral operators are introduced in Section 4. The action of these Fourier integral operators on the quantum scale is analyzed in Section 5. In Section 6, the preceding results contribute to eliminate the potential $V(hx)$ in the quantum scale and the problem is reduced to standard propagation estimates of quantum scattering theory. Applications are developed in Section 7.

2. Preliminaries

Notations

Passing from the quantum scale to the macroscopic scale and reverse are performed by applying or conjugating with the unitary dilation operators D_h defined by

$$(D_h u)(x) = \frac{1}{h^{d/2}} u\left(\frac{x}{h}\right),$$

and its inverse $D_h^{-1} = D_h^* = D_{1/h}$. Throughout this article, the Schwartz kernel of a continuous operator $K : \mathcal{C}_0^\infty(\mathbb{R}^d) \to \mathcal{D}'(\mathbb{R}^d)$ is denoted by $K(x,y)$. Note the identities

$$(D_h K D_h^*)(x,y) = \frac{1}{h^d} K\left(\frac{x}{h}, \frac{y}{h}\right) \qquad \text{and} \qquad (D_h^* K D_h)(x,y) = h^d K(hx, hy).$$

We set for short $H_0 = -\frac{1}{2}\Delta$, $H_U = -\frac{1}{2}\Delta + U(x)$, $H_V = -\frac{1}{2}\Delta + V(hx)$, $H = -\frac{1}{2}\Delta + U(x) + \Sigma(x,h) + V(hx)$, with the semi-classical equivalents $H_0^h = -\frac{h^2}{2}\Delta$, $H_U^h = -\frac{h^2}{2}\Delta + U(\frac{x}{h})$, $H_V^h = -\frac{h^2}{2}\Delta + V(x)$, $H^h = -\frac{h^2}{2}\Delta + U(\frac{x}{h}) + \Sigma(\frac{x}{h}, h) + V(hx)$. And the previous remark gives

$$H^h_{,0,U,V} = D_h H_{,0,U,V} D_h^*.$$

We also write systematically $\langle x \rangle$, $\hat{x}$ and $đx$ instead of $(1+|x|^2)^{1/2}$, $\frac{x}{\langle x \rangle}$ and $\frac{dx}{(2\pi)^d}$. The Fourier transform is normalized by taking

$$(Fu)(\xi) = \int_{\mathbb{R}^d} e^{-i\xi.x} u(x) dx \qquad \text{and} \qquad (F^{-1}u)(x) = \int_{\mathbb{R}^d} e^{ix.\xi} u(\xi) đ\xi.$$

Then $(2\pi)^{-d/2}F$ is unitary on $L^2(\mathbb{R}^d)$, $F^* = (2\pi)^d F^{-1}$, while a simple change of variables yields $FD_h^* = D_h F$ and $F^{-1}D_h^* = D_h F^{-1}$. For a quantity $q(\alpha,\beta)$, we write $q(\alpha,\beta) = O(\beta^n)$ or $q(\alpha,\beta) = o(\beta^n)$ when the ratio $\frac{q(\alpha,\beta)}{\beta^n}$ is bounded or converges to 0 uniformly with respect to α, and $q(\alpha,\beta) = O_\alpha(\beta^n)$ or $q(\alpha,\beta) = o_\alpha(\beta^n)$ when the estimates depend on the value of α. We say that a subset G of a Fréchet space F is bounded when every element of a complete family of semi-norms on F is bounded on G. Bounded subsets of $\mathcal{C}_0^\infty(\Omega)$ are sets of functions supported in a fixed compact subset of Ω and satisfying uniform $\mathcal{C}^\infty$ estimates. Finally, we say that symbols belong to or are uniformly bounded in $S(m^{-\infty}, g)$ when it is true for any $S(m^k, g)$, $k \in \mathbb{R}$.

Along this article we always consider the exact pseudo-differential calculus as presented in [20]-Chap XVIII or its semi-classical version, with symbols belonging to – or h-dependent symbols uniformly bounded in – some symbol class $S(m,g)$ (g σ-temperate and m σ-g-temperate). The metrics involved in this problem, primarily $g_0 = dx^2 + d\xi^2$ and $g_1 = \frac{dx^2}{\langle x \rangle^2} + d\xi^2$, are all splitted so that the Weyl-, the $(1,0)$- and the $(0,1)$-calculus are equivalent with explicit correspondances. As a consequence we call $OpS(m,g)$ the space of pseudo-differential ($h = 1$) operators with symbols in $S(m,g)$ without specifying the calculus. When necessary the three quantizations will be distinguished by writing them respectively $a^W(x, hD) = Op_W^h[a]$, $a^{(1,0)}(x, hD) = Op_{(1,0)}^h[a]$ and $a^{(0,1)}(x, hD) = Op_{(0,1)}^h[a]$, where the superscript ^{h} is obmitted when $h = 1$. Our analysis relies on the two following remarks.

Phase-space properties of wave operators

Under Hypothesis 1.1 a), the wave operator W_+ (resp. W_-) is a pseudo-differential operator in outgoing (resp. incoming) regions of the phase-space.

LEMMA 2.1. – *Let $\chi \in C_0^\infty((0,\infty))$ and $p_\pm(x,\xi) \in S(1,g_1)$ be such that*

$$\text{supp } (p_\pm) \subset \{(x,\xi) \in T^*\mathbb{R}^d,\ \hat{x}.\hat{\xi} \gtrless \sigma_\pm\} \quad \text{with } -1 < \sigma_\pm < 1. \tag{2.1}$$

We have

$$p_\pm^W(x,D)\chi(H_U)W_\pm - p_\pm^W(x,D)\chi(H_U) \in OpS(\langle\xi\rangle^{-\infty}\langle x\rangle^{1-\mu}, g_1), \tag{2.2}$$

and

$$W_\pm\chi(H_0)p_\pm^W(x,D) - \chi(H_0)p_\pm^W(x,D) \in OpS(\langle\xi\rangle^{-\infty}\langle x\rangle^{1-\mu}, g_1). \tag{2.3}$$

Proof. – We refer to the book of J. Derezinski and C. Gérard [10]-Section 4.13, where they prove

$$p_\pm^W(x,D)\chi(H_U)W_\pm - p_\pm^W(x,D)\chi(H_U)J_\pm \in OpS(\langle x\rangle^{-\infty}\langle\xi\rangle^{-\infty}, g_1),$$

and

$$W_\pm\chi(H_0)p_\pm^W(x,D) - J_\pm\chi(H_0)p_\pm^W(x,D) \in OpS(\langle x\rangle^{-\infty}\langle\xi\rangle^{-\infty}, g_1).$$

The operator $J_\pm$ is a modifier with kernel

$$J_\pm(x,y) = \int_{\mathbb{R}^d} e^{i(\Phi_\pm(x,\xi)-y.\xi)}a_\pm(x,\xi)\,đ\xi.$$

The symbol $a_\pm$ belongs to $S(1,g_1)$ and satisfies condition (2.1) for some $\sigma_\pm$ while $\Phi_\pm$ solves the Hamilton-Jacobi equation $p_U(x,\partial_x\Phi_\pm(x,\xi)) = p_0(\xi)$ on *supp* $a_\pm$. The estimates

$$|\partial_x^\alpha\partial_\xi^\beta(\Phi_\pm(x,\xi) - x.\xi)| \le C_{\alpha\beta}\langle x\rangle^{1-\mu-|\alpha|},$$

are derived in [30] from Hypothesis 1.1 a) and yield (2.2) (2.3). □

Matching between the two scales

The relationship between the metrics g_0 and g_1, respectively natural for semi-classical analysis and quantum scattering, is well known in the framework of second microlocalization around $T_0^*\mathbb{R}^d$ [4] [6]. Here it takes the following obvious form.

LEMMA 2.2. – *a) The dilation D_h correponds to the metaplectic mapping: $(x,h\xi) \to (hx,\xi)$ and we have*

$$D_h^*\mathrm{Op}_W^h[a(x,\xi)]D_h = D_h^*a^W(x,hD)D_h = a^W(hx,D) = \mathrm{Op}_W[a(hx,\xi)]. \tag{2.4}$$

b) The h-dependent symbol $a(hx,\xi,h)$ is uniformly bounded in $S(\langle\xi\rangle^{-\infty},g_1)$ as soon as $a(h)$ is uniformly bounded in $C_0^\infty(T^*\mathbb{R}^d)$.

3. Elimination of $U(\frac{x}{h})$ in the semi-classical scale

According to Remark 1.1, our aim is to determine the semi-classical measure set $\mathcal{M}(u^h(t), h)$ for $u^h(t) = e^{-i\frac{t}{h}H^h}(D_h W_+ F^{-1}\psi_+)$, $t \in (0, T_+)$ and $\psi_+ \in \mathcal{C}_0^\infty(\mathbb{R}^d \setminus \{0\})$. In order to get rid of the potential $U(\frac{x}{h})$, we need the following variation of the intertwinning relation $e^{-itH_U}W_+ = W_+ e^{-itH_0}$, of which the proof is deferred to Section 6.

PROPOSITION 3.1. – *For any $\psi_+ \in \mathcal{C}_0^\infty(\mathbb{R}^d \setminus \{0\})$, there exists a positive constant ε_{ψ_+} so that for $\varepsilon \in (0, \varepsilon_{\psi_+})$*

$$(3.1) \qquad e^{-i\frac{\varepsilon}{h}H}W_+F^{-1}\psi_+ - W_+e^{-i\frac{\varepsilon}{h}H_V}F^{-1}\psi_+ = O_{\psi_+}(\varepsilon) \quad in\ L^2(\mathbb{R}^d).$$

Proof of Theorem 1.1. – We establish (1.7) in four steps : a) construction of ε-dependent cut-offs in the phase-space, b) semi-classical propagation out of $\underset{j\in\mathbb{N}}{\cup} T^*_{x_j}\mathbb{R}^d$, c) quantum scale analysis based on Proposition 3.1, d) sharp estimates for the elements of $\mathcal{M}(u^h(t), h)$. In a), b) and c) the real numbers $\varepsilon \in (0, \varepsilon_1)$, with $\varepsilon_1 \le \varepsilon_{\psi_+}$ small enough, and $t \in (0, T_+)$ are supposed to be fixed.

a) For $s \in (0, T_+)$, we set $K_s = \Phi_V(s)[\{0\}\text{supp }\psi_+]$ and we deduce from the definition (1.6) of T_+ that $(\cup_{s\in[\varepsilon,t]} K_s)$ and $(\underset{j\in\mathbb{N}}{\cup} T^*_{x_j}\mathbb{R}^d)$ do not intersect. Since $(\underset{s\in[\varepsilon,t]}{\cup} K_s)$ is compact and $\underset{j\in\mathbb{N}}{\cup} T^*_{x_j}\mathbb{R}^d$ is closed by Hypothesis 1.1 b), there exists a positive constant $C_{\varepsilon,t}$ so that

$$\text{dist}(\bigcup_{s\in[\varepsilon,t]} K_s, T^*_{x_j}\mathbb{R}^d) > 2C_{\varepsilon,t}\langle x_j\rangle, \qquad \forall j \in \mathbb{N}.$$

Note that the factor $\langle x_j\rangle$ is due to finite speed propagation corresponding to the boundedness of supp ψ_+. By (1.8) and the regularity of the flow Φ_V, we can take ε_1 small enough so that

$$K_{\varepsilon'} \subset \left\{(x,\xi) \in T^*\mathbb{R}^d,\ x.\xi > 0 \text{ and } \frac{2}{C_{\psi_+}} < \frac{1}{2}|\xi|^2 < \frac{C_{\psi_+}}{2}\right\}, \qquad \forall \varepsilon' \in (0, \varepsilon_1),$$

where the positive constant C_{ψ_+} is taken large enough and only depends on supp ψ_+. As a consequence, we can find an open neighbourhood $\Omega_{\varepsilon,t}$ of K_0, $\overline{\Omega_{\varepsilon,t}}$ compact, so that

$$(3.2) \qquad \text{dist}(\bigcup_{s\in[\varepsilon,t]} \Phi_V(s)\overline{\Omega_{\varepsilon,t}}, T^*_{x_j}\mathbb{R}^d) > C_{\varepsilon,t}\langle x_j\rangle, \qquad \forall j \in \mathbb{N},$$

and

$$(3.3) \qquad \Phi_V(\varepsilon)\Omega_{\varepsilon,t} \subset \left\{(x,\xi) \in T^*\mathbb{R}^d,\ x.\xi > 0 \text{ and } \frac{1}{C_{\psi_+}} < \frac{1}{2}|\xi|^2 < C_{\psi_+}\right\}.$$

In connection with (3.2), we introduce a cut-off function $\chi_{\varepsilon,t} \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ so that $0 \le \chi_{\varepsilon,t} \le 1$, $\chi_{\varepsilon,t} \equiv 1$ on $\underset{s\in[\varepsilon,t]}{\cup} \Phi_V(s)\overline{\Omega_{\varepsilon,t}}$ and $\chi_{\varepsilon,t} \equiv 0$ on $\underset{j\in\mathbb{N}}{\cup}\{x \in \mathbb{R}^d, |x - x_j| \le \frac{C_{\varepsilon,t}}{2}\langle x_j\rangle\}$. For any $a \in \mathcal{C}_0^\infty(\Phi_V(t)\Omega_{\varepsilon,t})$, we define for $s \in [\varepsilon, t]$ $a(s) = \Phi_V^*(t-s)a = a \circ \Phi_V(t-s)$. Then the symbols $a(s)$, $s \in [\varepsilon, t]$, are uniformly bounded in $\mathcal{C}_0^\infty(T^*\mathbb{R}^d)$ and satisfy

$$\text{supp } a(s) \subset\subset \Phi_V(s)\Omega_{\varepsilon,t}, \tag{3.4}$$

$$\partial_s a(s) = -\left\{\frac{1}{2}|\xi|^2 + V(x), a(s)\right\}, \tag{3.5}$$

and

$$\chi_{\varepsilon,t}(x)a(x,\xi;s) \equiv a(x,\xi;s). \tag{3.6}$$

b) For a given $a \in \mathcal{C}_0^\infty(\Phi_V(t)\Omega_{\varepsilon,t})$, we consider the function of $s \in [\varepsilon, t]$, $f^h(s) = (u^h(s), a^W(x, hD; s)u^h(s))$, of which the derivative equals

$$\begin{aligned}(f^h)'(s) =&(u^h(s), \left(\frac{i}{h}[H^h, a^W(x,hD;s)] - \left\{\frac{1}{2}|\xi|^2 + V(x), a(s)\right\}^W(x,hD)\right)u^h(s))\\ =&(u^h(s), \left(\frac{i}{h}[H_V^h, a^W(x,hD;s)] - \left\{\frac{1}{2}|\xi|^2 + V(x), a(s)\right\}^W(x,hD)\right)u^h(s))\\ &+\sum_{j\in\mathbb{N}}(u^h(s), \frac{i}{h}\left[U_j\left(\frac{x-x_j}{h}\right), a^W(x,hD;s)\right]u^h(s)).\end{aligned}$$

By semi-classical calculus in $S(\langle\xi\rangle^2, dx^2 + \frac{d\xi^2}{\langle\xi\rangle^2})$, the first term of the right-hand side is $O_{a,\varepsilon,t}(h)$, while (3.6) imply

$$\begin{aligned}&\frac{i}{h}\left[U_j\left(\frac{x-x_j}{h}\right), a^W(x,hD;s)\right]\\ &\quad= \frac{i}{h}\left[U_j\left(\frac{x-x_j}{h}\right)\chi_{\varepsilon,t}(x)a^W(x,hD;s)\chi_{\varepsilon,t}(x)\right.\\ &\qquad\left.-\chi_{\varepsilon,t}(x)a^W(x,hD;s)\chi_{\varepsilon,t}(x)U_j\left(\frac{x-x_j}{h}\right)\right] + O_{a,\varepsilon,t}(h^\infty),\end{aligned}$$

in $\mathcal{L}(L^2(\mathbb{R}^d))$ for all $j \in \mathbb{N}$. By the uniform boundedness of U_j in $S(\langle x\rangle^{-\mu}, g_1)$ and the support conditions on $\chi_{\varepsilon,t}$, we have

$$\begin{aligned}\left\|\chi_{\varepsilon,t}(x)U_j\left(\frac{x-x_j}{h}\right)\right\|_{\mathcal{L}(L^2)} &\leq \left\langle\frac{1}{h}\text{dist }(x_j, \text{supp }\chi_{\varepsilon,t})\right\rangle^{-\mu}\\ &\leq \left\langle\frac{C_{\varepsilon,t}\langle x_j\rangle}{2h}\right\rangle^{-\mu} \leq C'_{\varepsilon,t}\langle x_j\rangle^{-\mu}h^\mu.\end{aligned}$$

