On the Herman-Kluk Semiclassical Approximation

Didier Robert

Département de Mathématiques

Laboratoire Jean Leray, CNRS-UMR 6629

Université de Nantes, 2 rue de la Houssinière,

F-44322 NANTES Cedex 03, France

didier.robert@univ-nantes.fr

Abstract

For a subquadratic symbol H on $\mathbb{R}^d \times \mathbb{R}^d = T^*(\mathbb{R}^d)$, the quantum propagator of the time dependent Schrödinger equation $i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$ is a Semiclassical Fourier-Integral Operator when $\hat{H} = H(x, \hbar D_x)$ ($\hbar$-Weyl quantization of H). Its Schwartz kernel is describe by a quadratic phase and an amplitude. At every time t, when $\hbar$ is small, it is "essentially supported" in a neighborhood of the graph of the classical flow generated by H, with a full uniform asymptotic expansion in $\hbar$ for the amplitude.

In this paper our goal is to revisit this well known and fondamental result with emphasis on the flexibility for the choice of a quadratic complex phase function and on global L^2 estimates when $\hbar$ is small and time t is large. One of the simplest choice of the phase is known in chemical physics as Herman-Kluk formula. Moreover we prove that the semiclassical expansion for the propagator is valid for $|t| << \frac{1}{4\delta}|\log \hbar|$ where $\delta > 0$ is a stability parameter for the classical system.

1 Introduction and Results

Let us consider the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi(t)}{\partial t} = \widehat{H}(t)\psi(t), \ \ \psi(t = t_0) = \psi_0, \tag{1.1}$$

where ψ is an initial state, $\hat{H}(t)$ is a quantum Hamiltonian defined as a continuous family of self-adjoint operators in the Hilbert space $L^2(\mathbb{R}^d)$, depending on time t and on the Planck constant $\hbar > 0$, which plays the role of a small parameter in the system of units considered in this paper. $\hat{H}(t)$ is supposed to be the $\hbar$-Weyl-quantization of a classical smooth observable $H(t, X)$, $X = (x, \xi) \in \mathbb{R}^d \times \mathbb{R}^d$ (see [27] for more details concerning semiclassical Weyl quantization).

Our main results concern subquadratic hamiltonians H; that means here that $H(t, X)$ is continuous in $t \in \mathbb{R}$, C^∞ smooth in $X \in \mathbb{R}^{2d}$ and satisfies, for every $\gamma \in \mathbb{N}^{2d}$, $|\gamma| \geq 2$,

$$|\partial_X^\gamma H(t, X| \leq C_{T,\gamma}, \ \ \forall t, |t - t_0| \leq T, \ \ \forall X \in \mathbb{R}^{2d} \tag{1.2}$$

where $\partial_X = \frac{\partial}{\partial X}$ and $C_{T,\gamma} > 0$.

Let us introduce some classes of symbols ("classical observables") defined as follows. Let be $m, n \in \mathbb{N}$.

Definition 1.1 *We say that a symbol s is in $\mathcal{O}_m(n)$ if s is a smooth function on the Euclidian space $\mathbb{R}^n$ such that for every $\gamma \in \mathbb{N}^n$, $|\gamma| \geq m$ we have*

$$|s|_{\infty,\gamma} := \sup_{X \in \mathbb{R}^n} |\partial_X^\gamma s(X)| < +\infty \tag{1.3}$$

If $s(\varepsilon)$ depends on a parameter $\varepsilon \in P$ we say that $s(\varepsilon)$ is bounded in $\mathcal{O}_m(n)$ if for every γ, we have

$$\sup_{\varepsilon \in P} |s(\varepsilon)|_{\infty,\gamma} < +\infty.$$

It is well known that the subquadratic assumption entails that equation (1.1) is solved by a unique quantum unitary propagator in $L^2(\mathbb{R}^d)$ such that $\psi_t = U(t,t_0)\psi_0$, $\forall t \in \mathbb{R}$. For the same reason, the classical dynamics is also well defined $\forall t \in \mathbb{R}$. $z_t = (q_t, p_t)$ is the classical path in the phase space $\mathbb{R}^{2d}$ such that $z_{t_0} = z$ and satisfying

$$\begin{cases} \dot{q}_t = \partial_p H(t, q_t, p_t) \\ \dot{p}_t = -\partial H_q(t, q_t, p_t), \quad q_{t_0} = q, \ p_{t_0} = p \end{cases} \tag{1.4}$$

It defines an Hamiltonian flow : $\phi^t(z) = z_t$ ($\phi^{t_0}(z) = z$). Let us introduce the stability Jacobi matrix of this Hamiltonian flow : $F(t) = \partial_z \phi^t(z)$. $F(t)$ is a $2d \times 2d$ symplectic matrix with four $d \times d$ blocks, $F(t) = \begin{pmatrix} A_t & B_t \\ C_t & D_t \end{pmatrix}$, where

$$A_t = \frac{\partial q_t}{\partial q}, \ B_t = \frac{\partial q_t}{\partial p}, \ C_t = \frac{\partial p_t}{\partial q}, \ D_t = \frac{\partial p_t}{\partial p} \tag{1.5}$$

We also introduce the classical action

$$S(t,z) = \int_{t_0}^{t} (p_s \cdot \dot{q}_s - H(s, z_s))ds \tag{1.6}$$

where $u \cdot v$ denote the usual scalar product for $u, v \in \mathbb{R}^d$, and the phase function

$$\boxed{\Phi(t,z;x,y) = S(t,z) + p_t \cdot (x - q_t) - p \cdot (y - q) + \frac{i}{2}\left(|x - q_t|^2 + |y - q|^2\right)} \tag{1.7}$$

For applications it is useful to introduce semi-classical subquadratic symbols. These symbols have an asymptotic expansion in the semiclassical parameter $\hbar > 0$, $H^\hbar(t, X) \asymp \sum_{j \geq 0} \hbar^j H_j(t, X)$ such that the following conditions are satisfied.

$$\forall j \geq 0, \ H_j(t, \bullet) \in \mathcal{O}_{(2-j)_+}(2d) \ \text{ and are bounded in } \mathcal{O}_{(2-j)_+}(2d) \text{ for } t \in \mathbb{R}, \tag{1.8}$$

$$\forall N \geq 1, \hbar^{-N-1}\Big(H(t, X) - \sum_{0 \leq j \leq N} \hbar^j H_j(t, X)\Big) \text{ is bounded in } \mathcal{O}_0 \text{ for } t \in \mathbb{R} \text{ and } \hbar \in]0,1]. \tag{1.9}$$

Let us recall the definition of Weyl quantization. For any symbol s in $\mathcal{O}_m(2d)$, and for any $\psi \in \mathcal{S}(\mathbb{R}^d)$, we have

$$Op_\hbar^w[s]\psi(x) = (2\pi\hbar)^{-d} \iint_{\mathbb{R}^{2d}} e^{\frac{i}{\hbar}(x-y)\cdot\xi} s\Big(\frac{x+y}{2}, \xi\Big)\psi(y)dyd\xi. \tag{1.10}$$

We shall also use the notation $\hat{s} = Op_\hbar^w[s]$.

The Herman-Kluk formula is included in the following asymptotic result which will be discussed in details in this paper. This formula was discovered by several authors in the chemical-physics litterature in the eighties. We refer to the introductions of [22] and [29] for interesting historical expositions. It is rather surprising that until the recent paper [29] there was no explicit connexion in the mathematical litterature between the Herman-Kluk formula and Fourier-Integral Operators with complex phases.

Theorem 1.2 *Let be $H^\hbar(t)$ a time dependent semiclassical subquadratic Hamiltonian and $K^\hbar(t; x, y)$ be the Schwartz kernel of its propagator $U^\hbar(t, t_0)$. Then there exists a semi-classical symbol of order 0, $a^\hbar(t; z) = \sum\limits_{0 \le j < +\infty} a_j(t; z)\hbar^j$ where a_j is continuous in t,*

$$K^\hbar(t; x, y) \asymp \int_{\mathbb{R}^{2d}} e^{\frac{i}{\hbar}\Phi(t, z; x, y)} a(\hbar; t; z) dz \tag{1.11}$$

in the L^2 uniform norm. More precisely, if we denote

$$K^{(\hbar, N)}(t; x, y) = (2\pi\hbar)^{-3d/2} \int_{\mathbb{R}^{2d}} e^{\frac{i}{\hbar}\Phi(t, z; x, y)} \Big(\sum_{0 \le j \le N} a_j(t; z)\hbar^j\Big) dz \tag{1.12}$$

and $U^{(\hbar, N)}(t, t_0)$ the operator, in $L^2(\mathbb{R}^d)$, with the Schwartz kernel $K^{(\hbar, N)}(t; x, y)$, then, for every $T > 0$ and every $N \ge 1$, there exists $C(T, N) > 0$ such that for the L^2 operator norm we have

$$\|U\hbar(t, t_0) - U^{(\hbar, N)}(t, t_0)\| \le C(T, N)\hbar^{N+1}, \quad \forall t, |t - t_0| \le T, \; \hbar \in]0, 1]. \tag{1.13}$$

The leading term is

$$a_0(t; z) = \det{}^{1/2}(A_t + D_t + i(B_t - C_t)) \exp\Big(-i \int_{t_0}^{t} H_1(z_s) ds\Big) \tag{1.14}$$

where the square root is defined by continuity starting from $t = t_0$ ($a_0(t_0; z) = 2^{d/2}$).
Moreover, the amplitudes a_j are smooth functions defined by transport equations (see the proof below) and, for every $T > 0$ they are bounded in $\mathcal{O}_0$ for $|t| \le T$.

