Uniform Semi-classical Estimates for the Propagation of Quantum Observables

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Abstract

We prove here that the semi-classical asymptotic expansion for the propagation of quantum observables, for C^∞-Hamiltonians growing at most quadratically at infinity, is uniformly dominated at any order, by an exponential term who's argument is linear in time. In particular, we recover the Ehrenfest time for the validity of the semi-classical approximation. This extends the result proved in [BGP]. Furthermore, if the Hamiltonian and the initial observables are holomorphic in a complex neighborhood of the phase space, we prove that the quantum observable is an analytic semi-classical observable. Other results about the large time behavior of observables with emphasis on the classical dynamic are also given. In particular, precise Gevrey estimates are established for classically integrable systems.

1 Introduction and main results

According to the Bohr's correspondance principle, the quantum evolution of an observable is close to its classical evolution as the Planck constant $\hbar$ is small. In the mathematical literature this result is known as Egorov Theorem [Ho, Ro]. But usually this result is proved for finite time and the asymptotics hold in the C^∞ (Poincaré) sense. Here we put emphasis on large time behavior of asymptotic expansions in $\hbar$, in the C^∞ case as well as in the analytic (or Gevrey) case. In the book [Iv] (section 2.3, Propagation of singularities along long bicharacteristics) one can find related results for the C^∞ case. But our results are more explicite. Many years ago, physicists conjectured that semi-classical approximation is still valid in large time interval with length $T(\hbar) \approx \log(\hbar^{-1})$ which is called Erhenfest time [Ch, Za]. That kind of result was rigorously proved for propagation of coherent states in [CR] (and in [HJ] in the analytic case). In [BGP] the authors have established long time estimates for the propagation of quantum observable. The main goal of this paper is to

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prove more accurate estimates in $\hbar$ and time. In particular, if the data are holomorphic in a complex neighborhood of the real phase space, then the semi-classical expansion of the time dependent quantum observable holds with an exponentially small remainder term, for time interval with length of order $\log(\hbar^{-1})$. Let us denote by $X = \mathbb{R}^n$ the configuration space of a classical mechanical system with n degrees of freedom. The corresponding phase space Z is identified with $\mathbb{R}^{2n}$ equipped with the symplectic form σ defined by

$$\sigma(z; z') = \langle Jz, z' \rangle. \tag{1}$$

where $\langle , \rangle$ is the Euclidean scalar product and J is the $2n \times 2n$ matrix

$$J = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}. \tag{2}$$

A generic point in Z is denoted z and its coordinates by (q, p) where $q, p \in \mathbb{R}^n$.
A classical Hamiltonian is a smooth real function $H : Z \to \mathbb{R}$. Our basic example will be $H(q,p) = \frac{\|p\|^2}{2m} + V(q)$ $(m > 0)$ where $\|p\|^2 = < p, p >$. We could also consider a Riemannian manifold (X, g). In what follows we put emphasis on the case $X = \mathbb{R}^n$.
The motion of the classical system is determined by the system of Hamilton's equations

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}(q,p), \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}(q,p). \tag{3}$$

The equations (3) generate a flow Φ^t on the phase space Z, defined by
$\Phi^t(q(0), p(0)) = (q(t), p(t))$; $\Phi^0 = \mathbb{1}$. Φ^t exists locally by the Cauchy-Lipchitz Theorem for O.D.E. But we need more assumptions on H to define Φ^t globally on Z. Φ^t defines a symplectic diffeomorphism (canonical transformation) group of transformations on Z. Let us consider a classical observable A, i.e A a smooth complex valued function defined on phase space Z. The time evolution of A can be easily computed

$$\frac{d}{dt} A(\Phi^t(z)) = \{H, A\}(\Phi^t(z)), \quad z = (q,p) \tag{4}$$

where $\{H, A\}$ is the Poisson bracket defined by

$$\{H, A\} = \partial_q H \cdot \partial_p A - \partial_p H \cdot \partial_q A. \tag{5}$$