By referring again to Hypothesis 1.1 b), we conclude with

$$f^h(t) = f^h(\varepsilon) + O_{a,\varepsilon,t}(h^{\text{Inf}\{1,\mu-1\}}). \tag{3.7}$$

c) Next we estimate the value of $f^h(\varepsilon)$ by studying the evolution on the quantum scale. We conjugate with the dilations D_h the expression of $f^h(\varepsilon)$ and refer to (2.4),

$$f^h(\varepsilon) = (e^{-i\frac{\varepsilon}{h}H}W_+F^{-1}\psi_+, a^W(hx, D; \varepsilon)e^{-i\frac{\varepsilon}{h}H}W_+F^{-1}\psi_+).$$

By applying semi-classical Garding's inequality, $b^W(x, hD) \geq O_b(h)$ for $b \geq 0 \in S(1, g_0)$ (*see* [18]), to $\|a(\varepsilon)\|^2_{L^\infty} - a^W(hx, D; \varepsilon)^* a^W(hx, D; \varepsilon)$ we get

$$\|a^W(hx, D; \varepsilon)\|_{\mathcal{L}(L^2)} = \|a^W(x, hD; \varepsilon)\|_{\mathcal{L}(L^2)} \leq \|a(\varepsilon)\|_{L^\infty} + O_{a(\varepsilon)}(h),$$

where the right-hand side equals $\|\Phi_V(t-\varepsilon)^* a\|_{L^\infty} + O_{a(\varepsilon)}(h) = \|a\|_{L^\infty} + O_{a,\varepsilon,t}(h)$. Hence we infer from Proposition 3.1

$$f^h(\varepsilon) = (e^{-i\frac{\varepsilon}{h}H_V}F^{-1}\psi_+, W_+^* a^W(hx, D; \varepsilon)W_+ e^{-i\frac{\varepsilon}{h}H_V}F^{-1}\psi_+) + \|a\|_{L^\infty}O(\varepsilon) + O_{a,\varepsilon,t}(h),$$

where the complete hamiltonian has been replaced by H_V. The above identity also writes

$$\begin{aligned}(3.8)\ f^h(\varepsilon) &= (e^{-i\frac{\varepsilon}{h}H_V}F^{-1}\psi_+, a^W(hx, D; \varepsilon)e^{-i\frac{\varepsilon}{h}H_V}F^{-1}\psi_+)\\ &+ (e^{-i\frac{\varepsilon}{h}H_V}F^{-1}\psi_+, \big(W_+^* a^W(hx, D; \varepsilon)W_+ - a^W(hx, D; \varepsilon)\big)e^{-i\frac{\varepsilon}{h}H_V}F^{-1}\psi_+)\\ &+ \|a\|_{L^\infty}O(\varepsilon) + O_{a,\varepsilon,t}(h).\end{aligned}$$

By standard semi-classical arguments (*see* [16], [28]) the sequence $(e^{-i\frac{\varepsilon}{h}H_V^h}D_hF^{-1}\psi_+)_h$ has a unique semi-classical measure

$$(3.9)\qquad \mathcal{M}(e^{-i\frac{\varepsilon}{h}H_V^h}D_hF^{-1}\psi_+, h) = \{\Phi_V(\varepsilon)_*[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi)|^2]\}.$$

As a consequence, the first term of (3.8) equals, after conjugating with dilations D_h^* and recalling $a(\varepsilon) = \Phi_V(t-\varepsilon)^* a$,

$$\int_{T^*\mathbb{R}^d} a(x,\xi)d(\Phi_V(t)_*[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi)|^2]) + o_{a,\varepsilon,t}(h^0).$$

The above identification (3.9) combined with Proposition B.2 yields $e^{-i\frac{\varepsilon}{h}H_V}F^{-1}\psi_+ \overset{h\to 0}{\rightharpoonup} 0$ in $L^2(\mathbb{R}^d)$. Thus the second term of (3.8) is an $o_{a,\varepsilon,t}(h^0)$ correction term as soon as $W_+^* a^W(hx, D; \varepsilon)W_+ - a^W(hx, D; \varepsilon)$ is uniformly compact.

We next prove that this difference may be decomposed as a finite sum of terms KA^h or A^hK, where K is a fixed compact operator and A^h is uniformly bounded with respect to $h \in (0, h_0)$ on $L^2(\mathbb{R}^d)$. According to Lemma 2.2 b), the symbol $a(hx, \xi; \varepsilon)$ is uniformly bounded in $S(\langle\xi\rangle^{-\infty}, g_1)$ while (3.3) (3.4) imply

$$\text{supp } a(hx, \xi, \varepsilon) \subset \left\{(x,\xi) \in T^*\mathbb{R}^d, \hat{x}.\hat{\xi} > 0 \text{ and } \frac{1}{C_{\psi_+}} \leq \frac{1}{2}|\xi|^2 \leq C_{\psi_+}\right\}.$$

Thus we can find $\chi_{\psi_+} \in \mathcal{C}_0^\infty((0,\infty))$ and $p_+(x,\xi) = \chi_+(\hat{x}.\hat{\xi}) \in S(1,g_1)$ satisfying condition (2.1) so that $\chi_{\psi_+}(\frac{1}{2}|\xi|^2) \equiv 1$ and $p_+ \equiv 1$ on supp $a(hx,\xi;\varepsilon)$, for all $h \in (0,h_0)$. Pseudo-differential calculus in the metric g_1 and relation (A.15) now lead to

$$\begin{aligned}(3.10)\qquad a^W(hx,D;\varepsilon) =&\chi_{\psi_+}(H_U)^* p_+^W(x,D)^* a(hx,D;\varepsilon) p_+^W(x,D)\chi_{\psi_+}(H_U)\\ &+ R(a,\varepsilon,h)K_\mu.\end{aligned}$$

where K_μ denotes the operator $\langle x\rangle^{\mathrm{Sup}\{-1,1-\mu\}}\langle D\rangle^{-1} \in \mathrm{Op}S(\langle x\rangle^{\mathrm{Sup}\{-1,1-\mu\}}\langle\xi\rangle^{-1},g_1)$, compact on $L^2(\mathbb{R}^d)$ and $\|R(a,\varepsilon,h)\|$ uniformly bounded in $\mathcal{L}(L^2)$. Note that the inverse $K_\mu^{-1} = \langle D\rangle\langle x\rangle^{-\mathrm{Sup}\{-1,1-\mu\}}$ belongs to $\mathrm{Op}S(\langle x\rangle^{-\mathrm{Sup}\{-1,1-\mu\}}\langle\xi\rangle,g_1)$. Identity (2.2) may be written and

$$p_+^W(x,D)\chi_{\psi_+}(H_U)W_+ = p_+^W(x,D)\chi_{\psi_+}(H_U) + RK_\mu,$$

with $R \in \mathcal{L}(L^2(\mathbb{R}^d))$ and we obtain

$$\begin{aligned}&W_+^* a^W(hx,D;\varepsilon)W_+\\ &\quad= W_+^*\chi_{\psi_+}(H_U)^* p_+^W(x,D)^* a(hx,D;\varepsilon)p_+^W(x,D)\chi_{\psi_+}(H_U)W_+\\ &\qquad+ W_+^* R(a,\varepsilon,h)K_\mu W_+\\ &\quad= \left[K_\mu^* R^* + \chi_{\psi_+}(H_U)^* p_+^W(x,D)^*\right] a(hx,D;\varepsilon)\left[p_+^W(x,D)\chi_{\psi_+}(H_U)\right.\\ &\qquad\left.+RK_\mu\right] + W_+^* R(a,\varepsilon,h)K_\mu W_+.\end{aligned}$$

Expanding the right-hand side while referring again to (3.10) provides at once the expected form for the difference $W_+^* a^W(hx,D;\varepsilon)W_+ - a^W(hx,D;\varepsilon)$.

d) We gather the results of b) and c) and we get for all $a \in \mathcal{C}_0^\infty(\Phi_V(t)\Omega_{\varepsilon,t})$, $t \in (0,T_+)$, $\varepsilon \in (0,\varepsilon_1)$, the estimate

$$\begin{aligned}(3.11)\quad (u^h(t), a^W(x,hD)u^h(t)) = &\int_{T^*\mathbb{R}^d} a(x,\xi)d(\Phi_V(t)_*[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi)|^2])\\ &+ \|a\|_{L^\infty}O(\varepsilon) + o_{a,\varepsilon,t}(h^0).\end{aligned}$$

Let $t \in (0,T_+)$ be fixed and let $\mu(t)$ belong to $\mathcal{M}(u^h(t),t)$. By possibly extracting a subsequence $(u^{h'}(t))_{h'}$, we have

$$\lim_{h'\to 0}(u^{h'}(t), b^W(x,h'D)u^{h'}(t)) = \int_{T^*\mathbb{R}^d} b(x,\xi)d\mu(x,\xi;t), \qquad \forall b \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d).$$

Next we take $b \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d)$, $b \geq 0$. For any $\varepsilon \in (0,\varepsilon_1)$, we consider a cut-off function $\chi_\varepsilon \in \mathcal{C}_0^\infty(\Phi_V(t)\Omega_{\varepsilon,t})$ with $0 \leq \chi_\varepsilon \leq 1$ and $\chi_\varepsilon \equiv 1$ on a neighbourhood of $K_t = \mathrm{supp}\ (\Phi_V(t)_*[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi)|^2])$. Estimate (3.11) applies to $a = \chi_\varepsilon b$ and taking the limit as $h' \to 0$ yields

$$\begin{aligned}&\int_{T^*\mathbb{R}^d}(\chi_\varepsilon b)(x,\xi)d\mu(x,\xi;t)\\ &\quad= \int_{T^*\mathbb{R}^d} b(x,\xi)d(\Phi_V(t)_*[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi)|^2]) + \|\chi_\varepsilon b\|_{L^\infty}O(\varepsilon).\end{aligned}$$

The cut-off χ_ε was chosen so that $b \geq \chi_\varepsilon b$ and $\|\chi_\varepsilon b\|_{L^\infty} \leq \|b\|_{L^\infty}$ and we obtain for $\varepsilon \in (0, \varepsilon_1)$

$$\int_{T^*\mathbb{R}^d} b(x,\xi) d\mu(x,\xi;t) \geq \int_{T^*\mathbb{R}^d} (\chi_\varepsilon b)(x,\xi) d\mu(x,\xi;t)$$
$$\geq \int_{T^*\mathbb{R}^d} b(x,\xi) d(\Phi_V(t)_*[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi)|^2]) + \|b\|_{L^\infty} O(\varepsilon).$$

The limiting inequality as $\varepsilon \to 0$ holds for any $b \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d)$, $b \geq 0$, and we conclude

$$\mu(t) \geq \Phi_V(t)_*[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi)|^2]. \tag{3.12}$$

Finally, we recall that the total mass of $\mu(t)$ is estimated by $\overline{\lim_{h'\to 0}} \|u^{h'}\|^2_{L^2} = 1$ and the sequence of inequalities

$$1 \geq \int_{T^*\mathbb{R}^d} d\mu(x,\xi;t) \geq \int_{T^*\mathbb{R}^d} d(\Phi_V(t)_*[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi)|^2]) = 1,$$

transforms (3.12) into an equality. □

4. Canonical transformations leaving $T_0^*\mathbb{R}^d$ invariant

In view of proving Proposition 3.1, we construct in this section some canonical transformations which intertwin the classical hamiltonians $p_0(x,\xi) = 1/2|\xi|^2$ and $p_V(x,\xi) = \frac{1}{2}|\xi|^2 + V(x)$ while being equal to identity on the fiber $T_0^*\mathbb{R}^d$ conormal to the origin. Such transformations are parametrized at least locally by a phase $\varphi(x,\eta) - y.\eta$ where $\varphi(x,\eta)$ solves an eikonal equation (*see* [1], [13], [14]). For any positive constant $E > 1$, $B_\eta(E)$ and $S_\eta(E)$ will denote the open sets

$$B_\eta(E) = \{\eta \in \mathbb{R}^d_\eta,\ |\eta| < E\} \qquad \text{and} \qquad S_\eta(E) = \left\{\eta \in \mathbb{R}^d_\eta,\ \frac{1}{E} < |\eta| < E\right\}.$$

LEMMA 4.1. – *For any $E > 1$ and $\alpha \in (0,1)$, one can find an open ball $B_{x,E,\alpha} \subset \mathbb{R}^d_x$, centered at $x = 0$, and a function $\varphi(x,\eta) \in \mathcal{C}^\infty(B_{x,E,\alpha} \times \mathbb{R}^d)$ satisfying estimates* (A.5) *so that*

$$\begin{cases} \frac{1}{2}|\partial_x\varphi(x,\eta)|^2 + V(x) = \frac{1}{2}|\eta|^2, \\ \partial_x\varphi(0,\eta) = \eta, \quad \text{on } B_{x,E,\alpha} \times S_\eta(E), \\ \varphi|_{x.\eta=0} = 0, \end{cases} \tag{4.1}$$

and

$$\left|\partial^2_{x\eta}\varphi(x,\eta) - Id\right| \leq \alpha, \qquad \forall (x,\eta) \in B_{x,E,\alpha} \times \mathbb{R}^d. \tag{4.2}$$

Moreover the ball $B_{x,E,\alpha}$ can be taken small enough so that

$$\begin{cases} |\partial_\eta\varphi(x,\eta) - x| \leq \alpha|x| \\ |\partial_x\varphi(x,\eta) - \eta| \leq \alpha|\eta| \end{cases}, \qquad \forall (x,\eta) \in B_{x,E,\alpha} \times \mathbb{R}^d. \tag{4.3}$$

Proof. – For any fixed $\eta \in \mathbb{R}^d \setminus \{0\}$, the eikonal equation

$$\begin{cases} \frac{1}{2}|\partial_x \varphi_\eta(x)|^2 + V(x) = \frac{1}{2}|\eta|^2, \\ \partial_x \varphi_\eta(0) = \eta, \\ \varphi_\eta|_{x.\eta=0} = 0, \end{cases} \tag{4.4}$$

admits a unique solution in a neighbourhood of $x = 0$. If we set $(x(t), \xi(t)) = \Phi_V(t)(x_0, \xi_0)$ with x_0 close to 0 such that $x_0.\eta = 0$ and $\xi_0 = \sqrt{|\eta|^2 - V(x_0)}\frac{\eta}{|\eta|}$, then (x_0, t) defines a coordinates system in a neighbourhood of $x = 0$. Existence : One considers the dynamical system $\dot{x} = \partial_\xi p_V(x, \xi)$, $\dot{\xi} = -\partial_x p_V(x, \xi)$, $\dot{u} = \xi.\partial_\xi p_V(x, \xi)$ with initial data $x(0) = x_0$, $\xi(0) = \xi_0$, $u(0) = 0$ and one checks that $\varphi_\eta(x) = u(t, x_0, \xi_0)$ solves (4.4). Uniqueness : If φ_η is a solution, one considers the initial value problem $\dot{x} = \partial_\xi p_V(x, \partial_x \varphi_\eta(x))$ with $x(0) = x_0$ and one checks that the quantities $x(t)$, $\xi(t) = \partial_x \varphi(x(t, x_0))$ and $u(t) = \varphi(x(t, x_0))$ have to solve the above system. By the regularity of the flow Φ_V, the neighbourhood of $x = 0$ can be chosen independent of $\eta \in V_{\eta_0}$, where V_{η_0} is a small neighbourhood of $\eta_0 \neq 0$, and $\varphi_\eta(x)$ is a $\mathcal{C}^\infty$-function of η. By taking a finite covering of the compact set $\overline{S_\eta(2E)}$, we construct a global solution $\varphi_1(x, \eta)$ of (4.1) on $B_{x,E} \times \overline{S_\eta(2E)}$, where $B_{x,E}$ is a small ball around $x = 0$.