In [29] the authors give a rigorous proof of this result with an additionnal hypothesis : they assume that $H(x, \xi)$ is a polynomial in ξ. Here we consider more general subquadratic symbols. In particular our result applies to relativistic Hamiltonians like $\sqrt{1 + |\xi|^2} + V(x)$. Using a global diagonalization (see [28], section 3), the result can be extended to Dirac systems.

Similar results are true with more general quadratic phases and for systems with diagonalisable leading symbols (see [4, 28]). Let us define the quadratic phase

$$\Phi^{(\Theta_t, \Gamma)}(t, z; x, y) = S(t, z) + p_t \cdot (x - q_t) - p \cdot (y - q) + \frac{1}{2}\big(\Theta_t(x - q_t) \cdot (x - q_t) - \overline{\Gamma}(y - q).(y - q)\big) \tag{1.15}$$

where Γ, Θ_t are complex symmetrix matrices with a definite-positive imaginary part, Θ_t is C^1 in t. Γ is constant, Θ_t may depend smoothly on t and z such that the following condition is satisfied :

$$\exists c_T > 0, \; \Im\Theta_t v.v \ge \frac{1}{c_T}|v|^2, \quad \forall t, \; |t| \le T, \; \forall z \in \mathbb{R}^{2d} \tag{1.16}$$

$$\forall \gamma, |\gamma| \ge 1, \exists C_{T, \gamma}, \; \|\partial_z^\gamma \Theta_t\| \le C_{T, \gamma}, \; \forall z \in \mathbb{R}^{2d}, \forall |t| \le T. \tag{1.17}$$

So we have

Theorem 1.3 *Under the assumptions of* Theorem *1.2 and (1.16), (1.17), we have*

$$K(t; x, y) \asymp (2\pi\hbar)^{-3d/2} \int_{\mathbb{R}^{2d}} e^{\frac{i}{\hbar}\Phi^{(\Theta_t, \Gamma)}(t, z; x, y)} f(\hbar; t; z) dz \tag{1.18}$$

where $f(\hbar; t; z) = \sum\limits_{0 \le j < +\infty} f_j(t; z)\hbar^j$ with the same meaning as in Theorem 1.2.
In particular

$$f_0(t, z) = 2^{d/2}\det{}^{1/2}[M(\Theta_t, \Gamma)] \tag{1.19}$$

where

$$M(\Theta_t, \Gamma) = i\big(C + D\overline{\Gamma} - \Theta(A + B\overline{\Gamma})\big).$$

There exist several methods to prove this theorem. In [29] the authors prove it as a consequence of a symbolic calculus for FIO with complex quadratic phases. In [5] the authors proved a weaker result for $\Gamma = i\mathbb{I}$ and $\Theta_t = \Gamma_t$ is determined by the propagation of Gaussian coherent states: $\Gamma_t = (C + D\Gamma)(A + B\Gamma)^{-1}$ (see section 2 of this paper). Laptev-Sigal in [23] have also considered a similar formula for the propagator (see section 5 of this paper) but assume that the initial data has a compact support in momenta. Kay [22] explains how to compute all the semiclassical corrections a_j but did not give estimates on the error term, so its expansion is not rigorously established. Here we choose another approach, may be more explicit and simpler. We shall prove the general theorem 1.3 as a consequence of the particular case of Theorem 1.2 by using a real deformation of the phase $\Phi^{(\Theta_t, \Gamma)}$ on the simpler one $\Phi^{(i\mathbb{I}, i\mathbb{I})}$. Moreover we give a direct proof of Theorem 1.2, proving the necessary properties for Fourier integrals with complex quadratic phases. This way we can get easily explicit estimates for the error terms for large times.

Let us assume that conditions on $\hat{H}(t)$ are satisfied for $T = +\infty$. Moreover assume that there exists a positive real function $\mu(T) \geq 1$, $T > 0$, such that the classical flow ϕ^t satisfies, for every multiindex γ, $|\gamma| \geq 1$, we have for some $C_\gamma > 0$,

$$|\partial_z^\gamma \phi^{t,t'}(z)| \leq C_\gamma \mu(T)^{|\gamma|}, \text{ for } |t| + |t'| \leq T, \ \forall z \in \mathbb{R}^{2d} \tag{1.20}$$

We have discussed in [5] the condition (1.20). In particular this condition is fulfilled with $\mu(T) = \mathrm{e}^{\delta T}$ for $\delta = \sup\limits_{X \in \mathbb{R}^{2d}, t \in \mathbb{R}} \|J\partial_{X,X}^2 H(t, X)\|$.

Theorem 1.4 *Choosing the phase as in theorem 1.2, for $j \geq 0$ the amplitudes $a_j(t, z)$ satisfy the following estimates, for every multiindex γ there exist a constant $C_{j,\gamma}$ such that*

$$|\partial_z^\gamma a_j(t, z)| \leq C_{j\gamma} |\det^{1/2} M_t| \mu(t)^{4j + |\gamma|}, \ \forall t \in \mathbb{R}, \ \forall z \in \mathbb{R}^{2d}. \tag{1.21}$$

Hence we have the following Ehrenfest type estimate. For every $N \geq 1$ and every $\varepsilon > 0$ there exists $C_{N,\varepsilon}$ such that we have

$$\|U(t, t_0) - U^{(N)}(t, t_0)\| \leq C_{N,\varepsilon} \hbar^{\varepsilon(N+1)}, \ \forall t, |t| \geq \frac{1 - \varepsilon}{4\delta}, \ \forall \hbar \in]0, 1]. \tag{1.22}$$

In previous works an Ehrenfest time $T_E = c \log \hbar^{-1}$, $c > 0$, was estimated for propagation of Gaussians in [9] and propagation of observables in [6]. For Gaussians we got $c = \frac{1}{6\delta}$, for observables $c = \frac{1}{2\delta}$. In [29] the authors gave an Ehrenfest time without explicit estimate on c.

2 Gaussians Coherent States and Quadratic Hamiltonians

The phase functions $\Phi^{(\Theta, \Gamma)}$ in (1.7) and (1.15) are closely related with Gaussian coherent states. This can be seen by proving a particular case of Theorem.1.2 for quadratic time-dependent Hamiltonians:

$$H_t(q, p) = \frac{1}{2}\left(G_t q \cdot q + 2L_t q \cdot p + K_t p \cdot p\right)$$

where $q, p \in \mathbb{R}^d$, K_t, L_t, G_t are real, $d \times d$ matrices, continuous in time $t \in \mathbb{R}$, G_t, K_t are symmetric. The classical motion in the phase space is given by the linear differential equation

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = J.\begin{pmatrix} G_t & L_t^T \\ L_t & K_t \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix}, \quad J = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} \tag{2.23}$$

where L^T is the transposed matrix of L, J defines the symplectic form $\sigma(X, X') := JX \cdot X'$, $X = (x, \xi)$, $X' = (x', \xi')$.

This equation defines a linear symplectic transformation, F_t, such that $F_0 = \mathbb{I}$ (we take here $t_0 = 0$). It can be represented as a $2d \times 2d$ matrix which can be written as four $d \times d$ blocks :

$$F_t = \begin{pmatrix} A_t & B_t \\ C_t & D_t \end{pmatrix}. \tag{2.24}$$

The quantum evolution for the Hamiltonian $\hat{H}(t)$ is denoted by $U(t)$ ($U(0) = \mathbb{I}$). We can compute the matrix elements of $U(t)$ on the coherent states basis φ_z. This has been done in Littlejohn [24] (p.249, (6.36)), Bargmann [3], Fedosov [12], [10]. We follow here the presentation given in [10]. Let us introduce some notations which will be used later. g denotes the Gaussian function: $g(x) = \pi^{-d/4} e^{-|x|^2/2}$ and $\Lambda_\hbar$ is the dilation operator $\Lambda_\hbar \psi(x) = \hbar^{-d/4} \psi(\hbar^{-1/2}x)$. So $\varphi_0 = \Lambda_\hbar g$, and the general Gaussian coherent states are defined as follows.

$$\varphi_z^{(\Gamma)} = \hat{T}(z)\varphi^{(\Gamma)}, \tag{2.25}$$

where $\hat{T}(z)$ is the Weyl translation operator, $z = (q, p)$,

$$\hat{T}(z) = \exp\left(\frac{i}{\hbar}(p \cdot x - q \cdot \hbar D_x)\right) \tag{2.26}$$

where $D_x = -i\frac{\partial}{\partial x}$ and $z = (q, p) \in \mathbb{R}^d \times \mathbb{R}^d$. $\varphi^{(\Gamma)}$ is the Gaussian state:

$$\varphi^{(\Gamma)}(x) = (\pi\hbar)^{-d/4} a_\Gamma \exp\left(\frac{i}{2\hbar}\Gamma x.x\right) \tag{2.27}$$

where Γ is a complex symmetric matrix such that $\Im\Gamma$ is definite-positive, a_Γ is a normalization constant. ($a_\Gamma = \det^{1/4}\Im\Gamma$).
It is convenient to introduce here the Siegel space $\Sigma_+(d)$ of $d \times d$ complex matrices Γ such that $\Im\Gamma$ is definite-positive. (see in [13] properties of $\Sigma_+(d)$).