Here we have used the notation $\partial_q = \frac{\partial}{\partial q}$. Now let us assume that H, A are quantizable. That means that we can associate to them the quantum observables $\hat{H}$ and $\hat{A}$ i.e self-adjoint operators in $L^2(X)$. By solving formally the Schrödinger equation : $i\hbar\partial_t \psi_t = \hat{H}\psi_t$, we can define the one parameter group of unitary operators $U(t) = \exp\left(-\frac{it}{\hbar}\hat{H}\right)$. The quantum time evolution of $\hat{A}$ is then given by $\hat{A}(t) = U(-t)\hat{A}U(t)$ which satisfies the Heisenberg-von Neumann equation

$$\frac{d\hat{A}(t)}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}], \tag{6}$$

where $[K, B] = KB - BK$ is the commutator of K, B. We shall use here the $\hbar$-Weyl quantization defined for $A \in \mathcal{S}(Z)$ (the space of Schwartz functions) by the following formula, with $\psi \in \mathcal{S}(X)$,

$$\hat{A}\psi(x) = (2\pi\hbar)^{-n} \iint_Z A\left(\frac{x+y}{2}, p\right) \mathrm{e}^{i\hbar^{-1}\langle x-y, p\rangle} \psi(y) dy dp. \tag{7}$$

Let us now introduce a more general set of classical observables for which the $\hbar$-Weyl quantization is well defined and have nice properties [Ho, Ro].

Definition 1.1 *(i) $A \in \mathcal{O}(m)$, $m \in \mathbb{R}$, if and only if $Z \stackrel{A}{\to} \mathbb{C}$ is C^∞ in Z and for every multi-index $\gamma \in \mathbb{N}^{2n}$ there exists $C > 0$ such that*

$$|\partial_z^\gamma A(z)| \leq C\langle z\rangle^m, \ \forall z \in Z.$$

(ii) We say that A is a C^∞-semi-classical observable of weight m if there exists $\hbar_0 > 0$ and a sequence $A_j \in \mathcal{O}(m)$, $j \in \mathbb{N}$, so that A is a map from $]0, \hbar_0]$ into $\mathcal{O}(m)$ satisfying the following asymptotic condition : for every $N \in \mathbb{N}$ and every $\gamma \in \mathbb{N}^{2n}$ there exists $C_N > 0$ such that for all $\hbar \in]0, \hbar_0[$ we have

$$\sup_Z \langle z\rangle^{-m} \left| \partial_z^\gamma \left(A(\hbar, z) - \sum_{0 \leq j \leq N} \hbar^j A_j(z) \right) \right| \leq C_N \hbar^{N+1}. \tag{8}$$

A_0 is called the principal symbol, A_1 the sub-principal symbol of $\hat{A}$. The set of semi-classical observables of weight m is denoted by $\mathcal{O}_{sc}(m)$. By the $\hbar$-Weyl quantization, its range in $\mathcal{L}(\mathcal{S}(X))$ is denoted $\widehat{\mathcal{O}}_{sc}(m)$.

Notation : For any A and A_j's satisfying (8), we will write : $A(\hbar) \asymp \sum_{j\geq 0} \hbar^j A_j$ in $\mathcal{O}_{sc}(m)$.

Let us now recall the statement of the propagation Theorem which will be improved in this paper. The microlocal version of the result is due to Egorov [Eg]. R. Beals [Be] found a nice simple proof which is reproduced in [Ro].

Theorem 1.2 *Let us consider an Hamiltonian H and an observable A satisfying :*

$$|\partial_z^\gamma H_j(z)| \leq C_{\gamma j}, \text{ for } |\gamma| + j \geq 2 \tag{9}$$

$$\hbar^{-2}(H - H_0 - \hbar H_1) \in \mathcal{O}_{sc}(0), \tag{10}$$

$$|\partial_z^\gamma A(z)| \leq C_\gamma, \text{ for } |\gamma| \geq 1. \tag{11}$$

