Rend. Lincei Mat. Appl. 22 (2011), 17–28
DOI 10.4171/RLM/585

Mathematical Physics — *Global parametrices for the Schrödinger propagator and geometric approach to the Hamilton-Jacobi equation*, by Sandro Graffi and Lorenzo Zanelli.

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Abstract. — A result is announced concerning a family of semiclassical Fourier Integral Operators representing a global parametrix for the Schrödinger propagator when the potential is quadratic at infinity. The construction is based on the geometrical approach of the corresponding Hamilton-Jacobi equation and thus sidesteps the problem of the caustics generated by the classical flow. Moreover, a detailed study of the real phase function allows us to recover a WKB semiclassical approximation which necessarily involves the multivaluedness of the graph of the Hamiltonian flow past the caustics.

Key words: Schrödinger equation, global Fourier Integral Operators, multivalued WKB semiclassical method, symplectic geometry.

2000 Mathematics Subject Classification: 35A17, 35A27, 35Q41, 70H20, 81Q20

1. Introduction

The purpose of this paper is to announce some results about the construction of a global parametrix for the Schrödinger propagator.

Let us consider the initial value problem for the Schrödinger equation:

$$\begin{cases} i\hbar \dfrac{\partial \psi}{\partial t}(t,x) = -\dfrac{\hbar^2}{2m}\Delta\psi(t,x) + V(x)\psi(t,x), \\ \psi(0,x) = \varphi(x). \end{cases} \tag{1.1}$$

Here $\hbar$ is the Planck constant (divided by 2π) and m the mass of the particle. The potential $V \in C^\infty(\mathbb{R}^n;\mathbb{R})$ is assumed quadratic at infinity; namely, there is a constant $C > 0$ such that $|V(x)| \le C|x|^2$ for $|x| \to \infty$. In this case it is well known that the operator H in $L^2(\mathbb{R}^n)$ defined by the maximal action of $-\frac{\hbar^2}{2m}\Delta + V(x)$ is self-adjoint. Hence the Cauchy problem (1.1) considered in $L^2(\mathbb{R}^n)$ admits the unique global solution $\psi(t,x) = U_\hbar(t)\varphi(x)$, $\forall t \in \mathbb{R}$, $\forall \varphi \in L^2(\mathbb{R}^n)$. Here $t \mapsto U_\hbar(t) := e^{-iHt/\hbar} : L^2 \to L^2$, $t \in \mathbb{R}$ is the unitary group generated by the self-adjoint operator H and is known as the propagator of the Schrödinger equation (1.1).

The construction of a parametrix for the Schrödinger propagator under the form of a semiclassical Fourier integral operator (FIO) with phase given by the solution of the corresponding classical Hamilton-Jacobi equation can be considered the main motivating problem of semiclassical microlocal analysis (see e.g. [Sj], [Ro]). This construction amounts indeed to the mathematical justification of the well known time-dependent WKB approximation which is a standard method in quantum mechanics.

In the present conditions a parametrix of the propagator under the form of a semiclassical Fourier integral operator (WKB representation), with real phase given by the solution of the Hamilton-Jacobi equation generated by the symbol of the Schrödinger operator, has been constructed long ago by Chazarain [Ch] (for related results by the same technique see also [Fu], [Ki]; for recent related work see [MY], [Ya1], [Ya2]). The L^2 continuity of the FIO follows by the general result of Asada and Fujiwara [AF] on continuity of FIO with oscillatory kernels. However the solutions of the Hamilton-Jacobi equations develop caustics after a finite time, and this occurrence makes the construction only local with respect to time itself; the solution at an arbitrary time $T > 0$ requires multiple compositions of the local representations.

The occurrence of caustics is unavoidable; therefore the construction of a global (in time) parametrix for the propagator without the introduction of multiple convolutions requires more general techniques. A parametrix has been constructed through the method of complex-valued phase functions (as in [KS], [LS]), with related complex transport coefficients. A particularly convenient choice of the complex phase function (the Herman-Kluk representation) has been isolated in the chemical physics literature long ago ([H-K]). Its validity has been recently proved in [SwR] and [Ro2]. The complex phase function methods not only generate a parametrix for all times, but also make possible to extend the construction to potentials more singular at infinity. This case is impossible to deal within the standard WKB approximations in which the phase function solves the classical Hamilton-Jacobi equation, because the caustics appear as soon as $t > 0$. On the other hand, the standard WKB approximation has a direct relation with the underlying classical flow which is not shared by the above approaches.