Let us define the Fourier-Bargmann transform $\mathcal{F}_\mathcal{B}^{(\Gamma)}$ as follows, $\psi \in L^2(\mathbb{R}^d)$,

$$\mathcal{F}_\mathcal{B}^{(\Gamma)}[\psi](z) = (2\pi\hbar)^{-d/2}\langle\psi, \varphi_z^{(\Gamma)}\rangle. \tag{2.28}$$

$z \in \mathbb{R}^{2d}$, $\varphi_z^{(\Gamma)}$ is the following coherent state living at z, $z = (q, p) \in \mathbb{R}^d \times \mathbb{R}^d$, $x \in \mathbb{R}^d$,

$$\varphi_z^{(\Gamma)}(x) = (\pi\hbar)^{-d/4} a_\Gamma \exp\left(\frac{i}{\hbar}\left(p \cdot x - \frac{p \cdot q}{2}\right) + \frac{i\Gamma(x-q)\cdot(x-q)}{2\hbar}\right) \tag{2.29}$$

$\mathcal{F}_\mathcal{B}^{(\Gamma)}$ is an isometry from $L^2(\mathbb{R}^d)$ into $L^2(\mathbb{R}^{2d})$ (with the Lebesgue measures). If $\Gamma = i\mathbb{I}$ we denote $\mathcal{F}_\mathcal{B} = \mathcal{F}_\mathcal{B}^{i\mathbb{I}}$; its range consists of $F \in L^2(\mathbb{R}^{2d})$ such that $\exp\left(\frac{p^2}{2} + i\frac{q\cdot p}{2}\right) F(q,p)$ is holomorphic in $\mathbb{C}^d$ in the variable $q - ip$. In other words,

$$\mathcal{F}_\mathcal{B}\psi(z) = E_\psi(q - ip)\exp\left(-\frac{p^2}{2} - i\frac{q\cdot p}{2}\right) \tag{2.30}$$

where E_ψ is entire in $\mathbb{C}^d$ (see [25]). Moreover we have the inversion formula

$$\psi(x) = \int_{\mathbb{R}^{2d}} \mathcal{F}_\mathcal{B}^{(\Gamma)}[\psi](z)\varphi_z^{(\Gamma)}(x)dz, \text{ in the } L^2 - \text{sense.} \tag{2.31}$$

These properties are well known (see [25, 5]). Sometimes we shall use the shorter notation $\tilde{\psi}^\Gamma = \mathcal{F}_\mathcal{B}^{(\Gamma)}\psi$ and $\tilde{\psi}^\Gamma = \tilde{\psi}$.

Let us denote by $\hat{R}[F_t]$ the quantum propagator for the Hamiltonian $H(t)$ (this is the metaplectic representation of F_t) and $K^{(F_t)}$ its Schwartz kernel. We know that $\Lambda_\hbar \hat{R}[F_t]g$ is the following Gaussian state [10, 13],

$$\Lambda_\hbar \hat{R}[F_t]g(x) = (\pi\hbar)^{-d/4} a_\Gamma(t) \exp\left(\frac{i}{2\hbar}\Gamma_t x.x\right) \tag{2.32}$$

where $a_\Gamma(t) = [\det(A_t + \Gamma B_t)]^{-1/2}a_\Gamma$, the complex square root is computed by continuity * from $t = t_0 = 0$, and

$$\Gamma_t = (C_t + \Gamma D_t)(A_t + \Gamma B_t)^{-1}, \quad \Gamma_{t_0} = \Gamma. \tag{2.33}$$

Proposition 2.1 *We have the following exact formula*

$$K^{(F_t)}(x,y) = 2^{d/2}(2\pi\hbar)^{-3d/2}\det^{1/2}\left(\frac{M(\Theta_t,\Gamma)}{i}\right)\int_{\mathbb{R}^{2d}} e^{\Phi^{(\Theta,\Gamma)}(t,z;x,y)}dz \tag{2.34}$$

where $\Gamma, \Theta_t \in \Sigma_+(d)$, Θ_t *is* C^1 *in* t; $M(\Theta_t,\Gamma) = C + D\bar{\Gamma} - \Theta_t(A + B\bar{\Gamma})$ *and*

$$\Phi^{(\Theta_t,\Gamma)}(t,z;x,y) = \frac{1}{2}(q_t\cdot p_t - q\cdot p) + p_t\cdot(x-q_t) - p\cdot(y-q) + \frac{1}{2}\left(\Theta_t(x-q_t)\cdot(x-q_t) - \bar{\Gamma}(y-q).(y-q)\right)$$

Let us remark that here the action is $S(t,z) = \frac{1}{2}(q_t \cdot p_t - q \cdot p)$.

First of all let us remark that the integral (2.34) is an oscillating integral and is defined, as usual, by integrations by parts. We shall give two proofs of this formula.
Proof I. We start with any Γ_0 in the Siegel space $\Sigma_+(d)$. Using the formula

$$\psi(x) = (2\pi\hbar)^{-d}\int_{\mathbb{R}^{2d}}\langle\psi, \varphi_z^{\Gamma_0}\rangle\varphi_z^{\Gamma_0}dz$$

we get the formula

$$K^{(F_t)}(x,y) = (2\pi\hbar)^{-d}\int_{\mathbb{R}^{2d}}\overline{\varphi_z^{(\Gamma_0)}(y)}\varphi_{z_t}^{(\Gamma_t)}(x)dz \tag{2.35}$$

So, we get

$$K^{(F_t)}(x,y) = (2\pi\hbar)^{-3d/2}k_0(t)\int_{\mathbb{R}^{2d}} e^{\frac{i}{\hbar}\Phi^{(\Gamma_t,\Gamma_0)}(t,z;x,y)}dz, \tag{2.36}$$

where

$$k_0(t) = 2^{d/2}\frac{\det^{1/2}(\Im\Gamma_0)}{\det^{1/2}(A + B\Gamma_0)}$$

Now we shall transform the phase $\Phi^{(\Gamma_t,\Gamma_0)}$ into the phase $\Phi^{(\Theta,\Gamma_0)}$.
Let us introduce $\Theta(s) = s\Theta + (1-s)\Gamma_t$, $0 \le s \le 1$. We have $\Theta(s) \in \Sigma_+(d)$. We want to find $k(t,s)$ such that $k(t,0) = k_0(t)$ and

$$\frac{\partial}{\partial s}\left(k(t,s)\int_{\mathbb{R}^{2d}} e^{\frac{i}{\hbar}\Phi^{(\Theta_t,\Gamma_0)}(t,z;x,y)}dz\right) = 0, \quad \forall s \in [0,1]. \tag{2.37}$$

We have

$$\frac{\partial}{\partial s}e^{\frac{i}{\hbar}\Phi^{(\Theta_t,\Gamma_0)}} = \frac{i}{2\hbar}(\Theta_t - \Gamma_t)(x-q_t)\cdot(x-q_t)e^{\frac{i}{\hbar}\Phi^{(\Theta_t,\Gamma_0)}}.$$

The main trick used here and later in this paper, and also in all the previous papers on this subject ([23, 22, 29]), is to integrate by parts to convert each factor $(x - q_t)$ into $\hbar$, using the following equality

$$(\partial_q + \bar{\Gamma}\partial_p)\Phi^{\Theta,\Gamma} = \left(C^\tau + \bar{\Gamma}D^\tau - (A^\tau + \bar{\Gamma}B^\tau)\Theta\right)(x - q_t) \tag{2.38}$$

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*this definition of $\det^{1/2}$ is different that the $\det^{1/2}$ function on $\Sigma_+(d)$, this is explained in [10] to compute Maslov index

where A^τ denotes the transposed matrix of A. Let us introduce the matrix

$$M = M(\Theta, \Gamma) = C + D\bar{\Gamma} - \Theta(A + B\bar{\Gamma})$$

So we have

$$M^\tau(x - q_t)e^{\frac{i}{\hbar}\Phi^{(\Theta,\Gamma)}} = \frac{\hbar}{i}(\partial_q + \bar{\Gamma}\partial_p)e^{\frac{\hbar}{i}\Phi^{\Theta,\Gamma}}. \tag{2.39}$$

Let us remark that M is invertible. This is a consequence of the following Lemma (see [11], [13] or [28], appendix A, for proofs).

Lemma 2.2 *For every linear symplectic map in* $F : T^*(\mathbb{R}^d) \to T^*(\mathbb{R}^d)$, $F = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ *and every* $\Gamma \in \Sigma_+(d)$, $(A + B\Gamma)$, $(C + D\Gamma)$ *are non invertible in* $\mathbb{C}^d$ *and* $(C + D\Gamma)(A + B\Gamma)^{-1} \in \Sigma_+(d)$.