Then we have the following properties :
(a) For $\hbar$ small enough, $\hat{H}, \hat{A}$ are essentially self-adjoint operators in $L^2(X)$, with core $\mathcal{S}(X)$, hence the quantum evolution $U(t) = \exp(-\frac{it}{\hbar}\hat{H})$ is well defined for all $t \in \mathbb{R}$.
(b) For each $t \in \mathbb{R}$, $\hat{A}(t) = U(-t)\hat{A}U(t) \in \widehat{\mathcal{O}}_{sc}(1)$. Its symbol has an asymptotic expansion, such that $A(t) - A \circ \Phi^t \asymp \sum_{j\geq 1} \hbar^j A_j(t)$, holds in $\mathcal{O}_{sc}(0)$, uniformly in t, for t in a bounded interval. Moreover $A_j(t)$ can be computed by the following formulas

$$A_0(t, z) = A(\Phi^t(z)), \tag{12}$$

$$A_1(t, z) = \int_0^t \{A(\Phi^\tau), H_1\}\Phi^{t-\tau}(z)d\tau \tag{13}$$

and for $j \geq 2$, by induction,

$$A_j(t, z) = \sum_{\substack{|(\alpha,\beta)|+k+\ell=j+1 \\ 0\leq\ell\leq j-1}} \Gamma(\alpha, \beta) \int_0^t [(\partial_p^\alpha \partial_q^\beta H_k)(\partial_q^\alpha \partial_p^\beta A_\ell)(\tau)](\Phi^{t-\tau}(z))d\tau, \tag{14}$$

with

$$\Gamma(\alpha,\beta)=\frac{(-1)^{|\beta|}-(-1)^{|\alpha|}}{\alpha!\beta!2^{|\alpha|+|\beta|}}i^{-1-|(\alpha,\beta)|}.$$

where Φ^t is the classical flow defined by the principal term H_0.

Since our aim is to improve Theorem 1.2, let us recall here briefly the method to prove it. We admit here that $\hat{A},\hat{H}$ are essentially self-adjoint (for a proof see [Ro]). Let us remark that, under the assumption on H_0 in Theorem 1.2, the classical flow Φ^t exists globally in Z. Indeed, the Hamiltonian vector field $(\partial_\xi H_0,-\partial_x H_0)$ has at most a linear growth at infinity and hence no classical trajectory can blow up in a finite time. Moreover, using usual methods in non linear O.D.E (variation equation), we can prove that for every $\gamma\in\mathbb{N}^{2n}$, $|\gamma|\geq 1$ $\partial_z^\gamma A(\Phi^t)\in\mathcal{O}(0)$ is uniformly bounded for $z\in Z$ and t bounded. Now, from the Heisenberg equation and the classical equation of motion, we get

$$\frac{d}{ds}U(-s)\widehat{A_0}(t-s)U(s)=U(-s)\left\{\frac{i}{\hbar}[\hat{H},\widehat{A_0}(t-s)]-\{\widehat{H,A_0}\}(\Phi^{t-s})\right\}U(s),\tag{15}$$

where $A_0(t)=A(\Phi^t)$. But, from the product rule formula (see Appendix), the principal symbol of $\frac{i}{\hbar}[\hat{H},\widehat{A_0}(t-s)]-\{\widehat{H,A_0}\}(\Phi^{t-s})$ vanishes. So, in the first step, we get the error term

$$U(-t)\hat{A}U(t)-\widehat{A_0}(t)=\int_0^t U(-s)\left(\frac{i}{\hbar}[\hat{H},\widehat{A_0}(t-s)]-\{H,\widehat{A_0}\}\Phi^{t-s}\right)U(s)ds.\tag{16}$$

Now, it is not difficult to obtain, by induction on j, the full asymptotics in $\hbar$ (see [Ro] for details). ∎

Remark 1.3 *If $H=H_0$ is a polynomial function of degree ≤ 2 on the phase space Z then the propagation Theorem has a very simple form : $A(t)=A\circ\Phi^t$ and the remainder term is null ($U(t)$ is a metaplectic transformation).*
In [PU2] a semi-classical version of Egorov Theorem on compact manifolds is given.

Our first result is an improvement of Theorem 1.2 by giving estimates for large time, in the C^∞-case.