In a forthcoming paper [G-Z] we study the problem through the so-called geometric approach to the Hamilton-Jacobi equation (see e.g. [CZ], [Sik86]), in which a global generating function for the Lagrangian submanifold defined by the classical Hamiltonian flow is constructed. The main results, announced here, are the following ones.

In Theorem 1.1 a parametrix is obtained for the propagator $U(t) := e^{iHt/\hbar}$ valid for $t \in [0, T]$, $0 < T < \infty$, under the form of a family of semiclassical *global* Fourier Integral Operators (FIO), which extend to continuous operators in $L^2(\mathbb{R}^n)$. The corresponding phase function is *real* and generates the graph of the flow of the Hamiltonian $\mathscr{H} = \frac{p^2}{2m} + V(x)$. The proof of the L^2 continuity requires an argument different from the standard one of [AF]. This construction not only yields globality in time, but also helps to obtain a unified view of Fujiwara's as well as Chazarain's approaches on one side, and of the Laptev-Sigal one on the other side.

In Theorem 1.2 we prove that a WKB construction is still valid, necessarily multivalued because of the caustics.

2. Statement of the results

Adopting standard notations and terminology (see e.g. [We]), we denote by $\omega = dp \wedge dx = \sum_{i=1}^n dp_i \wedge dx^i$ the 2-form on $T^*\mathbb{R}^n$ that defines its natural symplectic structure. As usual, a diffeomorphism $\mathscr{C} : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$ is a *canonical transformation* if the pull back of the symplectic form is preserved, $\mathscr{C}^*\omega = \omega$.

We say that $L \subset T^*\mathbb{R}^n$ is a *Lagrangian submanifold* if $\omega|_L = 0$ and $\dim L = n = \frac{1}{2}\dim T^*\mathbb{R}^n$. In a natural way, a symplectic structure $\bar{\omega}$ on $T^*\mathbb{R}^n \times T^*\mathbb{R}^n \cong T^*(\mathbb{R}^n \times \mathbb{R}^n)$ is the twofold pull–back of the standard symplectic 2-form on $T^*\mathbb{R}^n$ defined as $\bar{\omega} := pr_2^*\omega - pr_1^*\omega = dp_2 \wedge dx_2 - dp_1 \wedge dx_1$. Similarly, $\Lambda \subset T^*\mathbb{R}^n \times T^*\mathbb{R}^n$ is called a Lagrangian submanifold of $T^*\mathbb{R}^n \times T^*\mathbb{R}^n$ if $\bar{\omega}|_\Lambda = 0$ and $\dim(\Lambda) = 2n$.

A Hamiltonian is a C^2-function $\mathscr{H} : T^*\mathbb{R}^n \to \mathbb{R}$ and its flow is the one-parameter group of canonical transformations $\phi^t_{\mathscr{H}} : U \subseteq T^*\mathbb{R}^n \to T^*\mathbb{R}^n$ solving Hamilton's equations

$$\dot{\gamma} = J\nabla\mathscr{H}(\gamma)$$

(J the unit symplectic matrix) with initial conditions $\gamma(0) = (x_0, p_0) \in U$.

The Hamilton-Helmholtz functional:

$$A[(\gamma^x, \gamma^p)] := \int_0^t [\gamma^p(s)\dot{\gamma}^x(s) - \mathscr{H}(\gamma^x(s), \gamma^p(s))]\, ds \tag{2.1}$$

is well defined and continuous on the path space $H^1([0,t]; T^*\mathbb{R}^n)$. The action functional:

$$\mathscr{A}[\gamma^x] := \int_0^t \mathscr{L}(\gamma^x(s), \dot{\gamma}^x(s))\, ds \tag{2.2}$$

is defined on $H^1([0,t]; \mathbb{R}^n)$.

Here of course $\mathscr{H} = \frac{p^2}{2m} + V(x)$; hence the Legendre transform guarantees the corrispondence of the stationary curves of these two functionals. Obviously the self-adjoint operator H in $L^2(\mathbb{R}^n)$ defined by the maximal action of $-\frac{\hbar^2}{2m}\Delta + V(x)$ is the quantization of $\mathscr{H}$ in the Schrödinger representation.