So we have

$$\bar{M} = C + D\Gamma - \bar{\Theta}(A + B\Gamma) = \big((C + D\Gamma)(A + B\Gamma)^{-1} - \bar{\Theta}\big)(A + B\Gamma)^{-1}$$

But $(C + D\Gamma)(A + B\Gamma)^{-1} - \bar{\Theta}) \in \Sigma_+(d)$ so is invertible.
Denote $M(t, s) = M(\Theta_s, \Gamma_t)$. Let us recall the Liouville formula

$$\partial_s \det\big(M(t, s)\big) = \det\big(M(t, s)\big) \mathrm{Tr}\Big(\partial_s M(t, s) M(t, s)^{-1}\Big). \tag{2.40}$$

So, integrating by parts in (q, p) we get

$$k(t, s) = k(t, 0)\frac{\det^{1/2}M(t, s)}{\det^{1/2}M(t, 0)} \tag{2.41}$$

Now we have to compute $\frac{k(t,0)}{\det^{1/2}M(t,0)}$. A simple computation gives $M(t, 0) = (D - \Gamma_t B)(\bar{\Gamma}_0 - \Gamma_0)$. The proof of (2.34) follows from the formula

$$\det(D - \Gamma_t B) = \det(A + B\Gamma_0)^{-1}. \tag{2.42}$$

This equality follows from the symplecticity of F ($D^\tau B = B^\tau D$). We have $B^\tau \Gamma_t B - D^\tau B = -(A + B\Gamma_0)^{-1}B$. So we get (2.42) if $\det B \neq 0$. The general case follows by a density argument. Let us remark that can exchange the role of Θ and Γ by considering the adjoint $U(t)^*$ of $U(t)$. $\square$
Proof II
We solve directly the Schrödinger equation

$$\big(i\hbar\frac{\partial}{\partial t} - \hat{H}(t)\big)\psi(t, x) = 0 \tag{2.43}$$

for any initial data $\psi(x) := \psi(0, x)$, $\psi \in \mathcal{S}(\mathbb{R}^d)$ using the ansatz

$$\psi(t, x) = (2\pi\hbar)^{-3d/2}k(t)\int_{\mathbb{R}^{2d} \times \mathbb{R}^d} e^{i\Phi^{(\Theta,\Gamma)}(t, z; x, y)}\psi(y)dzdy \tag{2.44}$$

We have to compute $k(t)$ such that $k(0) = 2^{d/2}$. Let us remark that if we integrate first in y then the integral (2.44) in z converges because the Fourier-Bargmann transform of ψ, $\mathcal{F}_\mathcal{B}\psi$, is in the Schwartz space $\mathcal{S}(\mathbb{R}^{2d})$.
For simplicity we assume here that $\Theta = \Gamma = i\mathbb{I}$. The general case can be reached by the same method or by using the deformation argument of proof I as we shall see later for more general Hamiltonians.
Here the Hamiltonian $\hat{H}(t)$ is a quadratic form. So using dilations we can assume that $\hbar = 1$. A simple computation left to the reader, gives the following

Lemma 2.3

$$(g^{-1}\hat{H}(t)g)(x) = Gx \cdot x + i(L + L^{\tau})x \cdot x - Kx \cdot x + \text{Tr}(K - iL) \tag{2.45}$$

where $g(x) = e^{-\frac{|x|^2}{2}}$.

So we get

$$(i\partial_t - \hat{H}(t))\psi(t) = (2\pi\hbar)^{-3d/2} \iint_{\mathbb{R}^{2d} \times \mathbb{R}^d} e^{\frac{i}{\hbar}\Phi^{(\Theta,\Gamma)}(t,z;x,y)} b(t,x,z)\psi(y)dzdy \tag{2.46}$$

where

$$b(t,z,z) = i\partial_t k(t) - k(t)\big(E(x - q_t) \cdot (x - q_t) + \text{Tr}(K - iL)\big)$$

As in proof I, we integrate by parts in the variable $z \in \mathbb{R}^{2d}$, using

$$(\partial_q - i\partial_p)\Phi = M^{\tau}(x - q_t)$$

with $M = C - B - i(A + D)$, which is invertible (see below Lemma 3.2). Using the Hamilton equation of motion we get

$$\dot{M} = -E(A - iB) - i(K - iL)M. \tag{2.47}$$

So, we find the following differential equation for $k(t)$,

$$\dot{k} = \frac{1}{2}\text{Tr}\big((M\dot{M})k. \tag{2.48}$$

Using the Liouville formula, we get again (2.34) for this particular phase. $\square$

3   Proof of Theorem 1.2 and Theorem 1.4

As usual for this kind of problems there are two steps : 1-Determine the amplitudes a_j solving by induction transport differential equations, 2-Estimate the error between the approximated propagator and the exact one.

3.1   Transport equations

It is convenient to write

$$e^{\frac{i}{\hbar}\Phi} = (\pi\hbar)^{d/2}\varphi_{z_t}(x)\bar{\varphi}_z(y)e^{\frac{i}{\hbar}(S(t,z)+(p\cdot q - p_t \cdot q_t)/2)} \tag{3.49}$$

Then we have to compute $\hat{H}^{\hbar}(t)\varphi_{z_t}$. It is not difficult to add contributions of the lower order terms of the Hamiltonian, so we shall assume for simplicity that $H^{\hbar}(t) = H_0(t) := H(t)$.

Lemma 3.1 *For every* $N \geq 2$ *we have*

$$\hat{H}(t)\varphi_{z_t}(x) = \sum_{|\gamma| \leq N} \frac{\hbar^{|\gamma|/2}}{\gamma!}\partial_X^{\gamma}H(t,z_t)\Pi_{\gamma}\Big(\frac{x - q_t}{\sqrt{\hbar}}\Big)\varphi_{z_t}(x) + \hbar^{(N+1)/2}T(z_t)\Lambda_{\hbar}Op_1^w[R_N(t,z_t)]g(x) \tag{3.50}$$

where

$$R_N(t,z_t,X) = \int_0^1 \frac{(1-s)^N}{N!} \sum_{|\gamma|=N+1} \partial_X^{\gamma}H(t,z_t + s\sqrt{\hbar}X)X^{\gamma}ds \tag{3.51}$$

and Π_{γ} *is a universal polynomial of degree* $\leq |\gamma|$ *which is even or odd according* $|\gamma|$ *is even or odd.*

Proof. Let us recall that $\varphi_z = \hat{T}(z)\Lambda_\hbar g$. In this proof we put $z_t = z$. An easy property of Weyl quantization gives

$$\Lambda_\hbar^{-1}\hat{T}(z)\hat{H}(t)\hat{T}(z)\Lambda_\hbar = Op_1^w[H(\sqrt{\hbar}\bullet+z)] \tag{3.52}$$

So the Lemma follows easily from the Taylor formula with integral remainder.$\square$

In this first step we don't take care of remainder estimates, this will be done in the next step. Let us denote $\mathcal{I}(a,\Phi)$ the formal operator having the Schwartz kernel

$$K_a(x,y) = (2\pi\hbar)^{-3d/2}\int_{\mathbb{R}^{2d}} e^{\frac{i}{\hbar}\Phi(t,z;x,y)}a(t,z)dz \tag{3.53}$$

From the Lemma 3.1 we can write

$$\hat{H}(t)\mathcal{I}(a,\Phi) \sim \mathcal{I}(b,\Phi), \quad \text{where}$$
$$b \sim \sum_\gamma \frac{\hbar^{|\gamma|/2}}{\gamma!}\partial_X^\gamma H(t,z_t)\Pi_\gamma\Big(\frac{x-q_t}{\sqrt{\hbar}}\Big)a \tag{3.54}$$

We have

$$\Pi_\gamma(x) = \sum_{\beta\leq\gamma} h_{\gamma,\beta}x^\beta \tag{3.55}$$

The quadratic part can be computed as for quadratic Hamiltonians and the linear part disappears with the classical motion. So we have

$$b \sim H(t,z_t)a + (\partial_q H(t,z_t) + i\partial_p H(t,z_t))\cdot(x-q_t)a +$$
$$\hbar\Big(E\big(\frac{x-q_t}{\sqrt{\hbar}}\big)\cdot\big(\frac{x-q_t}{\sqrt{\hbar}}\big) + \text{Tr}(K-iL)\Big)a \tag{3.56}$$

where we denote $\partial_{X,X}^2 H(t,X)$ the Hessian matrix of $H(t)$. We have

$$\partial_{X,X}^2 H(t,z_t) = \begin{pmatrix} G & L \\ L & K \end{pmatrix}, \quad E = G + 2iL - K. \tag{3.57}$$

with $G := \partial_{q,q}^2 H(t,z_t)$, $L := \partial_{q,p}^2 H(t,z_t)$, $K := \partial_{p,p}^2 H(t,z_t)$.

Here the stability matrix $F_t = \begin{pmatrix} A_t & B_t \\ C_t & D_t \end{pmatrix}$ satisfies $\dot{F}_t = J\partial_{X,X}^2 H(t,z_t)F_t$, $F_{t=0} = \mathbb{I}$.

As in the quadratic case we want to transform the power of $(x-q_t)$ into power of $\hbar$.