Theorem 1.4 *Let us assume that the Hamiltonian H and the observable A satisfy the assumptions of Theorem 1.2. Let us introduce an upper bound of the stability exponents of the classical system*

$$\Gamma:=\sup_{z\in Z}\|\!|J\nabla_z^{(2)}H_0(z)|\!\|,$$

where for any observable f, $\nabla_z^{(2)}f$ is the corresponding Hessian matrix [2]*. Then, for every $j\in\mathbb{N}$ and every multi-index γ such that $j+|\gamma|\geq 1$, there exists $C_{j,\gamma}>0$ such that for every $z\in Z$ and every $t\in\mathbb{R}$ we have*

$$|\partial_z^\gamma A_j(t,z)|\leq C_{j,\gamma}\exp(\Gamma(2j-1+|\gamma|)|t|).\tag{17}$$

[2] Here the norm of a symmetric matrix M is defined by $\|\!|M|\!\|=\sup_{\|x\|\leq 1}|<Mx,x>|$.

Furthermore we have the following estimates in L^2 operator-norm of the remainder term. For every $N \in \mathbb{N}$ there exists C_N such that for every $t \in \mathbb{R}$ we have

$$\|\hat{A}(t) - \sum_{0 \leq j \leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq C_N \hbar^{N+1} (1+|t|)^{N+\delta_n} \exp(\Gamma(2N+\delta_n)|t|), \tag{18}$$

where δ_n is a universal constant ($\delta_n \leq 5n+3$).

This result entails the following corollary about the Ehrenfest time for the validity of the semi-classical approximation.

Corollary 1.5 *Under the assumptions of Theorem 1.4, for every $N \geq 1$ there exists $C_N > 0$ such that for every $\varepsilon > 0$ and for $|t| \leq \frac{1-\varepsilon}{2\Gamma} \log(\hbar^{-1})$, we have*

$$\|\hat{A}(t) - \sum_{0 \leq j \leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq C_N \hbar^{\varepsilon N+1} \hbar^{\frac{\varepsilon-1}{2}(5n+3)}. \tag{19}$$

In particular the semi-classical asymptotic expansion is valid under the above condition on t.

Remarks in the case of "classical" energy observables *We shall see from the proof of Theorem 1.4 that if the expansion of H in $\hbar$ is even (in particular if H is "classical" : $H = H_0$) then the $\hbar$-expansion of $A(t)$ is even and the exponential term in (17) becomes $\exp(\Gamma(3j/2 - 1 + |\gamma|)|t|)$. In the remainder estimate (18) the $2N$ becomes also $3N/2$ so that in this case the Ehrenfest time is not smaller than $\frac{2}{3\Gamma} \log \hbar^{-1}$. More precisely, for every $\varepsilon > 0$ and for $|t| \leq \frac{2-\varepsilon}{3\Gamma} \log(\hbar^{-1})$, we have*

$$\|\hat{A}(t) - \sum_{0 \leq j \leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq C_N \hbar^{\frac{\varepsilon}{2}N+1} \hbar^{\frac{\varepsilon-2}{3}(5n+3)}. \tag{20}$$

We remember that some times ago, S. De Bièvre suggested that the Ehrenfest time could be greater that $\frac{1}{2\Gamma} \log \hbar^{-1}$. The above results confirm this guess. In section 5 we shall make more comments about this.

Remark 1.6 *In many cases the assumptions of Theorem 1.2 on the Hamiltonian H are not satisfied. In particular for Schrödinger Hamiltonian with non constant magnetic field with vector-potential $a(q)$, $H(q,p) = \|p - a(q)\|^2 + V(q)$ or for a quartic electric potential $H(q,p) = \|p\|^2 + \|q\|^4$ the second derivatives are not always bounded. But if the observable A is supported in a flow-invariant compact set $\bar{\Omega}$, of the phase space, then, using the functionnal calculus on $\hbar$-pseudodifferential operators (see [Ro]) we can get the same conclusion as in Theorem 1.4 with a constant Γ defined as follows.*