Definition 2.1. *A global generating function for a Lagrangian submanifold $L \subset T^*\mathbb{R}^n$ is a C^2 function $S : \mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}$ such that*

- $L = \{(x,p) \in T^*\mathbb{R}^n \mid p = \nabla_x S(x,\theta),\ 0 = \nabla_\theta S(x,\theta)\}$,
- $rank(\nabla^2_{x\theta}S\ \nabla^2_{\theta\theta}S)|_L = \max.$

Similarly, a global generating function for a Lagrangian submanifold $\Lambda \subset T^*\mathbb{R}^n \times T^*\mathbb{R}^n$ is a C^2 map $S : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}$ such that

- $\Lambda = \{(x,p;y,\eta) \in T^*\mathbb{R}^n \times T^*\mathbb{R}^n \mid p = \nabla_x S(x,\eta,\theta),\ y = \nabla_\eta S(x,\eta,\theta),\ 0 = \nabla_\theta S\}$,
- $rank(\nabla^2_{x\theta}S\ \nabla^2_{\eta\theta}S\ \nabla^2_{\theta\theta}S)|_\Lambda = \max.$

REMARK 2.2. *The set:*

$$\Sigma_S := \{(x, \eta, \theta) \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^k \mid 0 = \nabla_\theta S(x, \eta, \theta)\} \tag{2.3}$$

is also a submanifold of $\mathbb{R}^{2n+k}$ *diffeomorphic to* Λ.

We focus our attention on the graphs of a Hamiltonian flow $\phi^t_{\mathscr{H}} : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$, which correspond to a family of Lagrangian submanifolds in $T^*\mathbb{R}^n \times T^*\mathbb{R}^n$:

$$\Lambda_t := \{(y, \eta; x, p) \in T^*\mathbb{R}^n \times T^*\mathbb{R}^n \mid (x, p) = \phi^t_{\mathscr{H}}(y, \eta)\}$$

which is in turn generated by the family of global generating functions:

$$\Lambda_t = \{(y, \eta; x, p) \in T^*\mathbb{R}^n \times T^*\mathbb{R}^n \mid p = \nabla_x S,\ y = \nabla_\eta S,\ 0 = \nabla_\theta S(t, x, \eta, \theta)\}$$

explicitly constructed for arbitrarily large times in [G-Z], §3.

As is known, the technical tool of the generating function for Lagrangian manifolds has been developed in the context of symplectic geometry and variational analysis (see [AZ], [CZ], [Cha], [LSik], [Vit], [Sik86], [Sik]) to sidestep the locality in time generated by the occurrence of caustics.

We can now state the main results of [G-Z]. We assume:

$$V(x) = \langle Lx, x\rangle + V_0(x), \quad L \in GL(n), \quad \det L \neq 0; \tag{2.4}$$

$$V_0 \in C^\infty(\mathbb{R}^n), \quad |\partial_x^\alpha V_0(x)| \leq C_0. \tag{2.5}$$

Then:

THEOREM 2.3. *Let* (2.4) *and* (2.5) *be fulfilled. Let* $0 < T < \infty$ *and* $\varphi \in \mathscr{S}(\mathbb{R}^n)$. *Then the propagator* $U_\hbar(t)$ *admits the following parametrix:*

$$\psi(t, x) = (2\pi\hbar)^{-n} \sum_{j=0}^{\infty} \int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{(i/\hbar)(S(t,x,\eta,\theta) - \langle y, \eta\rangle)} \times \hbar^j b_j(t, x, \eta, \theta)\, d\theta\, d\eta \varphi(y)\, dy + O(\hbar^\infty) \tag{2.6}$$

Here:

$$k > CT^4 \sup_{|\alpha|+|\beta|\geq 2} \sup_{(x,p)\in\mathbb{R}^{2n}} |\partial_x^\alpha \partial_p^\beta \mathscr{H}(x, p)|^2 \tag{2.7}$$

for some (explicitly estimated) $C > 0$. *Moreover the following assertions hold:*

(1) S *generates the graph* Λ_t *of the Hamiltonian flow* $\phi^t_{\mathscr{H}} : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$ $\forall t \in [0, T]$:

$$\begin{aligned}\Lambda_t &:= \{(y, \eta; x, p) \in T^*\mathbb{R}^n \times T^*\mathbb{R}^n \mid (x, p) = \phi^t_{\mathscr{H}}(y, \eta)\} \\ &= \{(y, \eta; x, p) \in T^*\mathbb{R}^n \times T^*\mathbb{R}^n \mid p = \nabla_x S,\ y = \nabla_\eta S,\ 0 = \nabla_\theta S\}\end{aligned} \tag{2.8}$$