Let $\chi_E \in \mathcal{C}^\infty((0, \infty))$ be such that $0 \leq \chi_E \leq 1$, $\chi_E \equiv 1$ on $[\frac{1}{2E^2}, \frac{E^2}{2}]$ and $\chi_E \equiv 0$ on $(0, \frac{1}{2(2E)^2}] \cup [\frac{(2E)^2}{2}, \infty)$. We set

$$\varphi(x, \eta) = \chi_E\left(\frac{1}{2}|\eta|^2\right)\varphi_1(x, \eta) + \left(1 - \chi_E\left(\frac{1}{2}|\eta|^2\right)\right)x.\eta.$$

Then $\varphi \in \mathcal{C}^\infty(B_{x,E} \times \mathbb{R}^d)$ solves (4.1) on $(B_{x,E}) \times S_\eta(E)$ and satisfies (A.5) with

$$\partial^2_{x,\eta}\varphi(0, \eta) = \mathrm{Id}, \qquad \forall \eta \in \mathbb{R}^d,$$

because $\partial_x \varphi_1(0, \eta) = \eta$ and $\partial^2_{x\eta}\varphi_1(0, \eta) = \mathrm{Id}$ for $\eta \in \overline{S_\eta(2E)}$. Further we have for any $x \in B_{x,E}$

$$\begin{aligned} \partial_x \varphi(x, \eta) - \eta =& \chi_E\left(\frac{1}{2}|\eta|^2\right)[\partial_x \varphi_1(x, \eta) - \partial_x \varphi_1(0, \eta)], \\ \partial^2_{x\eta}\varphi(x, \eta) - \mathrm{Id} =& \chi_E\left(\frac{1}{2}|\eta|^2\right)[\partial^2_{x\eta}\varphi_1(x, \eta) - \partial^2_{x\eta}\varphi_1(0, \eta)] \\ &+ \partial_\eta\left(\chi_E\left(\frac{1}{2}|\eta|^2\right)\right)[\partial_x \varphi_1(x, \eta) - \partial_x \varphi_1(0, \eta)]. \end{aligned}$$

By the continuity of $\partial^2_{x\eta}\varphi_1$ and $\partial^3_{xx\eta}\varphi_1$ on $\overline{S_\eta(2E)} \times B_{x,E}$ and the compactness of $\overline{S_\eta(2E)}$, the ball $B_{x,E}$ can be reduced to $B_{x,E,\alpha}$ so that (4.2) and the second estimate of (4.3) hold. Finally, the first estimate of (4.3) is a direct outcome of $\varphi(0, \eta) = 0$ and (4.2) since

$$\partial_\eta \varphi(x, \eta) - x = \partial_\eta \varphi(0, \eta) + \int_0^1 x.\left[\partial^2_{x\eta}\varphi(tx, \eta) - Id\right]dt.$$

□

Remark 4.2. – a) The phase function φ cannot be extended to the whole phase-space while preserving estimate (4.2) because we do not control the size of the ball $B_{x,E,\alpha}$ for general potentials $V(x)$.

b) The above estimate (4.2) implies that the phase φ also satisfies condition (A.6).

For $a \in \mathcal{C}_0^\infty(B_{x,E,\alpha} \times S_\eta(E))$, the transport equation

$$\begin{cases} \partial_t b + \partial_x\varphi.\partial_x b + \frac{1}{2}\mathrm{Tr}[\partial_x^2\varphi]b = 0, \\ b|_{t=0} = a, \end{cases} \tag{4.5}$$

admits a unique solution $b(t)$, $t \in [0, \varepsilon_{E,\alpha,a}]$, uniformly bounded in $\mathcal{C}_0^\infty(B_{x,E,\alpha} \times S_\eta(E))$ provided that $\varepsilon_{E,\alpha,a}$ is small enough. The next proposition asserts that the h-Fourier integral operators $J^h(b(t),\varphi)$, defined as in (A.4), transform modulo an $O(h)$ error term the quantum evolution associated with the h-dependent hamiltonian H_0^h into the one associated with H_V^h.

PROPOSITION 4.3. – *Let $b(t)$, $t \in [0, \varepsilon_{E,\alpha,a}]$, be the symbols defined by* (4.5). *Then the estimate*

$$e^{-i\frac{t}{h}H_V^h} J^h(a,\varphi) - J^h(b(t),\varphi)e^{-i\frac{t}{h}H_0^h} = O_{E,a,\alpha}(h), \tag{4.6}$$

holds in $\mathcal{L}(L^2(\mathbb{R}^d))$ uniformly with respect to $t \in [0, \varepsilon_{E,\alpha,a}]$.

Proof. – The result is standard (*see* a.e. [28]) up to the fact that the phase function φ is not defined everywhere. We have to introduce cut-offs $\chi_1 \in \mathcal{C}_0^\infty(B_{x,E,\alpha} \times \mathbb{R}^d)$ and $\chi_2 \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d)$ so that

$$\chi_1(x, \partial_x\varphi(x,\eta)) \equiv 1 \quad \text{and} \quad \chi_2(\partial_\eta\varphi(x,\eta),\eta) \equiv 1, \tag{4.7}$$

on supp $b(t)$, for all $t \in [0, \varepsilon_{E,\alpha,a}]$. Proposition A.2 gives

$$J^h(b(t),\varphi) - \chi_1^{(1,0)}(x,hD)J^h(b(t),\varphi) = O_{E,a,\alpha}(h^2), \tag{4.8}$$

and

$$J^h(b(t),\varphi) - J^h(b(t),\varphi)\chi_2^{(1,0)}(x,hD) = O_{E,a,\alpha}(h^2), \tag{4.9}$$

in $\mathcal{L}(L^2(\mathbb{R}^d))$ (Indeed the remainder is $O_{E,a,\alpha}(h^\infty)$). By semi-classical calculus in $S(\langle\xi\rangle^2, dx^2 + \frac{d\xi^2}{\langle\xi\rangle^2})$ the operator $H_V^h\chi_1^{(1,0)}(x,hD)$ (resp. $\chi_2^{(1,0)}(x,hD)H_0^h$) is the sum of $p_{V,2}^{(1,0)}(x,hD;h)$ [resp. $p_{0,2}^{(1,0)}(x,hD;h)$] and an $O_{E,a,\alpha}(h^2)$ remainder in $\mathcal{L}(L^2(\mathbb{R}^d))$, with $p_{V,2}(h)$ (resp. $p_{0,2}(h)$) uniformly bounded in $\mathcal{C}_0^\infty(B_{x,E,\alpha} \times \mathbb{R}^d)$ (resp. $\mathcal{C}_0^\infty(T^*\mathbb{R}^d)$). Condition (4.7) on the cut-offs implies that $p_{V,2}(x,\partial_x\varphi(x,\eta);h)$ and $p_{0,2}(\partial_\eta\varphi(x,\eta),\eta;h)$ both coincide with $p_V(x,\partial_x\varphi(x,\eta)) \equiv p_0(\partial_\eta\varphi(x,\eta),\eta)$ on supp $b(t)$, $t \in [0, \varepsilon_{E,\alpha,a}]$, where the last equality is nothing but the eikonal equation (4.1). By referring again to Proposition A.2, the left-hand side of (4.6) equals

$$-\int_0^t e^{-i\frac{t-s}{h}H_V^h}\left[J^h\left(\partial_t b + \partial_x\varphi.\partial_x b + \frac{1}{2}\mathrm{Tr}[\partial_x^2\varphi]b, \varphi\right)\right]e^{-i\frac{s}{h}H_0^h}ds + O_{E,a,\alpha}(h),$$

and the first term vanishes by (4.5). □

5. Action of $J^h(a,\varphi)$ in the quantum scale

Let φ be the phase function defined in Lemma 4.1 for a given choice of (E,α). With the parameter α we control how the canonical transformation associated with φ is close to the identity. In this section we take advantage of this and give sharp estimates for the dilated form

$$G^h(a,\varphi) = D_h^* J^h(a) D_h, \tag{5.1}$$

of the Fourier integral operators $J^h(a,\varphi)$.

PROPOSITION 5.1. – *Let K be a compact subset of $S_\eta(E)$ and let $a \in \mathcal{C}_0^\infty(B_{x,E,\alpha} \times S_\eta(E))$ be such that $a \equiv 1$ on $\{0\} \times K$. Then the estimate*

$$G^h(a,\varphi)G^h(a,\varphi)^*(F^{-1}\psi) = (F^{-1}\psi) + o_{E,\alpha,a,\psi}(h^0), \tag{5.2}$$

holds for any $\psi \in L^2(\mathbb{R}^d)$ supported in K.

Proof. – According to (A.7) (A.8), we have

$$J^h(a,\varphi)J^h(a,\varphi)^* = \mathrm{Op}_W^h\left[|a|^2(x,\eta(x,\xi))|\mathrm{det}\partial^2_{x,\eta}\varphi(x,\eta(x,\xi))|)\right] + O_{E,\alpha,a}(h),$$

in $\mathcal{L}(L^2)$, where $\eta(x,\xi)$ is the inverse mapping of $\eta \to \xi(x,\eta) = \partial_x\varphi(x,\eta)$. After conjugating with dilations D_h^* we get by (2.4)

$$G^h(a,\varphi)G^h(a,\varphi)^* = \mathrm{Op}_W\left[|a|^2(hx,\eta(hx,\xi))|\mathrm{det}\partial^2_{x,\eta}\varphi(hx,\eta(hx,\xi))|)\right] + O_{E,\alpha,a}(h).$$

Like in the proof of Proposition B.2 we use

$$s - \lim_{h\to 0} G^h(a,\varphi)G^h(a,\varphi)^* = |a|^2(0,\eta(0,D)|\mathrm{det}\partial^2_{x,\eta}\varphi(0,\eta(0,D))|,$$

and we conclude by noting that $\eta(0,\xi)=\xi$ and $\partial^2_{x,\eta}\varphi(0,\xi) = Id$ for all $\xi \in S_\eta(E)$. □

PROPOSITION 5.2. – *By taking $0 < \alpha < \alpha_0$, $\alpha_0 < 1$ small enough, the following properties hold for any bounded subset $\mathcal{B}$ of $\mathcal{C}_0^\infty(B_{x,E,\alpha} \times S_\eta(E))$.*

a) For any $N \in \mathbb{R}$, we have

$$\|\langle x\rangle^N G^h(a,\varphi)\langle x\rangle^{-N}\|_{\mathcal{L}(L^2)} = O_{E,\alpha,\mathcal{B},N}(h^0), \qquad \forall a \in \mathcal{B}. \tag{5.3}$$

b) If $p_+, \tilde{p}_- \in S(1,g_1)$ satisfy condition (2.1) *with $\sigma_- < \sigma_+ + 2\log(1-\alpha)$ then we have the estimate*

$$\|\langle x\rangle^N \tilde{p}_-^W(x,D)G^h(a,\varphi)p_+^W(x,D)\|_{\mathcal{L}(L^2)} = O_{E,\sigma_-,\sigma_+,\alpha,\mathcal{B},N}(h^0), \qquad \forall a \in \mathcal{B}. \tag{5.4}$$

In order to establish this Proposition, we need a technical lemma of which the proof is adapted from [10] and [21]. For $\chi \in \mathcal{C}_0^\infty(B_{x,E,\alpha})$ and $a \in S(\langle x\rangle^N, g_1)$ we define the operator

$$\Gamma^h(a,\chi,\varphi)(x,y) = \int_{\mathbb{R}^d} e^{i[\frac{\varphi(hx,\eta)}{h} - y.\eta]}\chi(hx)a(x,\eta)đ\eta. \tag{5.5}$$

For the sake of conciseness we introduce the following notion of support: For a symbol $c(h) \in S(\langle x\rangle^N, g_1)$ and a set $F^h \subset T^*\mathbb{R}^d$ possibly depending on $h \in (0, h_0)$, we write

$$g_1 - \text{supp } c(h) \subset^h F^h, \tag{5.6}$$

if, for any $N' \in \mathbb{R}$, we have $c^h = c_{N'}(h) + r_{N'}(h)$ with supp $c_{N'}(h) \subset F^h$ while the semi-norms of $c_{N'}(h)$ (resp. $r_{N'}(h)$) are estimated in $S(\langle x\rangle^N, g_1)$ (resp. $S(\langle x\rangle^{N'}, g_1)$) by the semi-norms of $c(h)$ in $S(\langle x\rangle^N, g_1)$ uniformly with respect to $h \in (0, h_0)$. As a consequence of pseudo-differential calculus in the metric g_1, the product $c(x, D, h)c'(x, D, h)$, whatever the quantization is, is uniformly bounded in $\mathrm{Op}S(\langle x\rangle^{-\infty}, g_1)$ when $c(h)$ and $c'(h)$ are uniformly bounded in some $S(\langle x\rangle^N, g_1)$ with

$$g_1 - \text{supp } c(h) \subset^h F^h, \quad g_1 - \text{supp } c'(h) \subset^h F'^h \quad \text{and} \quad F^h \cap F'^h = \emptyset.$$

LEMMA 5.3. – *The following properties hold as soon as the parameter α satisfies $0 < \alpha < \alpha_0$ for some fixed $\alpha_0 << 1$.*

a) The operator $\Gamma^h(a(h), \chi, \varphi)\Gamma^h(b(h), \chi, \varphi)^*$ is uniformly bounded in $\mathrm{Op}S(\langle x\rangle^{N+N'}, g_1)$ when $a(h)$ and $b(h)$ respectively describe bounded subsets of $S(\langle x\rangle^N, g_1)$ and $S(\langle x\rangle^{N'}, g_1)$. Moreover if $\eta(x, \xi)$ is the inverse mapping of $\eta \to \xi(x, \eta) = \partial_x\varphi(x, \xi)$, its $(1,0)$-symbol $c(h)$ satisfies

$$g_1 - \text{supp } c(h) \subset^h \{(x, \xi) \in T^*\mathbb{R}^d,\ hx \in B_{x,E,\alpha} \text{ and } (x, \eta(hx, \xi)) \in A^h \cap B^h\},$$

when

$$g_1 - \text{supp } a(h) \subset^h A^h \quad \text{and} \quad g_1 - \text{supp } b(h) \subset^h B^h.$$

b) For $a(h)$ and $b(h)$, $h \in (0, h_0)$ uniformly bounded in $S(\langle x\rangle^N, g_1)$ and $\in S(\langle x\rangle^{N'}, g_1)$ there exists $c(h) \in S(\langle x\rangle^{N+N'}, g_1)$ uniformly bounded so that

$$\Gamma^h(a, \chi, \varphi)b^{(1,0)}(x, D) = \Gamma^h(c(h), \chi, \varphi),$$

with

$$g_1 - \text{supp } c(h) \subset^h \{(x, \xi) \in A^h,\ hx \in B_{x,E,\alpha} \text{ and } (h^{-1}\partial_\eta\varphi(hx, \xi), \xi) \in B^h\},$$

if

$$g_1 - \text{supp } a(h) \subset^h A^h \quad \text{and} \quad g_1 - \text{supp } b(h) \subset^h B^h.$$

Proof. – a) The proof is basically the same as for Proposition A.2 a). We write

$$\begin{aligned}
&\Gamma^h(a(h), \chi, \varphi)\Gamma^h(b(h), \chi, \varphi)^* \\
&= \int_{\mathbb{R}^d} e^{i\frac{\varphi(hx,\eta) - \varphi(hy,\eta)}{h}} \chi(hx)a(x, \eta; h)\bar{b}(y, \eta; h)\chi(hy)đ\eta \\
&= \int_{\mathbb{R}^d} e^{i(x-y).\int_0^1 \partial_x\varphi(thx + (1-t)hy, \eta)dt} \chi(hx)a(x, \eta; h)\bar{b}(y, \eta; h)\chi(hy)đ\eta \\
&= \int_{\mathbb{R}^d} e^{i(x-y).\xi}c(x, y, \xi; h)đ\xi.
\end{aligned}$$

We used the change of variable $\xi \to \eta(u,v,\xi)$ reverse to $\eta \to \xi(u,v,\eta) = \int_0^1 \partial_x\varphi(tu + (1-t)v,\eta)dt$ and we set

$$c(x,y,\xi;h) = \chi(hx)a(x,\eta(hx,hy,\xi);h)\bar{b}(y,\eta(hx,hy,\xi);h)\chi(hy).$$

This symbol $c(h)$ is uniformly bounded in $S(\langle x\rangle^N\langle y\rangle^{N'}, \frac{dx^2}{\langle x\rangle^2} + \frac{dy^2}{\langle y\rangle^2} + d\xi^2)$ and the result comes at once from Lemma A.1 b).