$$\Gamma := \sup_{\Omega} \|\!| J \nabla_z^{(2)} H_0(z) |\!\|$$

where A is such that $supp(A) \subset \Omega$. A more precise statement will be given at the end of section 2 *(see Proposition 2.7).*
As we can see from the proofs, the use of the numerical constant Γ is to control the exponential growth of the flow in time. Of course it is also possible to make directly some

growth assumptions on the flow or to make some geometrical assumptions on the classical Hamiltonian. This will be done in section 4 with periodic systems (see Proposition 2.8) and and stated in this section with integrable systems (see Theorem 1.13). Some extensions to manifolds are also clearly possible. But in general (compact) manifolds no exact global quantization procedure exists so it seems difficult to compute $\hat{A}_j(t)$ for $j \geq 2$ for non classical symbols.

As it is expected, the dependence in j, γ, N of the constants in Theorem 1.4 can be specified under analyticity assumptions on A and H. Let us first recall the following definition (see [BK, Sj]).

Definition 1.7 *Let $A(\hbar, z)$ be a C^∞-semi-classical observable, $A \in \mathcal{O}_{sc}(0)$. We say that $A(\hbar, z)$ is a semi-classical observable with a Gevrey index $\sigma \geq 1$, if the following conditions are satisfied, for some constant $C > 0$,*

$$\forall \gamma \in \mathbb{N}^{2n},\ \forall j \in \mathbb{N},\ \forall z \in Z,\ \text{we have } |\partial_z^\gamma A_j(z)| \leq C^{|\gamma|+j+1}(|\gamma|+j)!^\sigma; \tag{21}$$

$$\left| \partial_z^\gamma \left(A(\hbar, z) - \sum_{0 \leq j \leq N} \hbar^j A_j(z) \right) \right| \leq \hbar^{N+1} C^{|\gamma|+N+2}(|\gamma|+N+1)!^\sigma. \tag{22}$$

As usual, a semi-classical observable with a Gevrey index equal to 1 is said analytic.

Theorem 1.8 *Let us assume that the energy Hamiltonian H has an expansion in $\hbar$ such that $\hbar^{-2}(H - H_0 - \hbar H_1)$ is an analytic, semi-classical observable and that it exists some $\delta > 0$ such that H_0, H_1 and the initial observable A are holomorphic in the complex domain $D(\delta) := \{z \in \mathbb{C}^{2n}, \|\Im z\| < \delta\}$. Suppose moreover that $\nabla_z^{(2)} H_0$, $\nabla_z H_1$, $\nabla_z A$ are bounded and continuous in $D(\delta)$. Then, if we define*

$$\Gamma := \sup_{z \in D(\delta)} \|J \nabla_z^{(2)} H_0(z)\|,$$

we have the following improvement of Theorem 1.4, saying that $\hbar^{-1}(A(t,z) - A \circ \Phi^t)$ is an analytic semi-classical observable, with control in time. More explicitely, there exist constants $K_0 > 0, K_1 > 0$ such that for every $t \in \mathbb{R}$, $j \in \mathbb{N}$, $z \in Z$, $N \geq 1$ and $\hbar \in]0, 1]$,

$$|\partial_z^\gamma A_j(t,z)| \leq K_0(j+|\gamma|)! K_1^{j+|\gamma|}(1+|t|)^j \exp(\Gamma(2j-1+|\gamma|)|t|); \tag{23}$$

and the following estimate in L^2 operator-norm of the remainder term :

$$\|\hat{A}(t) - \sum_{0 \leq j \leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq \hbar^{N+1} K_0 (N+1)! K_1^{N+1} |t|(1+|t|)^{N+\delta_n} \exp(\Gamma(2N+\delta_n)|t|). \tag{24}$$

where $\delta_n \leq 5n+3$ is a universal constant.

Remark 1.9 *As in the C^∞-case, if the expansion of H in $\hbar$ is even then in the estimates (23) and (24), in the exponential term, the $2N$ becomes $3N/2$. This remark is an extension of the remark concerning the "classical" observables.*

We can deduce from Theorem 1.8 a semi-classical approximation of $A(t)$ with an exponentially small error in $\hbar$, for long time intervals.