(2) *$S \in C^\infty([0,T]\times\mathbb{R}^{2n}\times\mathbb{R}^k;\mathbb{R})$ and has the expression:*

$$S = \langle x,\eta\rangle - \frac{t}{2m}\eta^2 - t\langle Lx,x\rangle + \langle Q(t)\theta,\theta\rangle + \langle v(t,x,\eta),\theta + f(t,x,\theta)\rangle + \langle v(t,x,\eta,\theta),\theta\rangle + g(t,x,\eta,\theta). \tag{2.9}$$

Here $f(t,x,\theta):[0,T]\times\mathbb{R}^n\times\mathbb{R}^k\to\mathbb{R}^k$, $v(t,x,\eta,\theta):[0,T]\times\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^k \to\mathbb{R}^k$, $g(t,x,\eta,\theta):[0,T]\times\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^k\to\mathbb{R}$ and $C_{\alpha\beta\sigma}(T)>0$ are such that

$$\sup_{[0,T]\times\mathbb{R}^{2n+k}} [|\partial_x^\alpha\partial_\theta^\sigma f(t,x,\eta,\theta)| + |\partial_x^\alpha\partial_\eta^\beta\partial_\theta^\sigma g(t,x,\eta,\theta)| + |\partial_x^\alpha\partial_\eta^\beta\partial_\theta^\sigma v(t,x,\eta,\theta)|] \leq C_{\alpha\beta\sigma}(T).$$

The function $(x,\eta)\mapsto v(t,x,\eta):\mathbb{R}^n\times\mathbb{R}^n\to\mathbb{R}$ is linear $\forall t\in\mathbb{R}$, and $t\mapsto Q(t):[0,T]\to GL(k)$ with $Q(0)=0$.

(3) *The transport coefficients $b_j: j=0,\dots$ are determined by the first order PDE:*

$$\begin{cases} \partial_t b_0 + \frac{1}{m}\nabla_x S\nabla_x b_0 + \frac{1}{2m}\Delta_x S b_0(t,x,\eta,\theta) = \Theta_N, \\ b_0(0,x,\eta,\theta) = \rho(\theta). \end{cases} \quad j=0 \tag{2.10}$$

$$\begin{cases} \partial_t b_j + \frac{1}{m}\nabla_x S\nabla_x b_j + \frac{1}{2m}\Delta_x S b_j - \frac{i}{2m}\Delta_x b_{j-1} = 0, \\ b_j(0,x,\eta,\theta) = 0. \end{cases} \quad j\geq 1 \tag{2.11}$$

Here $\rho(\cdot)\in\mathscr{S}(\mathbb{R}^k;\mathbb{R}^+)$, $\int_{\mathbb{R}^k}\rho(\theta)\,d\theta = 1$ and $\Theta_N\in C_b^\infty(\mathbb{R}^{2n+k};\mathbb{R})$ fulfills:

$$\Pi^\alpha\Theta_N \in C_b^\infty(\mathbb{R}^{2n+k};\mathbb{R}), \quad 0\leq\alpha\leq N;$$

$$\Pi\Theta_N := \operatorname{div}_\theta\left(\Theta_N\frac{\nabla_\theta S}{|\nabla_\theta S|^2}\right).$$

(4) *$\forall 0\leq t\leq T$, $0\leq T<+\infty$, the expansion* (2.6) *generates an L^2 parametrix of the propagator $U(t)=e^{iHt/\hbar}$: each term is a continuos FIO on $\mathscr{S}(\mathbb{R}^n)$ denoted $B_j(t)$, $j=0,1,\dots$, which admits a continuous extension to $L^2(\mathbb{R}^n)$, and:*

$$e^{iHt/\hbar} = \sum_{j=0}^\infty B_j(t) + O(\hbar^\infty). \tag{2.12}$$

The notation $O(\hbar^\infty)$ means:

$$\|R_N(t)\|_{L^2\to L^2} \leq C_N(T)\hbar^{N+1}, \quad \forall N\geq 0,\ \forall t\in[0,T],$$

$$R_N(t) := U(t) - \sum_{j=0}^N B_j(t).$$

Moreover, the expansion (2.12) *does not depend on* ρ *provided* $\|\rho\|_{L^1} = 1$. *Namely, if* $\rho_1 \neq \rho_2$*:*

$$\sum_{j=0}^{N} B_j[\rho_1](t) - \sum_{j=0}^{N} B_j[\rho_2](t) = O(\hbar^{N+1}).$$

By applying the stationary phase theorem to the oscillatory integral (2.6), the integration over the auxiliary parameters θ can be eliminated and the WKB approximation to the evolution operator is recovered, necessarily multivalued on account of the caustics.