b) The kernel of $\Gamma^h(a(h),\chi,\varphi)b^{(1,0)}(x,D;h)$ writes

$$\int_{\mathbb{R}^{3d}} e^{i\frac{\varphi(hx,\eta)}{h} - x'.\eta}\chi(hx)a(x,\eta;h)e^{i(x'-y).\xi}b(x',\xi;h)đ\eta dx'đ\xi$$
$$= \int_{\mathbb{R}^d} e^{i\frac{\varphi(hx,\xi)}{h} - y.\xi}\chi(hx)c(x,\xi;h)đ\xi,$$

with

$$c(x,\xi;h) = \int_{\mathbb{R}^{2d}} e^{i[\frac{\varphi(hx,\eta)-\varphi(hx,\xi)}{h} - x'.(\eta-\xi)]}\chi'(hx)a(x,\eta)b(x',\xi)đ\eta dx',$$

and

$$\chi' \in \mathcal{C}_0^\infty(B_{x,E,\alpha}), \quad \chi' \equiv 1 \text{ on supp } \chi.$$

We set $r(u,\xi,\eta) = \int_0^1\int_0^1 [\partial_\eta\partial_x\varphi(su,(1-t)\xi + t\eta) - Id]dsdt$ so that $\frac{1}{h}[\varphi(hx,\eta) - \varphi(hx,\xi)] = (x + r(hx,\xi,\eta)x).(\eta-\xi)$ while estimate (A.5) yields $|\partial_u^\beta\partial_\xi^\gamma\partial_\eta^\delta r| \le C_{\beta\gamma\delta}$ and (4.3) gives $|r| \le \alpha$. We point out the identy

$$\partial_\eta[(x + r(hx,\xi,\eta)x).(\eta-\xi)] = \partial_\eta\varphi(hx,\eta) = x + r(hx,\eta,\eta)x, \tag{5.7}$$

and introduce the notations $r_\xi = r(hx,\xi,\eta)$, $r_\eta = r(hx,\eta,\eta)$. Let $\chi_\alpha \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ obey $\chi_\alpha \equiv 1$ for $|u| \le \alpha$ and $\chi_\alpha \equiv 0$ for $|u| \ge 2\alpha$. The symbol $c(x,\xi;h)$ is the sum

$$c_-(x,\xi;h) + c_+(x,\xi;h) = \int_{\mathbb{R}^{2d}} e^{i(x+r_\xi x - x').(\eta-\xi)}d_-(x,x',\xi,\eta;h)đ\eta dx'$$
$$+ \int_{\mathbb{R}^{2d}} e^{i(x-x').(\eta-\xi)}d_+(x,x',\xi,\eta;h)đ\eta dx',$$

with

$$d_-(x,x',\xi,\eta;h) = (1-\chi_\alpha)\left(\frac{x + r_\eta x - x'}{\langle x\rangle + \langle x'\rangle}\right)\chi'(hx)a(x,\eta)b(x',\xi),$$

and

$$d_+(x,x',\xi,\eta;h) = \chi_\alpha\left(\frac{x + r_\eta x - x' - r_\xi x}{\langle x\rangle + \langle x' + r_\xi x\rangle}\right)\chi'(hx)a(x,\eta)b(x' + r_\xi x,\xi).$$

Owing to (5.7) we have

$$-i\frac{(x + r_\eta x - x')}{|x + r_\eta x - x'|^2}.\partial_\eta e^{i(x + r_\xi - x').(\eta-\xi)} = e^{i(x+r_\xi - x').(\eta-\xi)}.$$

Integrations by part with this vector field and some integrations by parts with respect to x' in order to make the integral converge, ensure

$$|\partial_x^\beta \partial_\xi^\gamma c_-(x,\xi;h)| \leq C_{\beta\gamma M}\langle x\rangle^{-M}.$$

The second term writes

$$c_+(x,\xi;h) = e^{iD_x.D_\eta} d_+(x,x',\xi,\eta;h)\Big|_{\substack{x'=x\\ \eta=\xi}}.$$

Hence by referring to Lemma A.1, the proof is done as soon as

$$(5.8) \qquad |\partial_x^\beta \partial_{x'}^\gamma \partial_{\xi,\eta}^\delta d_+(x,x',\eta,\xi;h)| \leq C_{\beta,\gamma,\delta}\langle x\rangle^{N-|\beta|}\langle x'\rangle^{N'-|\gamma|}.$$

Indeed one easily checks

$$(5.9) \qquad \begin{aligned} &|\partial_x^\beta \partial_{x'}^\gamma \partial_{\xi,\eta}^\delta d_+(x,x',\xi,\eta;h)| \\ &\quad \leq C_{\beta,\gamma,\delta} \operatorname*{Sup}_{0\leq k\leq|\beta|+|\gamma|} \langle x\rangle^{N-|\beta|+k}\langle x'+r_\xi x\rangle^{N'-|\gamma|-k}. \end{aligned}$$

On the support of χ_α, we know $|x+r_\eta x - x' - r_\xi x| \leq 2\alpha(\langle x\rangle + \langle x'+r_\xi x\rangle)$. By taking into account $|r| \leq \alpha$ we obtain

$$|x| - |x'+r_\xi x| \leq |x - x' - r_\xi x| \leq 3\alpha(\langle x\rangle + \langle x'+r_\xi x\rangle),$$

so that $(1-3\alpha)|x| \leq (1+3\alpha)\langle x'+r_\xi x\rangle$ allows to replace the right-hand side of (5.9) by $C_{\beta,\gamma,\delta}\langle x\rangle^{N-|\beta|}\langle x'+r_\xi x\rangle^{N'-|\gamma|}$. We now assume $|x|,\ |x'| \geq 1$, which is the only interesting case and we use again $|r| \leq \alpha$,

$$\begin{aligned} |(1-2\alpha)|x| - |x'|| &\leq |x + r_\eta x - x' - r_\xi x| \\ &\leq 4\alpha(|x| + |x'| + \alpha|x|). \end{aligned}$$

Thus, by taking α_0 small enough and $0 < \alpha < \alpha_0$, we have $C^{-1}\langle x\rangle \leq \langle x'\rangle \leq C\langle x\rangle$ on the support of χ_α and (5.8) becomes a consequence of (5.9). $\square$

Proof of Proposition 5.2. – We first notice that $G^h(a,\varphi) = \Gamma^h(a(hx,\eta),\chi,\varphi)$ when $a \in \mathcal{C}_0^\infty(B_{x,E,\alpha} \times S_\eta(E))$ and $\chi \in \mathcal{C}_0^\infty(B_{x,E,\alpha})$, $\chi \equiv 1$ on supp a.

a) We remark that $\langle x\rangle^N = \mathrm{Op}^{(1,0)}[\langle x\rangle^N]$ and the previous lemma implies the uniform boundedness of $(G^h(a,\varphi)\langle x\rangle^N)(G^h(a,\varphi)\langle x\rangle^N)^*$ in $\mathrm{Op}S(\langle x\rangle^{2N},g_1)$. As a consequence the operators $(\langle x\rangle^{-N}G^h(a,\varphi)\langle x\rangle^N)(\langle x\rangle^{-N}G^h(a,\varphi)\langle x\rangle^N)^*$ and $\langle x\rangle^{-N}G^h(a,\varphi)\langle x\rangle^N$ are uniformly bounded on $L^2(\mathbb{R}^d)$.

b) Owing to part a) we can replace $p_+^W(x,D)$ by $p_+^{(1,0)}(x,D)$. Indeed the equivalence of Weyl- and $(1,0)$- calculus gives $p_+^W(x,D) = {p'}_+^{(1,0)}(x,D)$ with $g_1 -\mathrm{supp}\, {p'}_+ \subset^h \mathrm{supp}\, p_+$. Lemma 5.5 b), gives $G^h(a,\varphi)p_+^{(1,0)}(x,D) = \Gamma^h(c(h),\chi,\varphi)$ where $c(h)$ is bounded in $S(1,g_1)$ with

$$g_1 - \mathrm{supp}\ c(h) \subset^h \{(x,\xi) \in T^*\mathbb{R}^d,\ hx \in B_{x,E,\alpha}\ h^{-1}\widehat{\partial_\eta\varphi(hx,\xi)}.\hat{\xi} \geq \sigma_+\}.$$

For $u \neq 0$ we calculate $\partial_u(\hat{u}).\delta u = \langle u\rangle^{-1}(\delta u - \frac{u.\delta u}{\langle u\rangle^2}u)$, from which we conclude that the inequality $|u-v| \leq \alpha|u|$ implies

$$|\hat{v}-\hat{u}| \leq \int_0^1 \frac{|v-u|}{|u+t(v-u)|}dt \leq \int_0^1 \frac{\alpha}{1-\alpha t}dt = -\log(1-\alpha). \tag{5.10}$$

Thus we deduce $g_1 - \text{supp } c(h) \subset^h \{\hat{x}.\hat{\xi} \geq \sigma_+ + \log(1-\alpha)\}$ from estimate (4.3). By Lemma 5.5 a), the operator

$$(G^h(a,\varphi)p_+^{(1,0)}(x,D))(G^h(a,\varphi)p_+^{(1,0)}(x,D))^* = \Gamma^h(c(h),\chi,\varphi)\Gamma^h(c(h),\chi,\varphi)^*$$

is uniformly bounded in $\text{Op}S(1,g_1)$ and the g_1-support of its $(1,0)-$symbol is $h-$included in $\{\hat{x}.\widehat{\eta(hx,\xi)} \geq \sigma_+ + \log(1-\alpha)\}$. We refer again to (4.3), $|\eta(hx,\xi)-\xi| \leq \alpha|\eta(hx,\xi)|$, and we conclude from (5.10) that the $(1,0)$-symbol of $(G^h(a,\varphi)p_+^{(1,0)}(x,D))(G^h(a,\varphi)p_+^{(1,0)}(x,D))^*$ satisfies

$$g_1 - \text{supp } d(h) \subset^h \{\hat{x}.\hat{\xi} \geq \sigma_+ + 2\log(1-\alpha) > \sigma_-\}.$$

As a consequence the operator

$$(p_-^W(x,D)G^h(a,\varphi)p_+^{(1,0)}(x,D))(p_-^W(x,D)G^h(a,\varphi)p_+^{(1,0)}(x,D))^*,$$

is uniformly bounded in $\text{Op}S(\langle x\rangle^{-\infty},g_1)$, which yields the result. □

6. Elimination of $V(hx)$ in the quantum scale

Proposition 3.1 is a triviality when $V \equiv 0$ (and $\Sigma \equiv 0$). Here we get rid of the semi-classical potential V with the help of the Fourier integral operators $J^h(a,\varphi)$ studied in the two previous sections. For a data $\psi_+ \in \mathcal{C}_0^\infty(\mathbb{R}^d \setminus \{0\})$, we take the constant $E > 1$ so that supp $\psi_+ \subset S_\eta(E)$. We fix σ_+, σ_- and α so that $-1 < \sigma_- < \sigma_+ < 1$, $0 < \alpha < \alpha_0$ and $\sigma_- < \sigma_+ + 2\log(1-\alpha)$. Note that in Proposition 4.1, the ball $B_{x,E,\alpha}$ can also be chosen small enough so that

$$\text{dist}\left(2\overline{B_{x,E,\alpha}}, x_j\right) \geq C_0\langle x_j\rangle, \qquad \forall j \in \mathbb{N}, \quad j \neq 0, \tag{6.1}$$

for some positive constant C_0. This condition will help in the treatment of Σ.. For $a \in \mathcal{C}_0^\infty(B_{x,E,\alpha} \times S_\eta(E))$ such that $a \equiv 1$ on $\{0\}$supp ψ_+, we consider the solution $b(s)$ of (4.5) for $s \in [0,\varepsilon_{E,\alpha,a}]$. All this choices of E, α, a and $\varepsilon_{E,\alpha,a}$ essentially depend on ψ_+ and the constant ε_{ψ_+} of Proposition 3.1 is nothing but $\varepsilon_{E,\alpha,a}$.

Proof of Proposition 3.1. – The boundedness of W_+, $e^{-\frac{i\varepsilon}{h}H}$ and $e^{-\frac{i\varepsilon}{h}H_V}$ and Proposition 5.1 imply

$$\begin{aligned}&\left(e^{-\frac{i\varepsilon}{h}H}W_+ - W_+e^{-\frac{i\varepsilon}{h}H_V}\right)(F^{-1}\psi_+)\\ &\quad = \left(e^{-\frac{i\varepsilon}{h}H}W_+ - W_+e^{-\frac{i\varepsilon}{h}H_V}\right)G^h(a,\varphi)G^h(a,\varphi)^*(F^{-1}\psi_+) + o_{\psi_+}(h^0).\end{aligned}$$

By differentiating with respect to ε and applying the intertwining property $H_U W_+ = W_+ H_0$ we get

$$\left(e^{-\frac{i\varepsilon}{h}H}W_+ - W_+ e^{-\frac{i\varepsilon}{h}H_V}\right)(F^{-1}\psi_+)$$
$$= -i\int_0^{\varepsilon} e^{-i\frac{\varepsilon-s}{h}H}h^{-1}(\Sigma(x;h)W_+ + [V(hx),W_+])e^{-\frac{is}{h}H_V}G^h(a,\varphi)$$
$$G^h(a,\varphi)^*(F^{-1}\psi_+)ds \ + o_{\psi_+}(h^0).$$

Since $\psi_+ \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, $\langle x\rangle^{N_0}F^{-1}\psi_+$ belongs to $L^2(\mathbb{R}^d)$ for $N_0 > 0$. Owing to Proposition 5.2 a) the operator $\langle x\rangle^{N_0}G^h(a,\varphi)\langle x\rangle^{-N_0}$ is bounded and it suffices to find an $N_0 > 0$ so that

$$h^{-1}(\Sigma(x;h)W_+ + [V(hx),W_+])e^{-\frac{is}{h}H_V}G^h(a,\varphi)\langle x\rangle^{-N_0}, \tag{6.2}$$

is bounded on $L^2(\mathbb{R}^d)$ uniformly with respect to $s \in [0,\varepsilon_{E,\alpha,a}]$ and $h \in (0,h_0)$. Before going further, we must note that estimates (4.8) (4.9) can be easily extended to any $\chi_1,\chi_2 \in S(1,g_0)$ which satisfy condition (4.7) (simply insert cut-offs with the proper support conditions like we did for p_V and p_0). Especially, if $\chi_x \in \mathcal{C}_0^\infty(2B_{x,E,\alpha})$ with $\chi_x \equiv 1$ on $(1+\alpha)B_{x,E,\alpha}$ and $\chi_\xi \in \mathcal{C}_0^\infty((0,\infty))$ with $\chi_\xi \equiv 1$ on $[\frac{(1-\alpha)^2}{2E^2}, \frac{E^2}{2(1-\alpha)^2}]$, then we get after conjugating with dilations

$$G^h(a,\varphi) = \chi_x(hx)G^h(a,\varphi) + O_{\psi_+}(h^2) = G^h(a,\varphi)\chi_x(hx) + O_{\psi_+}(h^2)$$
$$= \chi_\xi(H_0)G^h(a,\varphi) + O_{\psi_+}(h^2) = G^h(a,\varphi)\chi_\xi(H_0) + O_{\psi_+}(h^2)$$

in $\mathcal{L}(L^2(\mathbb{R}^d))$. Therefore we can always insert a cut-off $\chi_x(hx)$ or $\chi_\xi(H_0)$ just before or after a factor $G^h(a,\varphi)$ without changing the final estimates. We replace $G^h(a,\varphi)\langle x\rangle^{-N_0}$ by $G^h(a,\varphi)\chi_\xi(H_0)\langle x\rangle^{-N_0}$ and by conjugating (4.6) with dilations we transform the operator (6.2) into

$$h^{-1}(\Sigma(x;h)W_+ + [V(hx),W_+])G^h(b(s),\varphi)e^{-i\frac{s}{h}H_0}\chi_\xi(H_0)\langle x\rangle^{-N_0} + O_{\psi_+}(1).$$