Lemma 3.2 *Let us denote* $M_t = (C_t - B_t) - i(A_t + D_t)$. *We have*

$$\big|\det M_t\big| \geq 2^{-d}, \quad \text{and} \tag{3.58}$$

$$\hbar(\partial_q - i\partial_p)e^{\frac{i}{\hbar}\Phi} = iM_t^\tau(x-q_t)e^{\frac{i}{\hbar}\Phi} \tag{3.59}$$

Proof. For simplicity, let us forget the lower index t.
Let us consider the $2d\times 2d$ matrix

$$\mathbb{I} + F + iJ(\mathbb{I}-F) = \begin{pmatrix} \mathbb{I}+A-iC & B+i(\mathbb{I}-D) \\ C-i(\mathbb{I}-A) & \mathbb{I}+D+iB \end{pmatrix} = \begin{pmatrix} \mathbb{I}+A-iC & -i(D+iB)+i \\ i(A-iC) & \mathbb{I}+D+iB \end{pmatrix} \tag{3.60}$$

Using the Lemma 4 in [13], Appendix A, we get

$$\det(\mathbb{I}+F+iJ(\mathbb{I}-F)) = \det\big((\mathbb{I}+A-iC)(\mathbb{I}+D+iB)-(A-iC-\mathbb{I})(D+iB-\mathbb{I})\big) = 2^d\det\big(A+D+i(B-C)\big) \tag{3.61}$$

Using that F is symplectic, we get

$$(\mathbb{I}+F+iJ(\mathbb{I}-F))^*(\mathbb{I}+F+iJ(\mathbb{I}-F)) = (\mathbb{I}+F^\tau)(\mathbb{I}+F)+(1-F^\tau)(\mathbb{I}-F) \geq \mathbb{I}_{2d} \tag{3.62}$$

hence (3.58) follows.

Let us recall classical computations for the derivatives of the action

$$\partial_q S = (\partial_q q_t)^\tau p_t - p \tag{3.63}$$
$$\partial_p S = (\partial_p q_t)^\tau p_t \tag{3.64}$$

Then we can compute $\partial_q \Phi$, $\partial_p \Phi$ and we get (3.59). $\square$

Integrate by parts like in the quadratic case, we get

$$(i\hbar\partial_t - \hat{H}(t))\mathcal{I}(a, \Phi) \asymp \mathcal{I}(f, \Phi) \tag{3.65}$$

where

$$f \sim i\hbar\big(\partial_t a - \frac{1}{2}\mathrm{Tr}\big(\dot{M}M^{-1}\big)a$$
$$+ \sum_{|\gamma|\geq 3} \frac{\hbar^{|\gamma|/2}}{\gamma!}\partial_X^\gamma H(t, z_t)\Pi_\gamma\Big(\frac{x - q_t}{\sqrt{\hbar}}\Big)a \tag{3.66}$$

Hence using the Liouville formula, we get the first term

$$a_0(t, z) = 2^{d/2}\det{}^{1/2}\big(iM\big) \tag{3.67}$$

We shall obtain the next terms a_j by successive integrations by parts. This is solved more explicitly with the following Lemma.

Lemma 3.3 *For any symbol $b \in \mathcal{O}_0(2d)$, and every multiindex $\alpha \in \mathbb{N}^{2d}$ we have*

$$\int_{\mathbb{R}^{2d}} (x - q_t)^\alpha \mathrm{e}^{\frac{i}{\hbar}\Phi}b(z)dz = \sum_{\frac{|\alpha|}{2}\leq|\beta|\leq|\alpha|} \hbar^{|\beta|} \int_{\mathbb{R}^{2d}} f_{\alpha,\beta}(t, z)\mathrm{e}^{\frac{i}{\hbar}\Phi}\partial_z^\beta b(z)dz \tag{3.68}$$

where $f_{\alpha,\beta}(t, z)$ are symbols of order 0, uniformly bounded in $\mathcal{O}_0(2d)$ on bounded time intervals. They only depend on the classical flow $\phi^t(z)$ and its derivatives.
More precisely, let us assume that there exists a non positive function $\mu(T)$ such that for every $\gamma \in \mathbb{N}^{2d}$ we have

$$\sup_{|a|\leq T} |\partial_z^\gamma\phi^t(z)| \leq C_\gamma\mu(T)^{|\gamma|} \tag{3.69}$$

Then we have

$$|\partial_z^\epsilon f_{\alpha,\beta}(z)| \leq C_{\alpha,\beta;\epsilon}\mu(T)^{|\alpha|-|\beta|+|\epsilon|} \tag{3.70}$$

Proof. The Lemma is easily obtained by induction on $|\alpha|$ using Lemma 3.2 $\square$

Now, to determine the transport equation, we solve inductively on $j \geq 0$, the equation

$$(i\hbar\partial_t - \hat{H}(t))\mathcal{I}\Big(\sum_{0\leq k\leq j+1} \hbar^k a_k(t), \Phi\Big) = O(\hbar^{j+2}) \tag{3.71}$$

Reasoning by induction on $j \geq 0$, we get the transport equation for $a_{j+1}(t)$ by cancellation of the coefficient of $\hbar^{j+1}$ in (3.71).

$$\partial_t a_{j+1}(t, z) = \frac{1}{2}\mathrm{Tr}\big(\dot{M}M^{-1}\big)a_{j+1}(t, z) + b_j(t, z), \quad a_{j+1}(0, z) = 0, \tag{3.72}$$

where

$$b_j(t, z) = \sum_{|\alpha|+2k\leq 2(j+2)} F_{j,k,\alpha}(t, z)\partial_z^\alpha a_k(t, z). \tag{3.73}$$

Moreover, $F_{j,k,\alpha}(t,z)$ depends only on the classical flow $\phi^t(z)$ and its derivatives and satisfies

$$|\partial_z^\gamma F_{j,k,\alpha}(t,z)| \leq C_{j,k,\alpha,\gamma}\mu(T)^{2(j-k+2)+|\gamma|-|\alpha|} \tag{3.74}$$

where $C_{j,k,\alpha,\gamma}$ only depends on $\sup_{|t|\leq T}|H(t)|_{\infty,\gamma}$, $2 \leq |\gamma| \leq j+2$.

So we get, for every $j \geq 0$,

$$a_{j+1}(t,z) = \int_0^t \det{}^{1/2}\big(M(t,z)M(s,z)^{-1}\big)b_j(s,z)ds \tag{3.75}$$

Moreover, from (3.73) and (3.74), we get the following estimate, for every $j \geq 0$, $|t| \leq T$, $z \in \mathbb{R}^{2d}$,

$$|\partial_z^\gamma a_j(t,z)| \leq C_{j,\gamma}|\det{}^{1/2}M(t,z)|\mu(T)^{4j+|\gamma|} \tag{3.76}$$

with the same remark as in (3.74) for the constant $C_{j,\gamma}$.

3.2 Error estimates

Let us denote

$$\mathcal{R}_N(t) = (i\hbar\partial_t - \hat{H}(t))\mathcal{I}\big(a^{(N)}(t), \Phi\big) \tag{3.77}$$

where $a^{(N)}(t) = \displaystyle\sum_{0\leq k\leq N} \hbar^k a_k$. Using Duhamel formula we have

$$\|U^\hbar(t) - U^{N,\hbar}(t)\| \leq \hbar^{-1}\int_0^t \|\mathcal{R}(s)\|ds \tag{3.78}$$

where $t_0 = 0$, $U^\hbar(t) = U^\hbar(t,0)$, $U^{N,\hbar}(t) = \mathcal{I}\big(a^{(N)}(t), \Phi\big)$.

So we have to estimate $\|\mathcal{R}_N(t)\|$. Let us denote $K^{(N)}(x,y)$ the Schwartz kernel of $\mathcal{R}_N(t)$ and $\tilde{K}^{(N)}(X,Y)$ the Schwartz kernel of $\mathcal{R}_N(t)$ in the Fourier-Barmann representation :

$$\tilde{K}^{(N)}(X,Y) = \iint_{\mathbb{R}^d\times\mathbb{R}^d} K^{(N)}(x,y)\varphi_X(y)\overline{\varphi_Y(x)}dxdy. \tag{3.79}$$

Let be $\tilde{\mathcal{R}}_N(t)$ the operator with Schwartz kernel $\tilde{K}^{(N)}(X,Y)$. The following Lemma is well known. Here we forget N and t for simplicity.

Lemma 3.4 *We have the L^2 norm estimate*

$$\|\mathcal{R}\|_{L^2(\mathbb{R}^d)} \leq (2\pi\hbar)^{-d}\|\tilde{\mathcal{R}}\|_{L^2(\mathbb{R}^d)} \tag{3.80}$$

In particular we have

$$\|\mathcal{R}\|_{L^2(\mathbb{R}^d)} \leq (2\pi\hbar)^{-d}\max\left\{\sup_Y\int|\tilde{K}(X,Y)|dX, \sup_X\int|\tilde{K}(X,Y)|dY\right\} \tag{3.81}$$

Proof For inequality (3.80) we use that the Fourier-Bargmann transform is an isometry. Inequality (3.81) is known as Carleman (or Schur) L^2 estimate.$\square$

Using Lemma 3.1 we get

$$\tilde{K}^{(N)}(X,Y) = 2^{-3d/2}(\pi\hbar)^{-d}\int_{\mathbb{R}^{2d}}\langle \hat{T}(z_t)\Lambda_\hbar Op_1^w[R_N(t)]g, \varphi_Y\rangle\langle\varphi_X, \varphi_z\rangle a^{(N)}(t,z)e^{\frac{i}{\hbar}\delta(t,z)}dz \tag{3.82}$$

where $\delta(t,z) = S(t,z) + \frac{p \cdot q - p_t \cdot q_t}{2}$.