Theorem 2.4. *Let* $V(x) = \frac{1}{2}|x|^2 + V_0(x)$ *with*

$$\sup_{x \in \mathbb{R}^n} \|\nabla^2 V_0(x)\| < 1;$$

let $\hat{\varphi}_\hbar(\eta)$ *be the* $\hbar$*-Fourier transform of the initial datum* φ. *Then* $\forall t \in [0, T]$, $t \neq (2\tau + 1)\frac{\pi}{2}$, $\tau \in \mathbb{N}$, *there exists a finite open partition* $\mathbb{R}^n \times \mathbb{R}^n = \bigcup_{\ell=1}^{\mathcal{N}} D_\ell$ *such that the solution of* (1.1) *can be represented as:*

$$\psi(t,x) = \int_{\mathbb{R}^n} \hat{U}_\hbar(t,x,\eta)\hat{\varphi}_\hbar(\eta)\, d\eta, \quad 0 \leq t \leq T,\ t \neq (2\tau+1)\frac{\pi}{2}$$

$$\hat{U}_\hbar(t,x,\eta)|_{D_\ell} = \sum_{\alpha=1}^{\ell} e^{(i/\hbar)S_\alpha(t,x,\eta)} |\det \nabla_\theta^2 S(t,x,\eta,\theta_\alpha^*(t,x,\eta))|^{-1/2} \times e^{(i\pi/4)\sigma_\alpha} b_{\alpha,0}(t,x,\eta) + O(\hbar) \tag{2.13}$$

$$S_\alpha := S(t,x,\eta,\theta_\alpha^*(t,x,\eta)), \quad b_{\alpha,0} := b_0(t,x,\eta,\theta_\alpha^*(t,x,\eta)),$$

$$\sigma_\alpha := sgn \nabla_\theta^2 S(t,x,\eta,\theta_\alpha^*(t,x,\eta))$$

where $\mathcal{N}$ *is a t-dependent natural and:*

(i) *On each* D_ℓ *the equation* $0 = \nabla_\theta S(t,x,\eta,\theta)$ *has* ℓ *smooth solutions* $\theta_\alpha^*(t,x,\eta)$, $1 \leq \alpha \leq \ell$.
(ii) *Any function* $S_\alpha(t,x,\eta)$ *solves locally the Hamilton-Jacobi equation:*

$$\frac{|\nabla_x S_\alpha|^2}{2m}(t,x,\eta) + V(x) + \partial_t S_\alpha(t,x,\eta) = 0$$

(iii) *An explicit upper bound on the t-dependent natural* $\mathcal{N}$ *is given by formula* (2.64) *of* [G-Z].

Example. In the harmonic oscillator case $V(x) = \frac{1}{2}x^2$ and the phase function is exactly quadratic:

$$S(t,x,\eta,\theta) = \langle x,\eta\rangle - \frac{t}{2}(\eta^2 + x^2) + \langle v(t,x,\eta),\theta\rangle + \langle Q(t)\theta,\theta\rangle.$$

It admits a unique ($\mathcal{N} = 1$) smooth global critical point $\theta^*(t, x, \eta)$ on $(x, \eta) \in \mathbb{R}^{2n}$ for $t \in [0, T]$, $t \neq (2\tau + 1)\frac{\pi}{2}$, $\tau \in \mathbb{N}$. Hence the series (2.13) reduces to just one term conciding with the well known Mehler formula:

$$\psi(t, x) = \int_{\mathbb{R}^n} e^{(i/(\hbar \cos(t)))(\langle x, \eta \rangle - (\sin(t)/2)(\eta^2 + x^2))} \frac{1}{\cos(t)} \hat{\varphi}_\hbar(\eta)\, d\eta$$

Remarks.