Next we consider the cut-offs $\chi_+,\tilde\chi_- \in \mathcal{C}_0^\infty([-1,1])$ with $\chi_+ \equiv 1$ on $[\frac{\sigma_++1}{2},1]$ and $\chi_+ \equiv 0$ on $[-1,\sigma_+]$ while $\tilde\chi_- \equiv 1$ on $[-1,\frac{-1+\sigma_-}{2}]$ and $\tilde\chi_- \equiv 0$ on $[\sigma_-,1]$ and we set $p_+(x,\xi) = \chi_+(\hat x.\hat\xi)$, $p_- = 1 - p_+$, $\tilde p_-(x,\xi) = \tilde\chi_-(\hat x.\hat\xi)$ and $\tilde p_+ = 1 - \tilde p_-$. Standard microlocal propagation estimate given in [10]-Section 4.12 imply $\langle x\rangle^{N_0}p_-^W(x,D)e^{-i\frac{s}{h}H_0}\chi_\xi(H_0)\langle x\rangle^{-N_0} = O_{\psi_+}(1)$ and we are lead to check the boundedness of

$$h^{-1}(\Sigma(x;h)W_+ + [V(hx),W_+])G^h(b(s),\varphi)\langle x\rangle^{-N_0},$$

and

$$h^{-1}(\Sigma(x;h)W_+ + [V(hx),W_+])G^h(b(s),\varphi)p_+^W(x,D).$$

The symbols $b(s)$, p_+ and $\tilde p_-$ satisfy the assumptions of Proposition 5.2 so that the operator $\langle x\rangle^{N_0}G^h(b(s),\varphi)\langle x\rangle^{-N_0}$ and the factor $\{\ldots\}$ of the decomposition

$$\begin{aligned}G^h(b(s),\varphi)p_+^W(x,D) =&\chi_\xi(H_0)(\tilde p_+ + \tilde p_-)G^h(b(s),\varphi)p_+^W(x,D) + O_{\psi_+}(h^2)\\ =&\langle x\rangle^{-N_0}\big\{\langle x\rangle^{N_0}\chi_\xi(H_0)\langle x\rangle^{-N_0}\big\}\big\{\langle x\rangle^{N_0}\tilde p_- G^h(b(s),\varphi)p_+^W(x,D)\big\}\\ &+ \chi_\xi(H_0)\tilde p_+\big\{G^h(b(s),\varphi)p_+^W(x,D)\big\} + O_{\psi_+}(h^2),\end{aligned}$$

are uniformly bounded operators. Hence the problem amounts to the uniform boundedness of

$$h^{-1}(\Sigma(x;h)W_+ + [V(hx), W_+])\langle x\rangle^{-N_0}, \tag{6.3}$$

and

$$h^{-1}(\Sigma(x;h)W_+ + [V(hx), W_+])\chi_\xi(H_0)\tilde{p}_+^W(x,D)\chi_x(hx). \tag{6.4}$$

We have

$$\left|h^{-1}V(hx)\langle x\rangle^{-\mu}\right| \le \left|\left(\int_0^1 \partial_x V(thx)dt\right).\frac{x}{\langle x\rangle^{\mu}}\right| \le C, \tag{6.5}$$

while Peetre's inequality gives

$$\begin{aligned} \left|h^{-1}\Sigma(x;h)\langle x\rangle^{-\mu}\right| &\le Ch^{-1}\sum_{j\neq 0}\left\langle x - \frac{x_j}{h}\right\rangle^{-\mu}\langle x\rangle^{-\mu} \\ &\le Ch^{-1}\sum_{j\neq 0}\left\langle \frac{x_j}{h}\right\rangle^{-\mu} \le Ch^{\mu-1}. \end{aligned} \tag{6.6}$$

The smoothness of the wave operator, that $\langle x\rangle^N W_\pm \langle x\rangle^{-N-\delta}$ for $\delta > 0$ (*see* [10]-Section 4.6), and the above estimates yield the uniform boundedness of (6.3) in $\mathcal{L}(L^2(\mathbb{R}^d))$ as soon as $N_0 > \mu$.

Next we prove the boundedness of (6.4). By (2.3), we know that $W_+\chi_\xi(H_0)\tilde{p}_+^W(x,D)$ belongs to $\mathrm{Op}S(1,g_1)$. We introduce a cut-off $\chi_x' \in \mathcal{C}_0^\infty(2B_{x,E,\alpha})$ so that $\chi_x' \equiv 1$ on $\mathrm{supp}\chi_x$. Pseudo-differential calculus in $S(1,g_1)$ yields the boundedness of

$$A\chi_x(hx) - \chi_x'(hx)A\chi_x(hx),$$

in $\mathrm{Op}S(\langle x\rangle^{-\infty}, g_1)$ for $A = \chi_\xi(H_0)\tilde{p}_+^W(x,D)$ or $A = W_+\chi_\xi(H_0)\tilde{p}_+^W(x,D)$. Then by referring again to (6.5) (6.6) the problem is reduced to estimating

$$h^{-1}\Sigma(x;h)\chi_x'(hx),$$

and

$$\begin{aligned} &\left[h^{-1}(\chi'V)(hx), W_+\chi_\xi(H_0)\tilde{p}_+^W(x,D)\chi(hx)\right] \\ &\quad - W_+\left[h^{-1}(\chi'V)(hx), \chi_\xi(H_0)\tilde{p}_+^W(x,D)\chi(hx)\right]. \end{aligned}$$

For the first operator we have

$$\left|\frac{1}{h}\Sigma(x;h)\chi_x'(hx)\right| \le C\frac{1}{h}\sum_{j\neq 0}\left\langle\frac{hx-x_j}{h}\right\rangle^{-\mu}\chi_x'(hx) \le C\frac{1}{h}\sum_{j\neq 0}\left\langle\frac{C_0\langle x_j\rangle}{h}\right\rangle^{-\mu} \le Ch^{\mu-1},$$

where we used condition (6.1). By noting the uniform boundedness of $h^{-1}(\chi_x'V)(hx)$ in $S(\langle x\rangle, g_1)$, the estimate of the second term comes again from pseudo-differential calculus. This ensures that the $\mathcal{L}(L^2(\mathbb{R}^d))$-norm of (6.4) is also an $O_{\psi_+}(1)$ and the proof is complete. □

7. Applications

Our results are not realy satisfactory from one point of view: The asymptotic evolution described in Theorem 1.1 is not well posed in terms of semi-classical measures, even after a second microlocalisation if we refer to Proposition B.2 c). We recall that the commutation relation $SH_0 = H_0 S$ yields the natural decomposition $\hat{S} = \int_{(0,\infty)}^{\oplus} S(\lambda)d\lambda$ where $S(\lambda)$ belongs to $\mathcal{L}(L^2(S^{d-1}))$. Under the short range assumption Hypothesis 1.1 a), $S(\lambda)$ is continuous with respect to λ. If we follow the normalization of [22], it writes $\mathrm{Id} - 2\pi i(2\lambda)^{\frac{d-2}{2}}T(\lambda)$ with $T(\lambda)$ compact. Thus the relation $\psi_+ = \hat{S}\psi_-$ gives

$$\psi_+(\xi) = \psi_-(\xi) - 2\pi i|\xi|^{d-2}\int_{S^{d-1}} T\left(\frac{|\xi|^2}{2}, \omega, \omega'\right)\psi_-(|\xi|\omega')d\omega'.$$

As an example if we multiply ψ_- by a phase and set $\psi'_-(\xi) = e^{ig(\xi)}\psi_-(\xi)$ with g real-valued, we do not change the modulus $|\psi'_-(\xi)| = |\psi_-(\xi)|$ and the incoming semi-classical measures are the same. Meanwhile, for $\psi'_+ = \hat{S}\psi'_-$, we generally obtain $|\psi'_+(\xi)| \neq |\psi_+(\xi)|$ even in dimension $d = 1$. Hence the outgoing semi-classical measure cannot be expressed as a function of the incoming one. We shall see in the first paragraph that this problem is solved by introducing another asymptotics in which the scattering cross sections proportional to $|T(\frac{|\xi|^2}{2}, \omega, \omega')|^2$ arise as the only significant parameters. This provides a dynamical approach to the scattering into cones problem already studied by several authors ([2], [12], [29]) via stationary theory. In the second paragraph, we reformulate our results in dimension $d = 1$ and give sketch of a link with linear Boltzmann equations.

In this section we consider semi-classical measures associated with bounded sequences of trace-class operators which are mixed states constructed as projection-valued Bochner integrals. If (M, ϱ) is a measured space, we call $L^1(M, \mathcal{J}_1)$ the space of Bochner integrable $\mathcal{J}_1$-valued functions. Since $\mathcal{J}_1$ is a separable Banach space, a function $P(m)$ is Bochner integrable if and only if it is weakly measurable and $\|P(m)\|_{\mathcal{J}_1} \in L^1(M)$ (*see* [31]). For $\mathcal{M}_b(T^*\mathbb{R}^d)$, the situation is different because it is neither separable as a Banach space nor a Banach space when endowed with its weak* topology. We say that an $\mathcal{M}_b(T^*\mathbb{R}^d)$-valued function $\mu(m)$, $m \in M$, is weak* integrable if it is weak* measurable, that is $\int_{T^*\mathbb{R}^d} a(x,\xi)d\mu(x,\xi;m)$ is measurable for any $a \in \mathcal{C}_0(T^*\mathbb{R}^d)$, and $\|\mu(m)\|_{\mathcal{M}_b} \in L^1(M)$. Then we can define the weak* integral $\int_M \mu(m)d\varrho(m)$ in $\mathcal{M}_b(T^*\mathbb{R}^d)$ by

$$\int_{T^*\mathbb{R}^d} a(x,\xi)d\left[\int_M \mu(m)d\varrho(m)\right](x,\xi) = \int_M \left[\int_{T^*\mathbb{R}^d} a(x,\xi)d\mu(x,\xi;m)\right]d\varrho(m),$$

$$\forall a \in \mathcal{C}_0(T^*\mathbb{R}^d),$$

for the right-hand side is defined for any $a \in \mathcal{C}_0(T^*\mathbb{R}^d)$ and estimated by

$$\left[\int_M \|\mu(m)\|_{\mathcal{M}_b} d\varrho(m)\right]\|a\|_{L^\infty}.$$

Note that a function $\mu(m)$ is weak* measurable if and only if $\int_{T^*\mathbb{R}^d} a(x,\xi)d\mu(x,\xi;m)$ is measurable for any $a \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d)$ because $\mathcal{C}_0^\infty(T^*\mathbb{R}^d)$ is sequentially dense in $\mathcal{C}_0(T^*\mathbb{R}^d)$. Moreover the integral of a weak* integrable function is completely defined by its values on $\mathcal{C}_0^\infty(T^*\mathbb{R}^d)$.

LEMMA 7.1. – *Let $(P(m;h))_{h\in(0,h_0)}$ be a sequence in $L^1(M,\mathcal{J}_1)$ so that, for ϱ-almost every m, $\|P(m;h)\|_{\mathcal{J}_1} \leq g(m)$ and $\mathcal{M}(P(m;h),h) = \{\mu(m)\}$, with $g \in L^1(M)$. Then the sequence of trace-class operators $\left(\int_M P(m;h)dm\right)_{h\in(0,h_0)}$ admits as unique semi-classical measure $\int_M \mu(m)dm$,*

$$\mathcal{M}\left(\int_M P(m;h)dm, h\right) = \left\{\int_M \mu(m)dm\right\}.$$

Proof. – For $a \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d)$, we have

$$\int_{T^*\mathbb{R}^d} a(x,\xi)d\mu(x,\xi;m) = \lim_{h\to 0} \mathrm{Tr}[P(m;h)a^W(x,hD)],$$

for ϱ-almost every m while $\|\mu(m)\|_{\mathcal{M}_b} \leq \overline{\lim_{h\to 0}} \|P(m;h)\|_{\mathcal{J}_1} \leq g(m)$. Thus $\mu(m)$ is weak* integrable. Moreover for $h > 0$, the operator $a^W(x,hD)$ belongs to $\mathcal{L}(L^2(\mathbb{R}^d)) = \mathcal{J}_1{}^*$ and we have

$$\mathrm{Tr}\left[\left(\int_M P(m;h)dm\right)a^W(x,hD)\right] = \int_M \mathrm{Tr}[P(m;h)a^W(x,hD)]dm.$$

We conclude by Lebesgue's Theorem.

7.1. Scattering into cones

In this paragraph we forget the positions x_j and the potentials U_j for $j \neq 0$ and we consider the d-dimensional case, $d > 1$. Further we need a stronger version of Hypothesis 1.1 a)

HYPOTHESIS 8.1. – $\mu > d$,
which ensures according to [22] the continuity of the kernel $T(\lambda,\omega,\omega')$ with respect to (λ,ω,ω'), $\lambda \neq 0$.

We follow the idea of Thirring in [29] who considers instead of a pure state a properly chosen mixed state which describes a beam of particles with a momentum distribution concentrated around a fixed $\xi_0 \neq 0$ and widely spread orthogonally to ξ_0 in the quantum scale. We focus the momentum around ξ_0 by introducing another small parameter ε while replacing ψ_- by a function of the form $\frac{1}{\varepsilon^{d/4}}\Psi(\frac{\xi-\xi_0}{\varepsilon^{1/2}})$, with $\Psi \in \mathcal{C}_0^\infty(\mathbb{R}^d \setminus \{0\})$, $\|\Psi\|_{L^2} = (2\pi)^{d/2}$. The mixed state is constructed by superposing projections on broadly translated copies of this wave function. We take

$$P(\varepsilon) = \int_{\{\xi_0\}^\perp} \chi(m)P(m;\varepsilon)dm$$

where $P(m;\varepsilon)$ is the orthogonal projection on $W_-F^{-1}[e^{-i\frac{m.\xi}{\varepsilon}}\frac{1}{\varepsilon^{d/4}}\Psi(\frac{\xi-\xi_0}{\varepsilon^{1/2}})]$ and where $\chi\in\mathcal{C}_0^\infty(\{\xi_0\}^\perp)$, $\chi\equiv 1$ in a neighbourhood of $m=0$. In order to keep a state from the C^*-algebras point of view (*see* [7], [11]), we may assume $\chi\geq 0$ and $\int_{\{\xi_0\}^\perp}\chi(m)dm=1$. By conjugating with dilations, we define

$$P(\varepsilon,h)=D_hP(\varepsilon)D_h^*=\int_{\{\xi_0\}^\perp}\chi(m)D_hP(m;\varepsilon)D_h^*dm,$$

where $D_hP(m;\varepsilon)D_h^*$ is the orthogonal projection on

$$D_hW_-F^{-1}\left[e^{-i\frac{m.\xi}{\varepsilon}}\frac{1}{\varepsilon^{d/4}}\Psi\left(\frac{\xi-\xi_0}{\varepsilon^{1/2}}\right)\right].$$

Since Ψ is compactly supported in $\mathbb{R}^d\backslash\{0\}$, the assumptions of Theorem 1.1 are satisfied for all the concerned pure states, for some T_+ and T_- which essentially depend on the trajectory passing through $(0,\xi_0)$. By Lemma 7.1, we can calculate for $t\in(-T_-,0)\cup(0,T_+)$ and for any fixed $\varepsilon>0$ the semi-classical measure of

$$P(t;\varepsilon,h)=e^{-i\frac{t}{h}H^h}P(\varepsilon,h)e^{i\frac{t}{h}H^h}=\int_{\{\xi_0\}^\perp}\chi(m)e^{-i\frac{t}{h}H^h}D_hP(m;\varepsilon)D_h^*e^{i\frac{t}{h}H^h}dm.$$

It is equal to the weak* integral

$$\begin{aligned}(7.1)\qquad \mu(t,\varepsilon)&=\int_{\{\xi_0\}^\perp}\chi(m)\Phi_V(t)_*\left[(2\pi)^{-d}\delta_{x=0}\frac{1}{\varepsilon^{d/2}}\left|\Psi\left(\frac{\xi-\xi_0}{\varepsilon^{1/2}}\right)\right|^2\right]dm\\ &=\Phi_V(t)_*\left[(2\pi)^{-d}\delta_{x=0}\frac{1}{\varepsilon^{d/2}}\left|\Psi\left(\frac{\xi-\xi_0}{\varepsilon^{1/2}}\right)\right|^2\right],\end{aligned}$$

when $t\in(-T_-,0)$ and to

$$\mu(t,\varepsilon)=\int_{\{\xi_0\}^\perp}\chi(m)\Phi_V(t)_*\left[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi;m,\varepsilon)|^2\right]dm$$

when $t\in(0,T_+)$, with $\psi_+(m,\varepsilon)=\hat{S}[e^{-i\frac{m.\xi}{\varepsilon}}\frac{1}{\varepsilon^{d/4}}\Psi(\frac{\cdot-\xi_0}{\varepsilon^{1/2}})]$. Since the transformation Φ_V is smooth with jacobian 1, its action on bounded measures commutes with weak* integration and we get

$$(7.2)\quad \mu(t,\varepsilon)=\Phi_V(t)_*\left[\int_{\{\xi_0\}^\perp}\chi(m)\left[(2\pi)^{-d}\delta_{x=0}|\psi_+(\xi;m,\varepsilon)|^2\right]dm\right],\qquad t\in(0,T_+).$$

The next proposition details the asymptotic behaviour of $\mu(t,\varepsilon)$ in the weak* topology as $\varepsilon\to 0$.