Using Weyl commutation formula we have

$$\langle \varphi_X, \varphi_z \rangle = \exp\left(-\frac{|X-z|^2}{4\hbar} + \frac{i}{2\hbar}\sigma(X,z)\right) \tag{3.83}$$

$$\langle \hat{T}(z_t)\Lambda_\hbar Op_1^w[R_N(t)]g, \varphi_Y \rangle = \langle Op_1^w[R_N(t)]g, g_{\frac{Y-z_t}{\sqrt{\hbar}}} \rangle. \tag{3.84}$$

We know the Wigner function $W_{0,Z}$ of the pair (g, g_Z), $Z \in \mathbb{R}^{2d}$ [28]

$$W_{0,Z}(X) = 2^{2d}\exp\left(-|X-\frac{Z}{2}|^2 - i\sigma(X,Z)\right) \tag{3.85}$$

By a well known property of Weyl quantization [13], for any symbol s, we have

$$\langle Op_1^w[s]g, g_Z \rangle = (2\pi)^{-d}\int_{\mathbb{R}^{2d}} s(X)W_{0,Z}(X)dX \tag{3.86}$$

We shall use the following Lemma

Lemma 3.5 Let be $f \in \mathcal{O}_0(2d)$. For every $\gamma \in \mathbb{N}^{2d}$ and $m > 0$ there exists $C_{\gamma,m}$ such that

$$\left|\int_{\mathbb{R}^{2d}} X^\gamma f(X)e^{-|X-Z|^2 - iJZ \cdot X}dX\right| \leq C_{\gamma,m}(1+|Z|)^{-m}\sup_{|\alpha| \leq m+|\gamma|;\ Y \in \mathbb{R}^{2d}}|\partial_Y^\alpha f(Y)| \tag{3.87}$$

Proof It is enough to assume $|Z| \geq 1$. We integrate m times by parts with the differential operator

$$\mathcal{L} = \frac{2(X-Z) - iJZ \cdot X}{4|X-z|^2 + |JZ|^2}\partial_X \tag{3.88}$$

using that $(\mathcal{L}^\tau)^m = \sum_{|\alpha| \leq m} l_{m,\alpha}\partial_X^\alpha$, with $|l_{m,\alpha}| \leq C_{m,\alpha}(|Z| + |X-Z|)^{-m}$, where

$\theta(X) = -|X-Z|^2 - iJZ \cdot X$. $\square$

So using Lemma 3.5 we get the following estimate : for every $N; N'$ there exists $C_{N,N'}$ (depending only on semi-norms $|H(t)|_{\infty,\gamma}$, $2 \leq |\gamma| \leq N + N'$, such that for $X, Y \in \mathbb{R}^{2d}$ and $|t| \leq T$ we have

$$|\tilde{K}^{(N)}(X,Y)| \leq C_{N,N'}(\mu(T))^{N+N'}\hbar^{\frac{N+1}{2}-d}\int_{\mathbb{R}^{2d}} e^{-\frac{|X-z|^2}{4\hbar}}\left(1 + \frac{|Y-z_t|}{\sqrt{\hbar}}\right)^{-N'}|a^{(N)}(t,z)|dz. \tag{3.89}$$

Let us denote $\phi^{*t} = \phi^{0,t} = (\phi^t)^{-1}$. We have the Lipchitz estimate, for $|t| \leq T$,

$$|\phi^{*,t}Y - z| \leq \mu(T)|Y - z_t| \tag{3.90}$$

So we get

$$\left|\int_{\mathbb{R}^{2d}} e^{-\frac{|X-z|^2}{4\hbar}}\left(1 + \frac{|Y-z_t|}{\sqrt{\hbar}}\right)^{-N'}dz\right| \leq C_{N'}\left(1 + \frac{|\phi^{t*}Y - X|}{\mu(T)\sqrt{\hbar}}\right)^{-N'} \tag{3.91}$$

and

$$|\tilde{K}^{(N)}(X,Y)| \leq C_{N,N'}(\mu(T))^{N+N'}\hbar^{\frac{N+1}{2}}\left(1 + \frac{|\phi^{t*}Y - X|}{\mu(T)\sqrt{\hbar}}\right)^{-N'}\sup_{z \in \mathbb{R}^{2d},|t| \leq T}|a^{(N)}(t,z)| \tag{3.92}$$

Then using Lemma 3.4 and choosing $N' > 2d$, we get the following uniform L^2 estimate for the remainder term, for $|t| \leq T$,

$$\|\mathcal{R}_N(t)\| \leq C_N(\mu(T))^{N+1}\hbar^{(N+1)/2}\sup_{z \in \mathbb{R}^{2d},|t| \leq T}|a^{(N)}(t,z)| \tag{3.93}$$

If T is fixed, pushing the expansion up to $2N$ instead of N we get easily Theorem 1.2 using Duhamel formula.

Using global estimates on $a_j(t,z)$ obtained from the transport equation (3.76) and pushing the asymptotic expansion up to $2N$, we get the proof of Theorem 1.4 using again Duhamel formula.

4 Varying phase. Proof of Theorem 1.3

To avoid technicalities we fix the time t. It would be not difficult to follow a time parameter t if necessary for application. So in this section ϕ is a symplectic diffeomorphism in $\mathbb{R}^{2d}$, such that ϕ, ϕ^{-1} are Lipchitz continuous and $\phi \in \mathcal{O}_1(2d)$.

We denote $z = (q, p) \in \mathbb{R}^{2d}$, $\phi(z) = (Q(z), P(z)) \in \mathbb{R}^d \times \mathbb{R}^d$ and S an action for ϕ, i.e a primitive on $\mathbb{R}^{2d}$ of the closed 1-form $PdQ - pdq$. We consider the following phases

$$\Phi^{(\phi,\Theta,\Gamma)}(z; x, y) = S(z) + P \cdot (x - Q) - p \cdot (y - q) + \frac{1}{2}\big(\Theta(x - Q) \cdot (x - Q) - \overline{\Gamma}(y - q).(y - q)\big) \quad (4.94)$$

This class of Fourier-Integral operators with complex quadratic phase was ready analyzed in [29]. We want here to show how to vary the choice of the matrices Θ, Γ for a given canonical transformation ϕ of $\mathbb{R}^{2d}$. As in section 3, let us denote $\mathcal{I}(a, \Phi)$ the operator with the Schwartz kernel

$$K_a(x, y) = (2\pi\hbar)^{-3d/2} \int_{\mathbb{R}^{2d}} \mathrm{e}^{\frac{i}{\hbar}\Phi^{(\phi,\Theta,\Gamma)}(z;x,y)} a(z) dz \quad (4.95)$$

where $a \in \mathcal{O}_0(2d)$, $\Phi = \Phi^{(\phi,\Theta,\Gamma)}$.

Using a Fourier-Bargmann transform and the following estimate : there exist $C > 0$, $c > 0$ such that for all $X \in \mathbb{R}^{2d}$ we have

$$|\langle \varphi^{\Gamma}, \varphi_X \rangle| \le C \exp\Big(-\frac{c|X|^2}{\hbar}\Big), \quad (4.96)$$

we can estimate the Fourier-Bargmann transform $\tilde{K}_a(X, Y)$ of K_a and prove that $\mathcal{I}(a, \Phi)$ is bounded in $L^2(\mathbb{R}^d)$ (see section 3, Lemma 3.5 and the section 5 below).

Our goal in this section is to prove the following result which gives Theorem 1.3 as a particular case.

Proposition 4.1 *Let be 4 matrices in $\Sigma_+(d)$, $\Theta, \Theta', \Gamma, \Gamma'$ and $a \in \mathcal{O}_0(2d)$. Θ, Θ' may be z dependent such that*

$$\exists c > 0, \; \Im\Theta^{(\prime)}v.v \ge c|v|^2, \; \forall z \in \mathbb{R}^{2d} \quad (4.97)$$

$$\forall \gamma, |\gamma| \ge 1, \exists C_\gamma, \; \|\partial_z^\gamma \Theta^{(\prime)}\| \le C_\gamma, \; \forall z \in \mathbb{R}^{2d}. \quad (4.98)$$

Then there exists a semi-classical symbol $a' \sim \sum_j \hbar^j a'_j$ of order 0 such that we have for the L^2 operator norm,

$$\mathcal{I}(a, \Phi^{(\phi,\Theta,\Gamma)}) = \mathcal{I}(a', \Phi^{(\phi,\Theta',\Gamma')}) + O(\hbar^\infty) \quad (4.99)$$

Moreover we have for the principal symbol a'_0 the formula

$$a'_0(z) = a_0(z)\frac{\det^{1/2}(M(1))}{\det^{1/2}(M(0))} \quad (4.100)$$

where $M(s) := C + D\overline{\Gamma} - \big((1 - s)\Theta + s\Theta'\big)(A + B\overline{\Gamma})$

Proof. The method is rather simple and is an extension of what we have already done for quadratic Hamiltonians (Proof I) except that here we have to solve transport equations in the deformation parameter s to get the lower order correction terms.