1. The construction of the phase function is based upon the Amann-Conley-Zehnder reduction technique of the action functional ([AZ], [CZ], [Car]). Namely:

$$S(t, x, \eta, \theta) = \langle x, \eta \rangle + \int_0^t [\gamma^p(s)\dot{\gamma}^x(s) - H(\gamma^x(s), \eta + \gamma^p(s))]\, ds|_{\gamma(t, x, \theta)(\cdot)} \tag{2.14}$$

where the curves $\Gamma(t, x, \theta) = (\gamma^x(t, x, \theta)(s), \gamma^p(t, x, \theta)(s))$ are parametrized as follows:

$$\Gamma(t, x, \theta) := \begin{cases} \gamma^x(t, x, \theta)(s) = x - \displaystyle\int_s^t \phi^x(t, x, \theta)(\tau)\, d\tau, \\ \qquad \phi^x = \theta^x(\cdot) + f^x(t, x, \theta)(\cdot), \\ \gamma^p(t, x, \theta)(s) = \displaystyle\int_0^s \phi^p(t, x, \theta)(\tau)\, d\tau, \\ \qquad \phi^p = \theta^p(\cdot) + f^p(t, x, \theta)(\cdot) \end{cases} \tag{2.15}$$

Here $\theta \in \mathbb{P}_M L^2([0, T]; \mathbb{R}^{2n}) \simeq \mathbb{R}^k$ ($\mathbb{P}_M$ is the finite dimensional Fourier orthogonal projector, $k = 2n(2M + 1)$) so that the parameters θ can be identified with the finite Fourier components of the derivatives of the curves γ.

(2.14) represents a *generating function with finitely many parameters*, and it is global if k, the number of parameters, fulfills the lower bound (2.7). In turn, the functions $(f^x, f^p) : [0, T] \times \mathbb{R}^n \times \mathbb{P}_M L^2 \to \mathbb{Q}_M L^2 \times \mathbb{Q}_M L^2$ are determined by a fixed point functional equation, essentially the $\mathbb{Q}_M$ projection of the Hamilton equations.

The parametrization (2.8) entails that S is a smooth solution of the problem:

$$\begin{cases} \dfrac{|\nabla_x S|^2}{2m}(t, x, \eta, \theta) + V(x) + \partial_t S(t, x, \eta, \theta) = 0, \\ S(0, x, \eta, \theta) = \langle x, \eta \rangle; \quad \nabla_\theta S(t, x, \eta, \theta) = 0. \end{cases} \tag{2.16}$$

2. Any function $S(t, x, \eta, \theta)$ solving (2.16), i.e. the Hamilton-Jacobi equation under the stationarity constraint $\nabla_\theta S = 0$, is the central object to determine the so called *geometrical solutions of the Hamilton-Jacobi equation* (see for example the recent works [Car], [B-C]). Generating functions are clearly not

unique and this is due to the presence of the θ-auxiliary parameters. Uniqueness holds instead for the geometry of set of critical points:

$$\Sigma_S := \{(x, \eta, \theta) \in \mathbb{R}^{2n+k} \mid \nabla_\theta S(t, x, \eta, \theta) = 0\}$$

which does not depend on S because it is globally diffeomorphic to Λ_t; a detailed study of Σ_S is done in Section 2. We recall (Section 3) that symbols coinciding on some open set $\Omega \supset \Sigma_S$ generate semiclassical Fourier Integral Operators differing only by terms $O(\hbar^\infty)$. This will allow us to select symbols in such a way to make essentially trivial the proof of the L^2 continuity of the associated operator.

3. The symbol b_0 solving the geometrical version (2.10) of the transport equation is

$$b_0(t, x, \eta, \theta) = \exp\left\{-\frac{1}{2m}\int_0^t \Delta_x S(\tau, \gamma^x(t, x, \theta)(\tau), \eta, \theta)\, d\tau\right\}\rho(\theta) \tag{2.17}$$

If $T_2 > T_1$, then $k(T_2) > k(T_1)$ so that $\Gamma(T_1, x, \theta) \subset \Gamma(T_2, x, \theta)$. In the limit $T \to \infty$, $\theta \to \phi \in L^2(\mathbb{R}^+; \mathbb{R}^{2n})$ and we get the simplified functional (still well defined):

$$b_0(t, x, \phi) = \exp\left\{\frac{1}{2m}\int_0^t \Delta_x V\Big(x - \int_\tau^t \phi^x(\lambda)\, d\lambda\Big)\, d\tau\right\}\rho(\phi) \tag{2.18}$$