PROPOSITION 7.2. – *For any $t\in(-T_-,0)\cup(0,T_+)$, the semi-classical measure $\mu(t,\varepsilon)$ satisfies*

$$(7.3)\qquad w^*-\lim_{\varepsilon\to 0}\mu(t,\varepsilon)=\Phi_V(t)_*[\delta_{x=0}\delta_{\xi=\xi_0}]=\delta_{\Phi_V(0,\xi_0;t)}.$$

More precisely, if $\mathcal{T}_{\xi_0}$ *denotes the compact phase-space trajectory* $\bigcup_{t\in[-T_-,T_+]} \Phi_V(0,\xi_0;t)$ *and if* $a \in \mathcal{C}_0(T^*\mathbb{R}^d)$ *with* supp $a \cap \mathcal{T}_{\xi_0} = \emptyset$ *then*

$$\int_{T^*\mathbb{R}^d} a d\mu(t,\varepsilon) = o_{a,t}(\varepsilon^\infty), \qquad \forall t \in (-T_-,0), \tag{7.4}$$

and

$$\begin{aligned}\int_{T^*\mathbb{R}^d} a d\mu(t,\varepsilon) &= \varepsilon^{d-1}\int_{T^*\mathbb{R}^d} a d\left[\Phi_V(t)_*\left[\delta_{x=0}\frac{(2\pi)^{d+1}}{|\xi_0|}\left|T\left(\frac{|\xi_0|^2}{2},\frac{\xi}{|\xi|},\frac{\xi_0}{|\xi_0|}\right)\right|^2\delta\left(\frac{|\xi|^2}{2}-\frac{|\xi_0|^2}{2}\right)\right]\right]\\ &\quad + o_{a,t}(\varepsilon^{d-1}), \qquad \forall t\in(0,T_+).\end{aligned}\tag{7.5}$$

Remark 7.3. – a) The limit (7.3) corresponds to the fact well-known by physicists that scattering cannot be observed along the trajectory of the incident beam. Scattering phenomena are marginal effects only detectable in the other directions, which is the meaning of (7.4) (7.5). Detailed description of scattering experiments may be found in [8] [24]. In the stationary approach, this aspect is contained in the compactness of the T-matrix [10] [22] or in the decay at infinity of the spherical waves in the Sommerfeld's decomposition of scattered plane waves (*see* [27]).

b) As this was done in [26], equality (7.5) allows to derive the expression of scattering cross section from their exact physical definition. The ε^{d-1} factor cancels with the incident current density $= O(\varepsilon^{d-1})$. The exact value of the scattering cross section is then $(2\pi)^{d+1}|\xi|^{d-3}|T(\frac{|\xi|^2}{2},\omega,\omega')|^2$ in agreement with [24].

Proof. – The results for $t<0$ are straightforward consequences of the compact support of Ψ. For $t>0$, it actually suffices to study the weak* limit of $\mu(0^+,\varepsilon)-\mu(0^-,\varepsilon)$ or as an equivalent of its projection on $\mathbb{R}^d_\xi$,

$$\int_{\{\xi_0\}^\perp}\chi(m)\left[|\psi_+(\xi;m,\varepsilon)|^2-\frac{1}{\varepsilon^{d/2}}\left|\Psi\left(\frac{\xi-\xi_0}{\varepsilon^{1/2}}\right)\right|^2\right]dm. \tag{7.6}$$

The function $\psi_+(m,\varepsilon)$ is given by

$$\begin{aligned}\psi_+(\xi;m,\varepsilon) =& e^{-i\frac{m.\xi}{\varepsilon}}\frac{1}{\varepsilon^{d/4}}\Psi\left(\frac{\xi-\xi_0}{\varepsilon^{1/2}}\right)\\ &-2\pi i\int_{\mathbb{R}^d}T\left(\frac{|\xi|^2}{2},\frac{\xi}{|\xi|},\frac{\xi'}{|\xi'|}\right)e^{-i\frac{m.\xi'}{\varepsilon}}\frac{1}{\varepsilon^{d/4}}\Psi\left(\frac{\xi'-\xi_0}{\varepsilon^{1/2}}\right)\delta\left(\frac{|\xi'|^2}{2}-\frac{|\xi|^2}{2}\right)d\xi',\end{aligned}$$

and its modulus satisfies

$$(7.7)\qquad |\psi_+(\xi;m,\varepsilon)|^2-\frac{1}{\varepsilon^{d/2}}\left|\Psi\left(\frac{\xi-\xi_0}{\varepsilon^{1/2}}\right)\right|^2$$
$$=2\mathbb{R}e\Big[-2\pi i\int_{\mathbb{R}^d}T\left(\frac{|\xi|^2}{2},\frac{\xi}{|\xi|},\frac{\xi'}{|\xi'|}\right)$$
$$\times e^{-i\frac{m.(\xi'-\xi)}{\varepsilon}}\frac{1}{\varepsilon^{d/2}}\Psi\left(\frac{\xi'-\xi_0}{\varepsilon^{1/2}}\right)\overline{\Psi}\left(\frac{\xi-\xi_0}{\varepsilon^{1/2}}\right)\delta\left(\frac{|\xi'|^2}{2}-\frac{|\xi|^2}{2}\right)d\xi'\Big]$$
$$+4\pi^2\int_{\mathbb{R}^{2d}}T\left(\frac{|\xi|^2}{2},\frac{\xi}{|\xi|},\frac{\xi'}{|\xi'|}\right)\overline{T}\left(\frac{|\xi|^2}{2},\frac{\xi}{|\xi|},\frac{\xi''}{|\xi''|}\right)$$
$$\times e^{-i\frac{m.(\xi'-\xi'')}{\varepsilon}}\frac{1}{\varepsilon^{d/2}}\Psi\left(\frac{\xi'-\xi_0}{\varepsilon^{1/2}}\right)\overline{\Psi}\left(\frac{\xi''-\xi_0}{\varepsilon^{1/2}}\right)$$
$$\delta\left(\frac{|\xi'|^2}{2}-\frac{|\xi|^2}{2}\right)\delta\left(\frac{|\xi''|^2}{2}-\frac{|\xi|^2}{2}\right)d\xi'd\xi''.$$

Next we calculate the action of the measure (7.6) on a test function $f\in\mathcal{C}_0(\mathbb{R}^d)$, which may be supposed compactly supported. The validity of the next calculations relies on Fubini's Theorem for compactly supported distributions. The first term of (7.7) provides the real part of

$$-4\pi i\int_{\mathbb{R}^{2d}}\hat{\chi}\left(\pi_{\{\xi_0\}^\perp}\left(\frac{\xi'-\xi}{\varepsilon}\right)\right)T\left(\frac{|\xi|^2}{2},\frac{\xi}{|\xi|},\frac{\xi'}{|\xi'|}\right)\frac{1}{\varepsilon^{d/2}}\Psi\left(\frac{\xi'-\xi_0}{\varepsilon^{1/2}}\right)\overline{\Psi}\left(\frac{\xi-\xi_0}{\varepsilon^{1/2}}\right)$$
$$\delta\left(\frac{|\xi'|}{2}-\frac{|\xi|}{2}\right)f(\xi)d\xi'd\xi,$$

where $\pi_{\{\xi_0\}^\perp}$ is the orthogonal projection on $\{\xi_0\}^\perp$. After the change of variables $u=\frac{\xi'-\xi}{\varepsilon}$, $v=\frac{1}{\varepsilon^{1/2}}(\frac{\xi+\xi'}{2}-\xi_0)$, we get

$$-4\pi i\int_{\mathbb{R}^{2d}}\hat{\chi}(\pi_{\{\xi_0\}^\perp}u)T\left(\frac{|\xi_0+\varepsilon^{1/2}v-\varepsilon u/2|^2}{2},\frac{\xi_0+\varepsilon^{1/2}v-\varepsilon u/2}{|\xi_0+\varepsilon^{1/2}v-\varepsilon u/2|},\frac{\xi_0+\varepsilon^{1/2}v+\varepsilon u/2}{|\xi_0+\varepsilon^{1/2}v+\varepsilon u/2|}\right)$$
$$\Psi(v+\varepsilon^{1/2}u/2)\overline{\Psi}(v-\varepsilon^{1/2}u/2)\varepsilon^d\delta(\varepsilon u.(\varepsilon^{1/2}v+\xi_0))$$
$$f(\xi_0+\varepsilon^{1/2}v-\varepsilon u/2)dudv.$$

Since the T-matrix is continuous by Hypothesis 8.1 and since $\int_{\{\xi_0\}^\perp}\hat{\chi}(u)du=(2\pi)^{d-1}$ the first term of (7.6) equals

$$(7.8)\qquad \varepsilon^{d-1}\frac{2(2\pi)^d}{|\xi_0|}\mathrm{Im}T\left(\frac{|\xi_0|^2}{2},\frac{\xi_0}{|\xi_0|},\frac{\xi_0}{|\xi_0|}\right)f(\xi_0)+o_f(\varepsilon^{d-1}).$$

The second term is derived from the second term of (7.7) and equals after the change of variables $u=\frac{\xi'-\xi''}{\varepsilon}$, $v=\frac{1}{\varepsilon^{1/2}}(\frac{\xi'+\xi''}{2}-\xi_0)$,

$$4\pi^2\int_{\mathbb{R}^{3d}}\hat{\chi}(\pi_{\{\xi_0\}^\perp}u)T\left(\frac{|\xi|^2}{2},\frac{\xi}{|\xi|},\frac{\xi_0+\varepsilon^{1/2}v+\varepsilon u/2}{|\xi_0+\varepsilon^{1/2}v+\varepsilon u/2|}\right)\overline{T}\left(\frac{|\xi|^2}{2},\frac{\xi}{|\xi|},\frac{\xi_0+\varepsilon^{1/2}v-\varepsilon u/2}{|\xi_0+\varepsilon^{1/2}v-\varepsilon u/2|}\right)$$
$$\Psi(v+\varepsilon^{1/2}u/2)\overline{\Psi}(v-\varepsilon^{1/2}u/2)\varepsilon^d\delta(\varepsilon u.(\varepsilon^{1/2}v+\xi_0))$$
$$\delta\left(\frac{|\xi_0+\varepsilon^{1/2}v-\varepsilon u/2|^2}{2}-\frac{|\xi|^2}{2}\right)f(\xi)dudvd\xi.$$

We refer again to the continuity of the T-matrix and get

$$(7.9)\qquad \varepsilon^{d-1}\int_{\mathbb{R}^d}\frac{(2\pi)^{d+1}}{|\xi_0|}\left|T\left(\frac{|\xi_0|^2}{2},\frac{\xi}{|\xi|},\frac{\xi_0}{|\xi_0|}\right)\right|^2\delta\left(\frac{|\xi|^2}{2}-\frac{|\xi_0|^2}{2}\right)f(\xi)d\xi\ +o_f(\varepsilon^{d-1}).$$

By adding (7.8) and (7.9), we check that

$$w^*-\lim_{\varepsilon\to 0}\mu(0^+,\varepsilon)-\mu(0^-,\varepsilon)=0,$$

which yields (7.3) for $t>0$. If we take a test function $f(\xi)$ such that $\xi_0\notin \operatorname{supp} f$, then the contribution of $\mu(0^-,\varepsilon)$ and of (7.8) vanishes while (7.9) leads to (7.5). □

7.2. Towards a linear Boltzmann equation

In dimension $d=1$, the T-matrix written as $(T(\xi,\xi),T(\xi,-\xi))$ is continuous with respect to $\xi\in\mathbb{R}\setminus\{0\}$ under Hypothesis 1.1 a). The relation $\psi_+=\hat{S}\psi_-$ reads

$$\begin{aligned}\psi_+(\xi)&=\psi_-(\xi)-\frac{2\pi i}{|\xi|}[T(\xi,\xi)\psi_-(\xi)+T(\xi,-\xi)\psi_-(-\xi)]\\&=\left(1-\frac{2\pi i}{|\xi|}T(\xi,\xi)\right)\psi_-(\xi)-\frac{2\pi i}{|\xi|}T(\xi,-\xi)\psi_-(-\xi).\end{aligned}$$

By taking into account the unitarity relation $-2\pi i(T-T^*)+4\pi^2TT^*=0$ and by introducing like in [9] [26] the reflection coefficient $R(\xi)=-\frac{2\pi i}{|\xi|}T(-\xi,\xi)$, we obtain

$$\begin{aligned}|\psi_+(\xi)|^2=&(1-|R(\xi)|^2)|\psi_-(\xi)|^2+|R(-\xi)|^2|\psi_-(-\xi)|^2\\&+2\mathbb{R}e\left[(1-\frac{2\pi i}{|\xi|}T(\xi,\xi))\frac{2\pi i}{|\xi|}\overline{T}(\xi,-\xi)\psi_-(\xi)\overline{\psi_-}(-\xi)\right].\end{aligned}$$

The outgoing semi-classical measure cannot generally be expressed in terms of the incoming one. Nevertheless if ψ_- is supported in $\xi>0$ or in $\xi<0$, we get the physically relevant expression

$$|\psi_+(\xi)|^2=(1-|R(\xi)|^2)|\psi_-(\xi)|^2+|R(-\xi)|^2|\psi_-(-\xi)|^2.$$

Now we consider the case with at most countable positions x_j and quantum potentials U_j, $j\in\mathbb{Z}$, which satisfy Hypothesis 1.1 a). We may assume $x_j<x_{j+1}$ and the finite case is described by taking $x_j=\pm\infty$ and $U_j\equiv 0$ for $j\gtrless\pm N_\pm$, for some $N_\pm\in\mathbb{N}$. With every U_j, $j\in\mathbb{Z}$, we associate the T-matrix T_j and the reflection coefficients $R_j(\xi)$. For every position x_j, $j\in\mathbb{Z}$, we introduce the "flow" $\check{\Phi}_V^j$, derived from Φ_V by changing the sign of the velocity each time that the trajectory crosses $T^*_{x_j}\mathbb{R}$. We also define the functions τ_j and ξ_j on $T^*\mathbb{R}^d$ by

$$\tau_j(x,\xi)=\operatorname{Sup}\{t\in(-\infty,0],\ \Phi_V(x,\xi;t)\in T^*_{x_j}\mathbb{R}\},$$

and

$$(x_j,\xi_j(x,\xi))=\Phi_V(x,\xi;\tau_j(x,\xi)),$$

with the conventions $\tau_j(x,\xi)=-\infty$ and $\xi_j(x,\xi)=0$ when $\{t\in(-\infty,0],\ \Phi_V(x,\xi;t)\in T^*_{x_j}\mathbb{R}\}$ is empty. The next Proposition shows that for some h-dependent mixed states P^h, the semi-classical measure of the sequence $(e^{-i\frac{t}{h}H^h}P^h e^{i\frac{t}{h}H^h})$ solves an evolution equation which looks like a linear Boltzmann equation.

PROPOSITION 7.4. – *Let* $g \in L^1(T^*\mathbb{R})$, $g \geq 0$, *be such that*

$$\Phi_V(t-s)\left[\Phi_V(s)\text{supp } g \cap T^*_{x_i}\mathbb{R}\right] \cap (\bigcup_{j\in\mathbb{Z}} T^*_{x_j}\mathbb{R}) = \emptyset, \quad \forall i \in \mathbb{Z}, \quad \forall t,s \in [0,T], \quad t > s. \tag{7.10}$$

Then there exists a bounded sequence of trace-class operators $(P^h)_{h\in(0,h_0)}$ *so that*

$$\mathcal{M}\left(e^{-i\frac{t}{h}H^h}P^h e^{i\frac{t}{h}H^h}, h\right) = \{f(t)\}, \quad \forall t \in [0,T), \\ f(t) = \Phi_V(t)_* g + \sum_{j\in\mathbb{Z}} 1_{(-t,0)}(\tau_j)\left[|R_j(-\xi_j)|^2 \check{\Phi}^j_V(t)_* g - |R_j(\xi_j)|^2 \Phi_V(t)_* g\right]. \tag{7.11}$$

Moreover if g *is continuous on* $T^*\mathbb{R}$, *the function* $f(t)$ *is piecewise continuous and solves in* $\mathcal{D}'(T^*\mathbb{R})$ *the equation*

$$\begin{cases} \partial_t f + \xi.\partial_x f - \partial_x V.\partial_\xi f \\ \quad = \sum_{j\in\mathbb{Z}} \delta_{x_j}(x) \int_{\mathbb{R}} [\sigma_j(\xi,\xi')f_j^-(\xi',t) \\ \qquad\qquad - \sigma_j(\xi',\xi)f_j^-(\xi,t)]\delta\left(\frac{|\xi'|^2}{2} - \frac{|\xi|^2}{2}\right)d\xi', \\ f_{t=0} = g, \end{cases} \tag{7.12}$$

where $f_j^-(\xi,t) = \lim_{\substack{(x,\eta)\to(x_j,\xi) \\ (x-x_j).\eta<0}} f(x,\eta;t)$ *and* $\sigma_j(\xi',\xi) = 4\pi^2|T_j(\xi',\xi)|^2$.