Corollary 1.10 *Under the assumptions of Theorem 1.8, for every $\varepsilon > 0, C > 0$, such that $\varepsilon + 2C\Gamma < 1$, there exist constant $K > 0$, $a > 0$, such that for $|t| \leq C\log(\hbar^{-1})$ and $N = [\frac{a}{\hbar^\varepsilon}]$ we have*

$$\|\hat{A}(t) - \sum_{0\leq j\leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq K \exp\left(-\frac{a}{\hbar^\varepsilon}\right). \tag{25}$$

In applications it can be useful to consider observables with support outside some given non empty open set. Such observables can not be analytic but can be in some Gevrey class $s > 1$. Let us introduce the following technical assumptions :

- (C.0) H is analytic in $D(\delta)$ and there exist $C > 0$, $M \geq 0$ such that

$$|H(z)| \leq C(1 + |z|)^M, \ \ \forall z \in D(\delta). \tag{26}$$

  Moreover $\hat{H}$ is supposed to be self-adjoint in $L^2(\mathbb{R}^n)$.

- (C.1) Let Ω be a bounded open subset of Z such that $\bar{\Omega}$ is Φ^t-invariant for every $t \in \mathbb{R}$ and A a smooth observable such that $\mathrm{supp}(A) \subset \Omega$.

- (C.2) A is Gevrey $s > 1$.

Let us define

$$\Gamma_\delta := \sup_{\Re z\in\Omega; \Im z<\delta} |||J\nabla_z^{(2)} H(z)|||.$$

Theorem 1.11 *Let us assume* (C.0), (C.1), (C.2). *Then we have the following estimates, for some constant K_0, K_1,*

$$|\partial_z^\gamma A_j(t,z)| \leq K_0(3j/2 + |\gamma|)!^s (j/2)!^{-1} K_1^{j+|\gamma|} |t|(1 + |t|)^j \exp(\Gamma_\delta(3j/2 + |\gamma|)|t|); \tag{27}$$

and the following estimate in L^2 operator-norm of the remainder term :

$$\|\hat{A}(t) - \sum_{0\leq j\leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq \hbar^{N+1} K_0 (N+1)!^{(3s-1)/2} K_1^{N+1} |t|(1+|t|)^N \exp(\Gamma_\delta(3N/2+\delta_n)|t|). \tag{28}$$

where δ_n is a universal constant. Moreover, as above, we have a long time approximation of $\hat{A}(t)$ with exponentially small error estimate :
for every $\varepsilon > 0, C > 0$, such that $\varepsilon(3s-1)/2 + 3C\Gamma/2 < 1$, there exist constants $K > 0$, $a > 0$, such that for $|t| \leq C\log(\hbar^{-1})$, $N = [\frac{a}{\hbar^\varepsilon}]$ and $\hbar \in]0, 1]$, we have

$$\|\hat{A}(t) - \sum_{0\leq j\leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq K \exp\left(-\frac{a}{\hbar^\varepsilon}\right). \tag{29}$$

Remark 1.12 *If in condition (C.1) $\bar{\Omega}$ in Φ^t-invariant for every $t \geq 0$ (resp $t \leq 0$) then all the conclusions of the previous theorem hold for $t \geq 0$ (resp. $t \leq 0$).*

The above results are general and do not depend on specific properties of the classical dynamic. Nevertheless some important systems in classical and quantum mechanics are integrable and for them we can prove much better results : the semiclassical expansions are valid for time less than some algebraic power $\hbar^{-1}$ instead of $O(\log(\hbar^{-1}))$ (which is optimal for instable systems). Let us first introduce the following analytic-integrability condition :

- (C.3) There exists a symplectic map χ from Ω into $\mathcal{A}\times\mathbf{T}^n$ where $\mathcal{A}$ is an open set in $\mathbb{R}^n$, $\mathbf{T}^n$ is an n-dimensional torus, such that

$$\chi(\Phi^t(z)) = (I(z), \varphi(z) + t\omega(I(z))), \quad \text{where } \chi(z) = (I(z), \varphi(z)), \forall z \in \Omega, \forall t \in \mathbb{R}. \quad (30)$$

  Moreover there exist complex open neighborhoods $\tilde{\Omega}$, $\tilde{\mathcal{A}}$, $\tilde{\mathbf{T}}^n$ of $\Omega, \mathcal{A}, \mathbf{T}^n$ such that χ is an analytic diffeomorphism from $\tilde{\Omega}$ onto $\tilde{\mathcal{A}}\times\tilde{\mathbf{T}}^n$.