The functional (2.18) is closely related to the zero-th order symbol of the Laptev-Sigal construction [LS]:

$$v_0(t, y, \eta) = \exp\left\{\frac{1}{2m}\int_0^t \Delta_x V(x^\tau(y, \eta))\, d\tau\right\}.$$

Namely, the functional is the same, but this is evaluated on the classical curves (with initial conditions $x^0(y, \eta) = y$, $p^0(y, \eta) = \eta$) instead of all the free curves used in (2.18) with regularity H^1 and boundary condition $\gamma^x(t, x, \phi)(t) = x$.

4. For potentials in the class (2.4) and $0 \le t \le T$ small enough no caustics develop, and there is a unique smooth solution $\theta^*(t, x, \eta)$ for $(x, \eta) \in \mathbb{R}^{2n}$. The stationary phase theorem yields the 0-th order approximation to the integral (2.6):

$$\begin{aligned}\hat{U}_\hbar^{(0)}(t, x, \eta) = {}& e^{(i/\hbar)S(t, x, \eta, \theta^*)}|\det \nabla_\theta^2 S(t, x, \eta, \theta^*)|^{-(1/2)} \\ & \times e^{(i\pi/4)\sigma} b_0(t, x, \eta, \theta^*) + O(\hbar)\end{aligned} \tag{2.19}$$

which coincide with the WKB semiclassical approximation. This fact suggests a relationship, at any order in $\hbar$, between the present construction and those of Chazarain [Ch] and Fujiwara [Fu]. This is the contents of Theorem 4.1.

5. The first three assertions of Theorem 1.2 essentially represent the counterpart (in the η variables) of a result of Fujiwara [Fu], valid under the additional

assumption that the number of classical curves connecting boundary data is finite.

As already mentioned, the phase of the FIO related to the Hamiltonian flow $\phi^t_{\mathscr{H}}$, which belong to the general setting of Hörmander [Ho], is represented by the generating functions constructed by the above method. The relevant analytical properties of the FIO such as asymptotic behaviour of the kernel and L^2-continuity depend on the topology of their critical points. Therefore we conclude this announcement by stating the result about the L^2 continuity of the present FIO, whose proof is done by an argument different from that of [AF].

First, we introduce the set of phase functions:

Definition 2.5. *The set of phase functions $S(t,x,\eta,\theta):[0,T]\times\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^k\to\mathbb{R}$ is the set of smooth global generating functions of the graphs $\Lambda_t\subset T^*\mathbb{R}^n\times T^*\mathbb{R}^n$ of the canonical maps $\phi^t_H:T^*\mathbb{R}^n\to T^*\mathbb{R}^n$, with the inititial condition $S(0,x,\eta,\theta)=\langle x,\eta\rangle$. Each Λ_t admits the parametrization:*

$$\begin{aligned}\Lambda_t &:= \{(y,\eta;x,p)\in T^*\mathbb{R}^n\times T^*\mathbb{R}^n \mid (x,p)=\phi^t_{\mathscr{H}}(y,\eta)\}\\ &= \{(y,\eta;x,p)\in T^*\mathbb{R}^n\times T^*\mathbb{R}^n \mid p=\nabla_x S,\ y=\nabla_\eta S,\ 0=\nabla_\theta S(t,x,\eta,\theta)\}\end{aligned}$$

The following property of the generating function S is proved in [G-Z], §3.

Proposition 2.6. *Consider the set of critical points*

$$\Sigma_S := \{(x,\eta,\theta)\in\mathbb{R}^{2n+k} \mid 0=\nabla_\theta S(t,x,\eta,\theta)\}. \tag{2.20}$$

Then:

(1) *Σ_S is a manifold globally diffeomorphic to Λ_t;*
(2) *Define the following set*

$$\Upsilon_S := \{(x,\eta,\theta)\in\mathbb{R}^{2n+k} \mid |x|^2+|\eta|^2>D(T)^2,\ |\theta|\le\tilde{K}_2(T)\lambda(x,\eta)\}. \tag{2.21}$$