Proof. – We split the initial data g into several parts. For $j \in \mathbb{Z}$, we set $g_j = g|_{x_{j-1}<x<x_j}$ and we define

$$\Gamma_{j,+} = \text{supp } g_j \cap (\bigcup_{s\in(0,T)} \Phi_V(-s)T^*_{x_j}\mathbb{R}),$$

$$\Gamma_{j,-} = \text{supp } g_j \cap (\bigcup_{s\in(0,T)} \Phi_V(-s)T^*_{x_{j-1}}\mathbb{R}),$$

and

$$g_{j,+} = g_j|_{\Gamma_{j,+}}, \qquad g_{j,-} = g_j|_{\Gamma_{j,-}}, \qquad g_{j,0} = g_j - g_{j,+} - g_{j,-}.$$

With $g_{j,0}$ we associate the h-dependent trace-class operator $\gamma^h_{j,0}$ defined for $h > 0$ as the Bochner integral $\gamma^h_{j,0} = \int_{T^*\mathbb{R}} g_{j,0}(x,\xi)\pi^h_{x,\xi}dxd\xi$, where $\pi^h_{x_0,\xi_0}$ is the orthogonal projection on some h-dependent wave function with semi-classical measure $\delta_{x=x_0,\xi=\xi_0}$. For almost every $(x,\xi) \in$ supp $g_{j,0}$ the trajectory $\bigcup_{t\in[0,T]} \Phi_V(x,\xi;t)$ remains at a finite distance of $\bigcup_{j\in\mathbb{Z}} T^*_{x_j}\mathbb{R}$ while the semi-classical measure of $\pi^h_{x,\xi}$ equals $\delta_{(x,\xi)}$. By the same argument as in the proof of Theorem 1.1 part b), one checks that the semi-classical measure of $e^{-i\frac{t}{h}H^h}\pi^h_{x,\xi}e^{i\frac{t}{h}H^h}$, $t\in[0,T)$ is $\Phi_V(t)_*\delta_{(x,\xi)}$ for almost every $(x,\xi)\in\operatorname{supp} g_{j,0}$. We refer to Lemma 7.1 and get

$$\mathcal{M}(e^{-i\frac{t}{h}H^h}\gamma^h_{j,0}e^{i\frac{t}{h}H^h},h)=\{\Phi_V(t)_*g_{j,0}\},\qquad \forall t\in[0,T).$$

On supp $g_{j,+}\subset T^*\mathbb{R}$ we take the coordinates $(s,\eta)\in(0,T)\times(0,+\infty)$ given by $(x,\xi)=\Phi_V(s)(x_j,\eta)$. The jacobian of the transformation $(s,\eta)\to(x,\xi)$ equals

$$\partial_s x\partial_\eta\xi-\partial_s\xi\partial_\eta x=\partial_\xi p_V\partial_\eta\xi+\partial_x p_V\partial_\eta x=\partial_\eta p_V=\eta.$$

If we set $g_{j,+}(x,\xi)=\tilde g_{j,+}(s,\eta)$ then $\tilde g_{j,+}\in L^1((0,T)\times(0,+\infty),\eta ds d\eta)$ with the same L^1-norm as $g_{j,+}$. By noting $L^1((0,T)\times(0,+\infty),\eta dsd\eta)=L^1((0,T),L^1((0,+\infty),\eta d\eta))$, we define for almost every $s\in(0,T)$ and $k\in\mathbb{Z}$ the L^2-functions

$$\psi_{j,+,-}(\eta;s,k)=1_{[2^k,2^{k+1}]}(\xi)\sqrt{2\pi\eta\tilde g_{j,+}(s,\eta)},$$

and

$$u^h_{j,+}(x;s,k)=h^{-1/2}(W_{-,j}F^{-1}\psi_{j,+,-})\left(\frac{x-x_j}{h}\right).$$

If $\pi^h_{j,+}(s,k)$ denotes the projection on $e^{i\frac{s}{h}H^h}u^h_{j,+}(s,k)$, then $\pi^h_{j,+}\in L^1((0,T)\times\mathbb{Z},\mathcal{J}_1)$ where the measure on $(0,T)\times\mathbb{Z}$ is the product of Lebesgue measure ds with the discrete measure δk. Indeed $\pi^h_{j,+}$ is weakly measurable while we have

$$\|\pi^h_{j,+}(s,k)\|_{\mathcal{J}_1}\le\|1_{[2^k,2^{k+1}]}(\eta)\eta\tilde g_{j,+}(s,\eta)\|_{L^1((0,+\infty))}.$$

Thus the Bochner integral $\gamma^h_{j,+}=\displaystyle\int_{(0,T)\times\mathbb{Z}}\pi^h_{j,+}(s,k)ds\delta k$ defines a bounded sequence of trace-class operators. For almost every (s,k), Theorem 1.1 applies by taking $T_-=s$ and $T_+=T-s$ and we have

$$\mathcal{M}(e^{-i\frac{t}{h}H^h}\pi^h_{j,+}(s,k)e^{i\frac{t}{h}H^h},h)=\{\mu^h_{j,+}(t;s,k)\},\qquad\forall t\in[0,T),$$

with

$$\mu^h_{j,+}(t;s,k)=\begin{cases}\Phi_V(t-s)_*\left[\delta_{x=x_j}1_{[2^k,2^{k+1}]}(\eta)\eta\tilde g_{j,+}(s,\eta)\right], & if\quad t<s,\\ \Phi_V(t-s)_*[\delta_{x=x_j}1_{[2^k,2^{k+1}]}(\eta)\eta[(1-|R_j(\eta)|^2)\tilde g_{j,+}(s,\eta) & \\ \qquad+|R_j(-\eta)|^2\tilde g_{j,+}(s,-\eta)]], & if\quad t>s.\end{cases}$$

Note that $\mu^h_{j,+}(0;s,k)$ writes $\delta_{s'=s}1_{[2^k,2^{k+1}]}(\eta)\tilde g_{j,+}(s,\eta)$ in the coordinates (s',η). Thus by Lemma 7.1, $g_{j,+}(x,\xi)=\tilde g_{j,+}(s',\eta)$ is the semi-classical measure of $\gamma^h_{j,+}$. For a general $t\in[0,T)$, the sequence $(e^{-i\frac{t}{h}H^h}\gamma^h_{j,+}e^{i\frac{t}{h}H^h})$ admits as unique semi-classical measure

$$\Phi_V(t)_*g_{j,+}+1_{(-t,0)}(\tau_j)[|R_j(-\xi_j)|^2\check\Phi^j_V(t)_*g_{j,+}-|R_j(\xi_j)|^2\Phi_V(t)_*g_{j,+}].$$

The treatment of $g_{j,-}$ is completely symmetric and we finally take $P^h=\sum_{j\in\mathbb{Z}}\gamma^h_{j,0}+\gamma^h_{j,+}+\gamma^h_{j,-}$. The expression (7.11) comes at once by linearity and L^1-estimates. For (7.12), we first notice that the function $f(x,\xi;t)$ defined by (7.11) solves the classical Liouville equation out of $\bigcup_{j\in\mathbb{Z}}T^*_{x_j}\mathbb{R}$. The right-hand side is directly related to the discontinuity on $T^*_{x_j}\mathbb{R}$. □

A. Pseudo-differential calculus

Pseudo-differential operators often appear with a kernel-symbol depending both on x and y. Estimates on the (x,ξ)-symbol can be generally derived for some class of splitted σ-temperate metrics. This is the object of the next lemma which has, as usual, a semi-classical counterpart.

LEMMA A.1. – *a) Let the σ-temperate metric g be splitted, $g_{x,\xi}(t_x,-t_\xi)=g_{x,\xi}(t_x,t_\xi)$, and let the weight m_2 be g-σ-temperate. Then the symbol*

$$(A.1)\qquad e^{iD_y.D_\eta}b(x,y,\xi,\eta)\Big|_{\substack{y=x\\ \eta=\xi}}=\sum_{k<N}\frac{(iD_y.D_\eta)^k}{k!}b(x,x,\xi,\xi)+R_N(b)(x,\xi),$$

belongs to $S(m_1m_2,g)$ and the remainder $R_N(b)\in S(\frac{m_1m_2}{\lambda^N},g)$ is a continuous function of $b\in S(m_1\otimes m_2,g\oplus g)$.

b) Assume further that the metric g writes $g_{x,\xi}(t_x,t_\xi)=\alpha_x(t_x)+\beta_{x,\xi}(t_\xi)$ and take the weights $m_1(x)$ and $m_2(x,\xi)$ so that m_2 and m_1m_2 are g-σ-temperate. Then the operator with kernel

$$A(x,y)=\int_{\mathbb{R}^d}e^{i(x-y).\xi}b(x,y,\xi)đ\xi,$$

belongs to $\mathrm{Op}S(m_1m_2,g)$ when $b\in S(m_1(x)m_2(y,\xi),g')$, with $g'_{x,y,\xi}(t_x,t_y,t_\xi)=\alpha_x(t_x)+\alpha_y(t_y)+\beta_{y,\xi}(t_\xi)$. Moreover the $(1,0)$-symbol $a(x,\xi)$ of A admits the expansion

$$(A.2)\qquad \begin{aligned}a(x,\xi)&=e^{iD_y.D_\xi}b(x,y,\xi)|_{y=x}\\&=\sum_{k<N}\frac{(iD_y.D_\xi)^k}{k!}b(x,x,\xi)+R_N(b)(x,\xi),\end{aligned}$$

where $R_N(b)\in S(\frac{m_1m_2}{\lambda^N},g)$ is a continuous function of $b\in S(m_1(x)m_2(y,\xi),g')$.

Proof. – a) The symbol (A.1) equals $c(x,x,\xi,\xi)$ with $c(x,y,\xi,\eta)=e^{iD_y.D_\eta}b(x,y,\xi,\eta)$. If $t^1_{x,\xi},\ldots,t^k_{x,\xi}\in T_{x,\xi}T^*\mathbb{R}^d$ with $g_{x,\xi}(t^i_{x,\xi})\le 1$ for $i=1\ldots k$ and if $b^{(k)}_{x,\xi}$ denotes the k-th derivative of b with respect to (x,ξ), then the symbol $m_1(x,\xi)^{-1}b^{(k)}_{x,\xi}(x,.,\xi,.)\cdot t^1_{x,\xi}\cdots t^k_{x,\xi}$ is bounded in $S(m_2,g)$ uniformly with respect to (x,ξ), $t^1_{x,\xi},\ldots,t^k_{x,\xi}$. Then, the splitting of the metric g ensures the uniform boundedness of $m_1(x,\xi)^{-1}c^{(k)}_{x,\xi}(x,.,\xi,.)\cdot t^1_{x,\xi}\cdots t^k_{x,\xi}$ in $S(m_2,g)$. Hence $c(x,y,\xi,\eta)\in S(m_1\otimes m_2,g\oplus g)$ which yields $c(x,x,\xi,\xi)\in S(m_1m_2,g)$. We conclude by referring to the usual expansion and estimates for $e^{iD_y.D_\xi}$ valid when the metric g is splitted.

b) The $(1,0)$-symbol $a(x,\xi)$ of A can be calculated as

$$a(x,\xi)=\int_{\mathbb{R}^d}e^{-i\xi.s}A(x,x-s)ds=\int_{\mathbb{R}^{2d}}e^{-i\eta.s}b(x,x+s,\xi+\eta)dsđ\eta,$$

and equals $c(x,x,\xi,\xi)$ with $c(x,y,\xi,\eta)=e^{iD_y.D_\eta}b(x,y,\eta)$. The assumptions on b and the metric imply $b(x,y,\eta)\in S(m_1\otimes m_2,g\oplus g)$ and part a) applies. □

Throughout this paper we use semi-classical Fourier integral operators

$$J^h(a,\varphi)(x,y) = \int_{\mathbb{R}^d} e^{\frac{i}{h}(\varphi(x,\eta)-y.\eta)} a(x,\eta)\frac{d\!\!\!{}^-\eta}{h^d}. \tag{A.4}$$

with $\varphi(x,\eta)$ only defined on $C_x \times C_\eta \subset T^*\mathbb{R}^d$, C_x and C_η open convex subsets of $\mathbb{R}^d$, and $a(x,\eta) \in S(1,g_0)$, supp $a \subset C_x \times C_\eta$. We further assume $\varphi \in \mathcal{C}^\infty(C_x \times C_\eta)$ and

$$|\partial_x^\alpha \partial_\eta^\beta \varphi(x,\eta)| \le C_{\alpha,\beta}, \qquad \forall (x,\eta) \in C_x \times C_\eta, \quad |\alpha| + |\beta| \ge 2, \tag{A.5}$$

$$|detM| \ge C_0 > 0, \qquad \forall M \in ch\{\partial^2_{x\eta}\varphi(x,\eta), (x,\eta) \in C_x \times C_\eta\} \tag{A.6}$$

where ch denotes the convex hull.

PROPOSITION A.2. – *a) For any pair of symbols, $a_i(h)$, $i = 1,2$, $h \in (0,h_0)$, uniformly bounded in $S(1,g_0)$ with* supp $a_i(h) \subset C_x \times C_\eta$, *the product $J^h(a_1(h),\varphi)J^h(a_2(h),\varphi)^*$ is an h-pseudo-differential operator. It equals*

$$J^h(a_1(h),\varphi)J^h(a_2(h),\varphi)^* = a_0^W(x,hD;h) + hr(x,hD;h), \tag{A.7}$$

where

$$a_0(x,\xi;h) = a_1(x,\eta(x,\xi);h)a_2(x,\eta(x,\xi);h)|\mathrm{det}\partial^2_{x,\eta}\varphi(x,\eta(x,\xi))|^{-1}, \tag{A.8}$$

$\xi \to \eta(x,\xi)$ is the inverse mapping of $\eta \to \xi(x,\eta) = \partial_x\varphi(x,\eta)$ and $r(x,\xi;h)$ is uniformly bounded in $S(1,g_0)$. As a consequence, $J^h(a_i(h),\varphi)$, $i = 1,2$, are uniformly bounded operators on $L^2(\mathbb{R}^d)$.

b) Assume that the symbols $a(h)$ and $b(h)$ are uniformly bounded in $S(1,g_0)$ with supp $a(h) \subset C_x \times C_\eta$ *and* supp $b(h) \subset C_x \times \mathbb{R}^d$. *Then the equality*

$$b^{(1,0)}(x,hD;h)J^h(a(h),\varphi) = J^h(c(h),\varphi), \tag{A.9}$$

holds for some $c(h)$ uniformly bounded in $S(1,g_0)$ with supp $c(h) \subset C_x \times C_\eta$. *Moreover $c(h)$ equals $c_0(h) + hc_1(h) + h^2r(h)$ where*

$$c_0(x,\eta;h) = b(x,\partial_x\varphi(x,\eta);h)a(x,\eta;h), \tag{A.10}$$

$$\begin{aligned} c_1(x,\eta;h) =& \frac{1}{i}\partial_\xi b(x,\partial_x\varphi(x,\eta);h)\partial_x a(x,\eta;h) \\ &+ \frac{1}{2i}\mathrm{Tr}[\partial_\xi^2 b(x,\partial_x\varphi(x,\eta);h)\partial_x^2\varphi(x,\eta)]a(x,\eta;h), \end{aligned} \tag{A.11}$$

and $r(h)$ is uniformly bounded in $S(1,g_0)$.

c) Assume that the symbols $a(h)$ and $b(h)$ are uniformly bounded in $S(1,g_0)$ with supp $a(h) \subset C_x \times C_\eta$ *and* supp $b(h) \subset \mathbb{R}^d \times C_\eta$. *Then the equality*

$$J^h(a(h),\varphi)b^{(1,0)}(x,hD;h) = J^h(d(h),\varphi), \tag{A.12}$$

holds for some $d(h)$ *uniformly bounded in* $S(1, g_0)$ *with* supp $d(h) \subset C_x \times C_\eta$. *Moreover* $d(h)$ *equals* $d_0(h) + hd_1(h) + h^2 r(h)$ *where*

$$(A.13) \qquad d_0(x, \eta; h) = a(x, \eta; h) b(\partial_\eta \varphi(x, \eta), \eta; h),$$

$$(A.14) \qquad d_1(x, \eta; h) = \frac{1}{i} \partial_\eta a(x, \eta; h) \partial_x b(\partial_\eta \varphi(x, \eta), \eta; h) + \frac{1}{2i} a(x, \eta; h) \mathrm{Tr}[\partial_x^2 b(\partial_\eta \varphi(x, \eta), \eta; h) \partial_\eta^2 \varphi(x, \eta)],$$

and $r(h)$ *is uniformly bounded in* $S(1, g_0)$.