Let us remark that this class of Fourier-integral operators is closed under adjointness :

$$\mathcal{I}(a, \Phi^{(\Theta,\Gamma)})^* = \mathcal{I}(a^*, \Phi^*), \quad (4.101)$$

where $a^*(Z) = \bar{a}(\phi^{-1}Z)$, $Z = (Q, P)$, $Z = \phi(z)$ and

$$\Phi^*(Z; x, y) = -S(\phi^{-1}Z) + p \cdot (x - q) - P \cdot (y - Q) +$$
$$\frac{1}{2}\big(\Gamma(x - q) \cdot (x - q) - \overline{\Theta}(y - Q).(y - Q)\big) \quad (4.102)$$

So by transitivity we can assume that $\Gamma = \Gamma'$. As in the quadratic Hamiltonian case let us introduce $\Theta_s = (1-s)\Theta + s\Theta'$, $\Phi^{(s)} = \Phi^{(\Theta_s,\Gamma)}$, $0 \leq s \leq 1$ and look for a semiclassical symbol $a^{(s)} = \sum_j \hbar^j a_j^{(s)}$ such that

$$\frac{\partial}{\partial s} \int_{\mathbb{R}^{2d}} e^{\frac{i}{\hbar}\Phi^{(s)}(z;x,y)} a^{(s)}(z)dz = O(\hbar^\infty), \quad \forall s \in [0,1] \tag{4.103}$$

But we have

$$\frac{\partial}{\partial s}\Phi^{(s)}(z;x,y) = \frac{i}{\hbar}(\Theta' - \Theta)(x-Q)\cdot(x-Q) \tag{4.104}$$

and we have to find a C^1 family symbol $a^{(s)}$, $0 \leq s \leq 1$ such that

$$\mathcal{I}\Big(\partial_s a^{(s)} + \frac{i}{\hbar}(\Theta' - \Theta)(x-Q)\cdot(x-Q)a^{(s)}, \Phi\Big) = O(\hbar^\infty) \tag{4.105}$$

The principal term $a_0' = a^{(1)}$ is computed as in the quadratic case.
Let us suppose for a moment that Θ, Θ' are constant. Then as in the quadratic case we have

$$(\partial_q + \bar\Gamma\partial_p)\Phi^{(s)} = \big(C^\tau + \bar\Gamma D^\tau - (A^\tau + \bar\Gamma B^\tau)\Theta_s\big)(x-Q) \tag{4.106}$$

where $A = \partial_q Q$, $B = \partial_p Q$, $C = \partial_q P$, $D = \partial_p P$ and $F = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ is a symplectic matrix.

We know that $M(s) := C + D\bar\Gamma - \Theta_s(A + B\bar\Gamma)$ is invertible so we can integrate by parts as in section 3. and as above we can achieve the proof of Proposition 4.1.
When Θ, Θ' are z dependent, the integrations by part are more tricky. We have to use

$$(\partial_q + \bar\Gamma\partial_p)\Phi^{(s)} = M\tau(s,z)(x-Q) + N(s,z)(x-Q,x-Q) \tag{4.107}$$

where $N(s,z)(x,y)$ is a bilinear application in $(x,y) \in \mathbb{R}^d \times \mathbb{R}^d$ into $d \times d$ matrices, with coefficients in $\mathcal{O}_0$ in z, C^1 in s.
Hence we have

$$(x-Q)e^{\frac{i}{\hbar}\Phi^{(\Theta,\Gamma)}} = \frac{\hbar}{i}(M^\tau)^{-1}(s,z)(\partial_q + \bar\Gamma\partial_p)e^{\frac{\hbar}{i}\Phi^{(\Theta,\Gamma)}} - M^\tau)^-(s,z)N(s,z)(x-Q,x-Q)e^{\frac{\hbar}{i}\Phi^{(\Theta,\Gamma)}} \tag{4.108}$$

So we apply (4.108) and the following lemmas to proceed like in section 3.

Lemma 4.2 *For any symbol $b \in \mathcal{O}_0(2d)$, for every multiindex $\alpha \in \mathbb{N}^{2d}$ and every $N \geq |\alpha|/2$ we have*

$$\int_{\mathbb{R}^{2d}} (x-Q)^\alpha e^{\frac{i}{\hbar}\Phi^{(s)}} b(z)dz = \sum_{\frac{|\alpha|}{2}\leq|\beta|\leq N} \hbar^{|\beta|}\int_{\mathbb{R}^{2d}} f_{\alpha,\beta}(s,z)e^{\frac{i}{\hbar}\Phi^{(s)}}\partial^\beta b(z)dz +$$

$$\sum_{|\beta|+|\gamma|=N+1,|\beta|\geq 1} \hbar^{|\gamma|}\int_{\mathbb{R}^{2d}} g_{\alpha,\beta}(s,z)(x-Q)^\beta e^{\frac{i}{\hbar}\Phi^{(s)}} g_{\beta,\gamma}\partial^\gamma b(z)dz \tag{4.109}$$

where $f_{\alpha,\beta}(s,z)$, $g_{\alpha,\beta}(s,z)$ are symbols of order 0, uniformly bounded in $\mathcal{O}_0(2d)$ for $s \in [0,1]$.

Lemma 4.3 *For every $b \in \mathcal{O}_0(2d)$ and $\beta \in \mathbb{N}^d$ we have the crude L^2 estimate, uniform in $s \in [0,1]$,*

$$\|\mathcal{I}((x-Q)^\beta b, \Phi^{(s)}\| = O(\hbar^{|\beta|/2}) \tag{4.110}$$

Using these two lemmas we get the full semiclassical symbol $a' \sim \sum_j \hbar^j a_j'$, where

$$a_0'(z) = a_0 \frac{\det^{1/2}(M(s))}{\det^{1/2}(M(0))} \tag{4.111}$$

and for $j \geq 1$, a_j' is computed by induction as solution for $s = 1$ of the differential equation

$$\partial_s a_j(s) = \text{Tr}\big(\dot{M}(s)M^{-1}(s)\big)a_j(s) + b_j(s), \quad a_j(0) = a_j. \tag{4.112}$$

where $b_j(s)$ depends on the $a_k(s)$, $k \leq j-1$ □

Remark 4.4 *Considering the adjoint operator, it is possible to exchange the role of the matrices Θ and Γ.*
If the symbol a depends smoothly on some parameter λ, it is not difficult to show that a' also depends smoothly in λ.

Proof of Lemma 4.2. This is done by an induction on N such that $\alpha \leq N$.□
Proof of Lemma 4.3. Let us begin by giving a simple proof of (4.96) when Θ is z dependent satisfying the assumptions (4.1). We shall prove the more general estimate, for every $\beta \in \mathbb{N}^d$ there exist $C > 0$, $c > 0$ such that

$$|\langle x^\alpha g^\Theta, g_Y \rangle| \leq C \mathrm{e}^{-c|Y|^2}, \quad \forall Y \in \mathbb{R}^{2d} \tag{4.113}$$

Let us denote $Y = (y, \eta) \in \mathbb{R}^d \times \mathbb{R}^d$. By a direct estimate we get easily,

$$|\langle x^\alpha g^\Theta, g_Y \rangle| \leq C \mathrm{e}^{-2c|y|^2}, \quad \forall (y, \eta) \in \mathbb{R}^{2d}. \tag{4.114}$$

Using Fourier transform and Plancherel formula, we exchange y and η and we get (4.113).
Now we can follow the method of section 3 to estimate L^2 norm of operators using a Fourier-Bargmann transformation.
Let be $\tilde{K}(X, Y)$ the Fourier-Bargmann kernel of $\mathcal{I}((x - Q)^\beta b, \Phi^{(s)})$. We have

$$\tilde{K}(X, Y) = 2^{-3d/2}(\pi\hbar)^{-d}\hbar^{|\alpha|/2} \int_{\mathbb{R}^{2d}} \langle \hat{T}(Z)\Lambda_\hbar(x^\beta g^\Theta), \varphi_Y \rangle \langle \varphi_X, \varphi_z \rangle b(z) \mathrm{e}^{\frac{i}{\hbar}\delta(t,z)} dz \tag{4.115}$$

where $Z = (Q, P) = \phi(z)$ and

$$|\langle \hat{T}(Z)\Lambda_\hbar(x^\beta g^\Theta), \varphi_Y \rangle| = |\langle x^\beta g^\Theta, g_{\frac{Y-Z}{\sqrt{\hbar}}} \rangle|. \tag{4.116}$$

So we get

$$|\tilde{K}(X, Y)| \leq C\hbar^{|\alpha|/2} \int_{\mathbb{R}^{2d}} \exp\left(-\frac{c}{\hbar}(|Y - \phi(z)|^2 + |X - z|^2)\right) dz \tag{4.117}$$

Using that ϕ is a Lipchitz canonical transformation, we have, for C_0 large enough and $c_0 > 0$ small enough,

$$|\tilde{K}(X, Y)| \leq C_0 \hbar^{|\alpha|/2} \exp\left(-\frac{c_0}{\hbar}(|Y - \phi(X)|^2\right) \tag{4.118}$$

Hence we get the proof of Lemma 4.3 using Lemma 3.4.□
we have proved Proposition 4.1 and Theorem 1.3.