Then for all $t>0$ Υ_S is free from critical points, i.e.:

$$\Upsilon_S\subset\mathbb{R}^{2n+k}\backslash\Sigma_S$$

We introduce now the relevant class of symbols associated to S. For $(x,\eta)\in\mathbb{R}^n\times\mathbb{R}^n$ set:

$$\lambda(x,\eta):=\sqrt{1+|x|^2+|\eta|^2}$$

Definition 2.7. *The set of symbols consists of all $b\in C^\infty([0,T]\times\mathbb{R}^{2n}\times\mathbb{R}^k;\mathbb{R})$ such that*

(i)

$$b(0,x,\eta,\theta)=\rho(\theta),\quad \rho(\cdot)\in\mathscr{S}(\mathbb{R}^k;\mathbb{R}^+),\quad \int_{\mathbb{R}^k}\rho(\theta)\,d\theta=1.$$

(ii) *For all multi-indices* α, β, σ *and* $t \in]0, T]$ *there are constants* $C^{\pm}_{\alpha,\beta,\sigma}(T) > 0$ *such that the following inequalities hold:*

$$(2.22)\qquad |b(t,x,\eta,\theta)| \leq \begin{cases} C^{+}(T)e^{\lambda(x,\eta)}e^{-|\theta|^2}, & (x,\eta,\theta) \notin \Upsilon_S \\ C^{-}(T)\lambda^{-n}(x,\eta)e^{-|\theta|^2}, & (x,\eta,\theta) \in \Upsilon_S \end{cases}$$

Finally, we introduce the class of global FIO associated to the Hamiltonian flow $\phi^t_{\mathscr{H}}$:

Definition 2.8. *Fix a phase function S as in Definition* 2.5, *and a symbol b as in Definition* 2.7. *Then the global* $\hbar$*-Fourier Integral Operator on* $\mathscr{S}(\mathbb{R}^n)$ *is defined as:*

$$(2.23)\quad B(t)\varphi(x) = (2\pi\hbar)^{-n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{(i/\hbar)(S(t,x,\eta,\theta)-\langle y,\eta\rangle)}b(t,x,\eta,\theta)\,d\theta\,d\eta\varphi(y)\,dy$$

In equivalent way, it can be rewritten in the form:

$$(2.24)\qquad B(t)\varphi(x) = (2\pi\hbar)^{-n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{(i/\hbar)\tilde{S}(t,x,y,u)}\tilde{b}(x,u)\,du\varphi(y)\,dy$$

where $u := (\eta,\theta)$, $\tilde{S}(t,x,y,u) := S(t,x,\eta,\theta) - \langle y,\eta\rangle$ *and* $\tilde{b}(t,x,u) := b(t,x,\eta,\theta)$. *Indeed, if S generates the Lagrangian submanifold* Λ, *then* $\tilde{S}$ *does the same in new variables:*

$$\Lambda = \{(x,p;y,\eta) \in T^*\mathbb{R}^n \times T^*\mathbb{R}^n \mid p = \nabla_x\tilde{S},\ \eta = -\nabla_y\tilde{S},\ 0 = \nabla_u\tilde{S}\}$$

Then the resut is:

Theorem 2.9. *Consider the FIO as in Definition* 2.8*:*

$$B(t)\varphi(x) = (2\pi\hbar)^{-n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^k} e^{(i/\hbar)(S(t,x,\eta,\theta)-\langle y,\eta\rangle)}b(t,x,\eta,\theta)\,d\theta\,d\eta\varphi(y)\,dy$$

Then $B(t) : \mathscr{S}(\mathbb{R}^n) \to \mathscr{S}(\mathbb{R}^n)$ *is continuous and admits a continuous extension as an operator in* $L^2(\mathbb{R}^n)$.

Remark 2.10. It is verified in [G-Z] that the exponential upper bound outside Υ_S is fulfilled by the symbol b_0 as well as by any other symbol b_j, $j = 1, \ldots$ appearing in the expansion of Theorem 1.1. It is moreover verified that on the domain Υ_S there are no critical points for the function S, and this leads to the required vanishing asymptotic behaviour of the type $\lambda^{-n}(x,\eta)$ in this region. This disjoint partition of $\mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n$ is motivated by the proof [G-Z] that the contribution of Υ_S to the FIO is of order $O(\hbar^\infty)$ and L^2-bounded. This setting allows us a very simple proof of global L^2 continuity.

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Received 14 June 2010,
and in revised form 26 July 2010.

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