Theorem 1.13 *Let us assume conditions* (C.0), (C.1), (C.2), (C.3). *Then we have the following Gevrey type estimates, for some constants* K_0, K_1,

$$|\partial_z^\gamma A_j(t,z)| \leq K_0(3j/2+|\gamma|)!^s (j/2)!^{-1} K_1^{j+|\gamma|}(1+|t|)^{|\gamma|+2j}; \quad (31)$$

and the following estimate in L^2 *operator-norm of the remainder term :*

$$\|\hat{A}(t) - \sum_{0\leq j\leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq \hbar^{N+1} K_0 (N+1)!^{(3s-1)/2} K_1^{N+1} |t|(1+|t|)^{2N+\delta_n} \quad (32)$$

where $\delta_n \leq 5n+3$ *is a universal constant. Moreover as above we have a long time approximation of* $\hat{A}(t)$ *with exponentially small error estimate :*
for every $\varepsilon > 0$, *there exist* $K > 0$, $a > 0$, *such that for* $|t| \leq C\hbar^{-1/2+\varepsilon}$ *and* $N = [\frac{a}{\hbar^{3\varepsilon/(2s-1)}}]$ *we have*

$$\|\hat{A}(t) - \sum_{0\leq j\leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq K \exp\left(-\frac{a}{\hbar^{3\varepsilon/(2s-1)}}\right). \quad (33)$$

Remark 1.14 *Many integrable systems satisfy condition* (C.3). *Let us assume that the system is analytic-integrable in the Liouville sense. That means that there exist n real-analytic Hamiltonians* F_1, ..., F_n *in* Ω *with* $F_1 = H$, *Poisson commuting,* $\{F_j, F_k\} = 0$. *Assume that* $F := (F_1, \cdots, F_n)$ *is a regular map from* $\bar{\Omega}$ *into* $\mathbb{R}^n$ *and that for every* $\lambda \in F(\Omega)$, $F^{-1}(\lambda) \cap \bar{\Omega}$ *is a compact and connected component of* $F^{-1}(\lambda)$. *Then revisiting the proof of Liouville Theorem (Arnold [AR]) we can prove that* (C.3) *is satisfied.*

Remark 1.15 *Let us recall that only even terms* A_j *appear in Theorem 1.13. In the more general case with non null subprincipal terms* ($H = H_0 + \hbar H_1$) *where* H_1 *is analytic and* H_0 *analytically integrable in* Ω *then odd terms contribute and in the above estimates we have to replace* $(3s-1)/2$ *by* $2s-1$. *In particular the exponential error estimate holds for a smaller time* $|t| \leq \hbar^{-1/3+\varepsilon}$.

Remark 1.16 *Estimates (18) and (24) improve results given in [Iv] and in [BGP] in different ways. In the* C^∞ *case, we get results similar to those of [BGP] without analyticity assumptions and with a better control for large time. In the analytic and Gevrey cases we get better estimates with respect to N and t (see (24)). Note that in [BGP] the* $A_j(t)$*'s are not defined through the algorithm (14).*
Similar exponential estimates were recently proved in [HJ] for propagation of Gaussian coherent states.