Proof. – a) The kernel of $J^h(a_1(h), \varphi) J^h(a_2(h), \varphi)^*$ equals

$$K(x, y, h) = \int_{\mathbb{R}^d} e^{i \frac{\varphi(x,\eta) - \varphi(y,\eta)}{h}} a_1(x, \eta; h) a_2(y, \eta; h) \frac{d\eta}{h^d} = \int_{\mathbb{R}^d} e^{\frac{i}{h}(x-y).\xi} b(x, y, \xi; h) \frac{d\xi}{h^d},$$

with

$$b(x, y, \xi; h) = a_1(x, \eta(x, y, \xi); h) a_2(y, \eta(x, y, \xi); h) |\mathrm{det} \partial_\xi \eta(x, y, \xi)|.$$

By (A.6) the mapping: $\eta \in C_\eta \rightarrow \xi(x, y, \eta) = \int_0^1 \partial_x \varphi(tx + (1-t)y, \eta) dt$, $x, y \in C_x$, is a diffeomorphism and $\eta(x, y, \xi)$ actually denotes its inverse. We conclude by applying the semi-classical version of Lemma A.1.

b) The kernel of $b^{(1,0)}(x, hD; h) J^h(a(h), \varphi)$,

$$K(x, y; h) = \int_{\mathbb{R}^{3d}} e^{\frac{i}{h}(x-x').\xi} b(x, \xi; h) e^{\frac{i}{h}(\varphi(x', \eta) - y.\eta)} a(x', \eta; h) \frac{d\xi dx' d\eta}{h^{2d}},$$

is the same as the one of $J^h(c(h), \varphi)$ with $c(h)$ given by

$$c(x, \eta; h) = \int_{\mathbb{R}^{2d}} b(x, \xi; h) a(x', \eta; h) e^{-\frac{i}{h}(x'-x).(\xi - \int_0^1 \partial_x \varphi(tx + (1-t)x', \eta) dt)} \frac{d\xi}{h^d} dx' = e^{ihD_z.D_\zeta} b\left(x, \zeta + \int_0^1 \partial_x \varphi(x + (1-t)z, \eta) dt; h\right) a(x + z, \eta; h) \Big|_{\substack{z=0 \\ \zeta=0}}.$$

The first right-hand side shows that the support of $c(h)$ is contained in $C_x \times C_\eta$. Meanwhile the estimates in $S(1, g_0)$ and expansions are derived from the last line by referring again to Lemma A.1.

c) Conjugating with $D_h F$ and taking the adjoint interchanges the x and ξ variables and this part is reduced to the former one.

Finally we need some functional calculus.

LEMMA A.3. – *If the potential* U *belongs to* $S(\langle x \rangle^{-N}, \frac{dx^2}{\langle x \rangle^2})$, $N \geq 0$, *and* $\chi \in \mathcal{C}_0^\infty((0, \infty))$, *then* $\chi(H_U)$ *belongs to* $\mathrm{Op}S(\langle \xi \rangle^{-\infty}, g_1)$ *and we have*

$$(A.15) \qquad \chi(H_U) - \chi(H_0) \in \mathrm{Op}S(\langle \xi \rangle^{-\infty} \langle x \rangle^{-N}, g_1).$$

Proof. – Let us first prove that $\chi(H_U) - \chi(H_0) \in \mathrm{Op}S(\langle\xi\rangle^{-4}\langle x\rangle^{-N}, g_1)$. By Helffer-Sjöstrand functional calculus formula [ ] [ ] [ ] we have

$$\chi(H_U) - \chi(H_0) = \frac{i}{2\pi}\int_{\mathbb{C}}\int_0^1 \partial_{\bar z}\tilde\chi(z)A_{tU}^{-1}(z)\langle D\rangle^{-2}UA_{tU}(z)^{-1}\langle D\rangle^{-2}dz\wedge d\bar z,$$

where $A_{tU}(z)$ is the operator $\langle D\rangle^{-2}(z - H_0 - tU)$ and $\tilde\chi$ is a compactly supported almost analytic extension of χ. We know $A_{tU}(z) \in \mathrm{Op}S(1, g_1)$ with uniform estimates when $z \in \mathrm{supp}\ \tilde\chi$ and we want to check that the k^{th} semi-norm in $S(1, g_1)$ of $A_{tU}(z)^{-1}$ is an $O_k(|\mathrm{Im}z|^{-N(k)})$ for some $N(k)$. We shall use Beals criterion [5] and estimate the multi-commutators

$$\langle x\rangle^{|\beta|}ad_x^\alpha ad_D^\beta A_{tU}(z)^{-1} = \langle x\rangle^{|\beta|}\sum_{\substack{(\alpha_1,\beta_1)+\cdots+(\alpha_l,\beta_l)=(\alpha,\beta)\\ |(\alpha_1,\beta_1)|\neq 0}} C_{\alpha_i,\beta_i}A_{tU}(z)^{-1}ad_x^{\alpha_1}ad_D^{\beta_1}A_{tU}(z)$$
$$A_{tU}(z)^{-1}\dots ad_x^{\alpha_l}ad_D^{\beta_l}A_{tU}(z)A_{tU}(z)^{-1}. \tag{A.16}$$

By taking $\beta = 0$ one readily gets $\|ad_x^\alpha A_{tU}(z)^{-1}\|_{\mathcal{L}(L^2)} = O_\alpha(|\mathrm{Im}z|^{N(\alpha)})$ from standard resolvent estimates. We notice the identity $x^n. = \sum_{p=0}^{n} C_n^p(ad_x^p.)x^{n-p}$ and we obtain

$$\|\langle x\rangle^n A_{tU}(z)^{-1}\langle x\rangle^{-n}\|_{\mathcal{L}(L^2)} \le C_\alpha|\mathrm{Im}z|^{N(n)},$$

which inserted in (A.16) provides the general estimate

$$\|ad_x^\alpha ad_D^\beta A_{tU}(z)^{-1}\|_{\mathcal{L}(L^2)} \le C_\alpha|\mathrm{Im}z|^{N(\alpha,\beta)}.$$

Finally we improve the power of $\langle\xi\rangle$ by writing

$$\chi(H_U) - \chi(H_0) = [\chi(H_U) - \chi(H_0)]\chi'(H_U) + \chi(H_0)[\chi'(H_U) - \chi'(H_0)],$$

for some $\chi' \in \mathcal{C}_0^\infty((0,\infty))$, $\chi' \equiv 1$ on supp χ. □

B. 2-microlocal measures

Throughout this paragraph, we identify the manifold $X = (T^*\mathbb{R}^d\backslash T_0^*\mathbb{R}^d)\cup S_{T_0^*\mathbb{R}^d}(T^*\mathbb{R}^d)$, endowed with its natural blow-up topology, with $[0,+\infty)\times S^{d-1}\times\mathbb{R}^d$ by $(x = r\theta, \xi) \leftrightarrow (r, \theta, \xi)$.

LEMMA B.1. – *Out of any bounded sequence (u^h) in $L^2(\mathbb{R}^d)$, one can extract a subsequence $(u^{h'})$ such that $D_{h'}^* u^{h'}$ converges weakly in $L^2(\mathbb{R}^d)$, $D_{h'}^* u^{h'} \overset{h'\to 0}{\rightharpoonup} v$, and find a non-negative measure $\mu \in \mathcal{M}_b(X)$ so that*

$$\lim_{h'\to 0}(u^{h'} - D_{h'}v, a^W(x, h'D)(u^{h'} - D_{h'}v)) = \int_X a(r,\theta,\xi)d\mu(r,\theta,\xi), \quad \forall a \in \mathcal{C}_0^\infty(X). \tag{B.1}$$

Notation

The set of all 2-microlocal measures, $\mu(r,\theta,\xi)$, associated with the sequence (u^h) will be denoted by $\mathcal{M}_2(u^h,h)$.

These 2-microlocal measures have also been introduced in another framework by C. Fermanian-Kammerer in [15] to which we refer the reader for additional information.

Proof. – We only consider real-valued symbols, the result for complex-valued symbols being deduced by linearity. Let $\varphi\in\mathcal{C}_0^\infty(\mathbb{R}^d)$ be a cut-off so that $\varphi\equiv 1$ in a neighbourhood of $x=0$. We write for any $a\in\mathcal{C}_0^\infty(X)$

$$a^W(x,hD)=D_h\mathrm{Op}_W[\varphi(x)a(hx,\xi)]D_h^*+D_h\mathrm{Op}_W[(1-\varphi(x))a(hx,\xi)]D_h^*,$$

where the first term is a Hilbert-Schmidt operator and the $L^2(T^*\mathbb{R}^d)$-convergence of the symbol gives

$$\lim_{h\to 0}\mathrm{Op}_W[\varphi(x)\alpha(hx,\xi)]=\mathrm{Op}_W[\varphi(x)\alpha(0,\xi)]\quad\text{in } \mathcal{J}_2, \tag{B.2}$$

while the second term is uniformly bounded $\mathrm{Op}S(\langle\xi\rangle^{-\infty},g_1)$. If the symbol $\sigma(h)$ is uniformly bounded in $S(1,\frac{dx^2}{\langle x\rangle^2}+\frac{d\xi^2}{\langle\xi\rangle^2})$ with $\sigma(x,\xi;h)-a(hx,\xi)\geq 0$, pseudo-differential calculus and Garding inequality lead to

$$\mathrm{Op}_W[\sigma(x,\xi;h)-(1-\varphi(x))a(hx,\xi)]=A^h+KB^h, \tag{B.3}$$

where A^h is a bounded non-negative operator, B^h is uniformly bounded on $L^2(\mathbb{R}^d)$ and $K=\langle x\rangle^{-1}\langle D\rangle^{-1}$ is compact.

Since, $\|D_h^*u^h\|_{L^2}\leq C$, we can consider a subsequence $(u^{h'})$ so that $D_{h'}^*u^{h'}\overset{h'\to 0}{\rightharpoonup}v$. By taking $\sigma(x,\xi;h)=\|a\|_{L^\infty}$ in (B.3) we obtain

$$\begin{aligned}&(u^{h'}-D_{h'}v,[\|a\|_{L^\infty}-a^W(x,h'D)](u^{h'}-D_{h'}v))\\&\quad\geq(D_h^*u^h-v,\mathrm{Op}_W[\varphi(x)a(hx,\xi)](D_h^*u^h-v))+(D_h^*u^h-v,KB^h(D_h^*u^h-v)).\end{aligned}$$

Hence the compactness of K and of the limit (B.2) give

$$\overline{\lim_{h'\to 0}}(u^{h'}-D_{h'}v,a^W(x,h'D)(u^{h'}-D_{h'}v))\leq C^2\|a\|_{L^\infty}. \tag{B.4}$$

Now let D be a countable set of elements of $\mathcal{C}_0^\infty(X)$ dense in $\mathcal{C}_0(X)$. For any fixed $\alpha\in D$ we can find a subsequence $(u^{h'_\alpha})$ so that $(u^{h'_\alpha}-D_{h'_\alpha}v,\alpha^W(x,h'_\alpha D)(u^{h'_\alpha}-D_{h'_\alpha}v))$ has a limit $\mu_\alpha\in\mathbb{C}$. By a diagonal extraction process, we can make the subsequence $u^{h'}$ independent of $\alpha\in D$ so that the mapping $\alpha\to\mu_\alpha$ defines a linear form μ_D on the vector space Span D. Owing to estimate (B.4), this linear form is continuous for the topology induced on Span D by the $\mathcal{C}_0(X)$-topology. By the density of D or Span D, this linear form extends uniquely as a bounded measure μ. The convergence for any $a\in\mathcal{C}_0^\infty(X)$ is again a consequence of (B.4). The positivity of the measure μ is easily checked by taking $a\in\mathcal{C}_0^\infty(X)$, $a\geq 0$, and $\sigma(x,\xi;h)=2a(hx,\xi)$ in (B.3). □

PROPOSITION B.2. – *a) If* $\mu \in \mathcal{M}_2(u^h, h)$ *where the sequence* (u^h) *satisfies* $\|u^h\|_{L^2} = 1$ *and* $D_h^* u^h \overset{h\to 0}{\rightharpoonup} v$ *in* $L^2(\mathbb{R}^d)$, *then*

$$1 - \|v\|_{L^2}^2 \geq \int_X d\mu(r, \theta, \xi). \tag{B.5}$$

b) If $\mu \in \mathcal{M}_2(u^h, h)$ *and* $D_h^* u^h \overset{h\to 0}{\rightharpoonup} v$, *then the measure* μ' *defined on* $T^*\mathbb{R}^d$ *by*

$$\mu' = \pi_*[\mu] + \delta_{x=0} \otimes |(Fv)(\xi)|^2 d\!\!{}^-\xi,$$

with $\pi(r, \theta, \xi) = (r\theta, \xi)$, *belongs to the semi-classical measures set* $\mathcal{M}(u^h, h)$.
c) If the semi-classical measures set $\mathcal{M}(u^h, h)$ *is reduced to one element* μ *such that supp* $\mu \cap T_0^*\mathbb{R}^d = \emptyset$ *and* $\int_{T^*\mathbb{R}^d} d\mu(x, \xi) = 1$ *while we assume* $\|u^h\|_{L^2} = 1$, *then* $\mathcal{M}_2(u^h, h) = \{\mu\}$ *and* $D_h^* u^h \overset{h\to 0}{\rightharpoonup} 0$.

Proof. – These three properties essentially rely on $s - \lim_{h\to 0} a^W(x, D; h) = a^W(x, D)$ on $L^2(\mathbb{R}^d)$, for any sequence $a(h)$ uniformly bounded in $S(1, g_0)$ converging to $a \in S(1, g_0)$ in the $\mathcal{C}^\infty$ topology (*see* [20]-Theorem 18.6.2).

a) Let $\chi \in \mathcal{C}_0^\infty(X)$ be such that $0 \leq \chi \leq 1$ and $\chi \equiv 1$ on a neighbourhood of $r = 0$. Then $\chi \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d)$ and we have

$$\begin{aligned}(u^h - D_h v, \chi^W(x, hD)(u^h - D_h v)) &= (u^h, \chi^W(x, hD)u^h) \\ &- 2\mathbb{R}e(D_h^* u^h, \chi^W(hx, D)v) + (v, \chi^W(hx, D)v).\end{aligned} \tag{B.6}$$

The first term of the right-hand side is bounded by 1 while the rest converges to $-\|v\|_{L^2}^2$.

b) is obtained by identifying $\mathcal{C}_0^\infty(T^*\mathbb{R}^d)$ as a subspace of $\mathcal{C}_0^\infty(X)$.

c) Assume $\mathcal{M}(u^h, h) = \{\mu\}$. We consider a subsequence $(u^{h'})$ such that $D_h^* u^h \overset{h'\to 0}{\rightharpoonup} v$ in $L^2(\mathbb{R}^d)$ and $\mathcal{M}_2(u^{h'}, h') = \{\mu'\}$. We take $\chi \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d \setminus T_0^*\mathbb{R}^d)$ and we have $s - \lim_{h'\to 0} \chi^W(h'x, D) = 0$ on $L^2(\mathbb{R}^d)$. Therefore, the characterization of semi-classical measures (1.5) and (B.6) lead to

$$\int_X \chi d\mu' = \lim_{h'\to 0} (u^{h'} - D_{h'} v, \chi^W(x, h'D)(u^{h'} - D_{h'} v)) = \int_{T^*\mathbb{R}^d} \chi d\mu.$$

From this and supp $\mu \cap T_0^*\mathbb{R}^d = \emptyset$, we conclude $\mu' \geq \mu$. But part a) gives $1 - \|v\|_{L^2}^2 \geq \int_X d\mu' \geq \int_{T^*\mathbb{R}^d} d\mu = 1$, which yields $v = 0$ and $\mu' = \mu$. By uniqueness, it is true for the whole sequence. □

ACKNOWLEDGEMENTS

The author would like to thank J.-M. Bony, P. Gérard and especially C. Gérard for profitable discussions and advices.

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(Manuscript received December 12, 1994;
revised May 31, 1995.)

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