5   Semiclassical Fourier Integral Operators

In [23], [8] and in the recent preprint [30], the authors have considered Fourier-integral operators defined by the following simpler phase

$$\Psi^{(\phi,\Theta)}(p; x, y) = S(y, p) + P \cdot (x - Q) + \frac{1}{2}\Theta(x - Q) \cdot (x - Q) \tag{5.119}$$

where $(Q, P) = \phi(y, p)$, ϕ is a bilipchitz canonical transformation like above, $\Theta \in \Sigma_+(d)$.
In [23] and [8] the authors have proved semiclassical expansions for the propagator of Schrödinger equation for initial data with a compact support. This result is extended in [30] for the Schrödinger Hamiltonian $-\hbar^2 \triangle + V$, to general data in L^2 with uniform norm estimates. We shall give here some extensions of results of [30] using the same techniques as in section 3 and 4, so we shall not repeat the details.
    Let us denote $\mathcal{J}(a, \Psi^{\phi,\Theta})$ the operator whose Schwartz kernel is

$$K(x, y) = (2\pi\hbar)^{-d} \int_{\mathbb{R}^d} \mathrm{e}^{\frac{i}{\hbar}\Psi^{(\phi,\Theta)}(p; x, y)} a(y, p) dp \tag{5.120}$$

A natural question discussed in this section is to compare the Fourier-Integral operators $\mathcal{I}(a, \Phi^{(\phi,\Theta,\Gamma)})$ defined with $2d$ "frequency variables" and $\mathcal{J}(a, \Psi^{(\phi,\Theta)})$ defined with d "frequency variables".
A Fourier integral operator in $L^2(\mathbb{R}^d)$ is always a quantization of a canonical transformation ϕ in the cotangent space $T^*(\mathbb{R}^d)$. A nice way to make clear this relationship is to use a Fourier-Bargmann transform (see [7, 31]). This can be easily done in the same way for Semiclassical-Fourier-Integral operators as we shall see now.

Definition 5.1 *A family of operators, depending on a small parameter $\hbar \in]0,1]$, $U^\hbar : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}'(\mathbb{R}^d)$ is a Semiclassical-Fourier-Integral operator of order $m \in \mathbb{R}$ associated to the canonical bilipchitz transformation $\phi : T^*(\mathbb{R}^d) \to T^*(\mathbb{R}^d)$, if for every N' we have $U^\hbar = U^\hbar_{N'} + R^\hbar_{N'}$, where $U^\hbar_{N'} : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}'(\mathbb{R}^d)$ and $\|R^\hbar_{N'}\| = O(\hbar^{N'})$ and for every $N \geq 0$ there exists C_N such that*

$$|\tilde{K}^\hbar(X,Y)| \leq C_N \hbar^{m-3d/2}\Big(1 + \frac{|Y - \phi(X)|}{\sqrt{\hbar}}\Big)^{-N}, \quad \forall X, Y \in \mathbb{R}^{2d}, \quad \hbar \in]0,1], \tag{5.121}$$

where $\tilde{K}^\hbar(X,Y)$ is the Schwartz kernel of $\mathcal{F}_\mathcal{B} U^\hbar_{N'} \mathcal{F}_\mathcal{B}^*$.

Remark 5.2 *1. In this definition, which coïncides with a definition given in [31] for $\hbar = 1$, a semiclassical-Fourier-Integral operator has, up to a negligible operator in $\hbar$, a kernel living in a neighborhood of the graph of a canonical transformation ϕ. But this definition says nothing concerning asymptotic expansion of $\tilde{K}^\hbar(X,Y)$ in a neighborhood of the graph of ϕ when $\hbar$ is small. So this definition is certainly too permissive. But for $\hbar$ fixed it is suitable as proven in [31].*

2. Using Carleman-Schur estimate, a semiclassical F.I.O of order 0 is uniformly bounded in $L^2(\mathbb{R}^d)$. This is a straightforward consequence of the definition. This class of semiclassical F.I.O of order 0 is clearly closed by composition.

3. In Definition 5.1 it is equivalent to use any Fourier-Bargmann transformation $\mathcal{F}_\mathcal{B}^{(\Gamma)}$, $\Gamma \in \Sigma_+(d)$.

4. There are other definitions of semiclassical F.I.O using Lagrangian analysis and real phase functions. For this point of view see for example [1].

5. Fourier-Integral operators with complex phase were used to study propagation of singularities of P.D.E. Many papers and books have been published on this subject, among them let us point out [2, 26, 32].

Now we shall see that the operators already considered in this paper are semiclassical-Fourier-Integral operators.

Proposition 5.3 *Let be amplitudes $a = a(x,z)$, $a \in \mathcal{O}_0(3d)$ and $u = u(x,y,p)$, $u \in \mathcal{O}_0(3d)$ and $\Theta, \Gamma \in \Sigma_+(d)$, Θ may depend in z or (y,p), such that (1.16), (1.17) are satisfied. Then $\mathcal{I}(a, \Phi^{(\phi,\Theta,\Gamma)})$ and $\mathcal{J}(u, \Psi^{\phi,\Theta})$ are semiclassical-Fourier-Integral operators of order 0.*

Proof. Concerning $\mathcal{I}(a, \Phi^{(\phi,\Theta,\Gamma)})$, we get the result following subsection 3.2, estimate (3.92).
The proof for $\mathcal{J}(u, \Psi^{\phi,\Theta})$ is almost the same. For simplicity we assume Θ constant. For Θ depending in (y,p) we could proceed as in section 4.
Let us denote $X = (\tilde{x}, \tilde{\xi})$, $Y = (\tilde{y}, \tilde{\eta})$. We want to estimate

$$\tilde{K}(X,Y) = (2\pi\hbar)^{-d} \iiint_{\mathbb{R}^{3d}} e^{\frac{i}{\hbar}\tilde{\Phi}} u(x,y,p)\,dp\,dx\,dy \tag{5.122}$$

where

$$\tilde{\Phi} = S(y,p) + P \cdot (x - Q) + \frac{\Theta}{2}(x - Q) \cdot (x - Q) +$$

$$\frac{i}{2}(\tilde{x} - y) \cdot (\tilde{x} - y) + \tilde{\xi} \cdot (\tilde{x} - y) + \frac{i}{2}(\tilde{y} - x) \cdot (\tilde{y} - x) + \tilde{\eta} \cdot (\tilde{y} - x) \tag{5.123}$$

Let us remark that we have : $F^{-1} = \begin{pmatrix} D^\tau & -B^\tau \\ -C^\tau & A^\tau \end{pmatrix}$ if $F = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$. So, because F^{-1} is symplectic, we know that $D^\tau - B^\tau \Theta$ is invertible. Hence we have

$$
\begin{align}
\partial_y \tilde{\Phi} &= (C^\tau - A^\tau \Theta)(x - Q) + (\tilde{\xi} - p) + i(\tilde{x} - y) \tag{5.124} \\
\partial_p \tilde{\Phi} &= (D^\tau - B^\tau \Theta)(x - Q) \tag{5.125} \\
\partial_x \tilde{\Phi} &= \Theta(x - Q) + (P - \tilde{\eta}) + i(\tilde{y} - x). \tag{5.126}
\end{align}
$$

So we get the necessary estimates on $\tilde{K}$ by integrations by parts using

$$
\begin{align}
\partial_y \tilde{\Phi} - (-A^\tau \Theta + C^\tau)(D^\tau - B^\tau \Theta)^{-1} \partial_p \Psi &= (\tilde{\xi} - p) + i(\tilde{x} - y) \tag{5.127} \\
\partial_x \tilde{\Phi} - \Theta(D^\tau - B^\tau \Theta)^{-1} \partial_p \Psi &= (P - \tilde{\eta}) + i(\tilde{y} - x) \tag{5.128}
\end{align}
$$

$\square$

The following result is a slight generalization of [23, 8, 30].

Theorem 5.4 *Under the assumptions of Theorem 1.2 and (1.16), (1.17), we have*

$$
K(t; x, y) \asymp (2\pi\hbar)^{-d} \int_{\mathbb{R}^d} e^{\frac{i}{\hbar} \psi^{(\phi^t, \Theta_t)}(t, y, p, x)} u(\hbar; t, y, p) dp \tag{5.129}
$$

where $u(\hbar; t, y, p) = \displaystyle\sum_{0 \le j < +\infty} u_j(t; y, p)\hbar^j$ has the same meaning as in Theorem1.2.
In particular

$$
u_0(t, y, p) = \det^{1/2}\Big(D - \Theta B\Big) \tag{5.130}
$$

Sketch of proof. These result can be proved following the same strategy as for proving Theorem 1.3.
We first prove the Theorem for some Θ ($\Theta = i\mathbb{I}$), following the proof of Theorem 1.2. then we can get the Theorem for any Θ by the variation argument as in the proof of Theorem 1.3. L^2 estimate for operator norm of Fourier-Integral operators is used to control the remainder terms. $\square$

Remark 5.5 *It is not difficult to adapt the proof of Theorem 1.4 concerning an Ehrenfest time estimate to the setting of Theorem 5.4.*

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