Remark 1.17 *The above results still hold true if the Hamiltonian H has singularities (like Coulomb ptentials) outside of Ω. This will be comment in section 4.*

Remark 1.18 *The above results are still valid for Hamiltonians H which admit singularities (e.g. Coulomb potential) outside Ω (see comments in section 4).*

Example 1.19 *Our results apply in particular to the following examples :*

1. *$H(q,p) = \|p\|^2 + V(q)$, $A(q,p) = q_1$ with V holomorphic in $\{q \in \mathbb{C}^n,\ \|\Im q\| < \delta\}$, for some $\delta > 0$ and such that*
$$\sup_{\{q\in\mathbb{C}^n,\ \|\Im q\|<\delta\}} \|\nabla_q^{(2)} V(q)\| < +\infty.$$
2. *$H(q,p) = \sqrt{1+\|p\|^2} + V(q)$ with V and A as above.*

A natural question in the study of remainders in Egorov's Theorem is to know in which way the error bounds are optimal. More precisely, this raises the question whether remainders actually do have exponential growth in generic cases. We treat this problem in section 6 through two examples of Schrödinger Hamiltonians for which exponential remainders are highlighted. The sections 2, 3 and 4 are respectively devoted to the proof of Theorems 1.4, 1.8 and 1.13. Another related problem is to study the evolution of the quantum observables $\hat{A}(t)$ along coherent states ϕ_z ($z \in Z$), defined by the mean value quantity $\langle \hat{A}U(t)\phi_z, U(t)\phi_z\rangle$, when $\hbar$ goes to zero. It's a kind of "weak" version of our main results. It is well known that as long as t (possibly depending on $\hbar$) is reasonably big then $U(t)\phi_z$ stays concentrated around the classical trajectory $\Phi^t(z)$. We give in section 5 estimates of the maximum duration of this phenomenon (Ehrenfest time) and discuss our results with similar previous ones.

2 The C^∞ case

The goal of this section is to prove Theorem 1.4. In order to control derivatives of observables moving along the classical flow, we shall use the Faà de Bruno formula [Co] :

Lemma 2.1 *Let $g : \mathbb{R}^d \to \mathbb{R}^d$ and $f : \mathbb{R}^d \to \mathbb{R}$ smooth enough mappings defined in suitable neighborhoods. Then for $\alpha \in \mathbb{N}^d$, we have*

$$\partial^\alpha (f\circ g) = \sum_{\gamma\neq 0, \gamma\leq\alpha} (\partial^\gamma f)\circ g \cdot \mathcal{B}_{\alpha,\gamma}[\partial^\beta g], \text{ where} \tag{34}$$

$$\mathcal{B}_{\alpha,\gamma}[\partial^\beta g] = \alpha! \sum_{\substack{\sum_\beta \beta = \gamma \\ \sum_\beta \beta |a_\beta| = \alpha}} \prod_{0\neq\beta\in\mathbb{N}^d} \frac{1}{a_\beta!}\left(\frac{\partial^\beta g}{\beta!}\right)^{a_\beta}.$$

In formula (34), β and a_β are multi-index and we have used the usual rules for multi-index. Let us explain one term. We have $g = (g_1, \cdots g_d) \in \mathbb{R}^d$, $a_\beta = (a_{\beta,1}, \cdots, a_{\beta,d})$, $\beta! = \beta_1! \cdots \beta_d!$, then

$$\left(\frac{\partial^\beta g}{\beta!}\right)^{a_\beta} = \left(\frac{\partial^\beta g_1}{\beta!}\right)^{a_{\beta,1}} \cdots \left(\frac{\partial^\beta g_d}{\beta!}\right)^{a_{\beta,d}}. \tag{35}$$

Our first step is to estimate the classical flow.

Lemma 2.2 *For every $\gamma \in \mathbb{N}^{2n}$, there exists $C_\gamma > 0$ such that*

$$\forall t \in \mathbb{R},\ \forall z \in Z,\quad \|\partial_z^\gamma \Phi^t z\| \leq C_\gamma \exp(|\gamma||t|\Gamma) \tag{36}$$

Proof : We proceed by induction on $|\gamma|$. We start with the Jacobi stability equation

$$\frac{d}{dt}\nabla_z \Phi^t(z) = J\nabla_z^{(2)} H_0(\Phi^t z)\nabla_z \Phi^t z. \tag{37}$$

Using the definition of Γ and the Gronwall inequality, we get (36) for $|\gamma| = 1$ with $C_\gamma = 1$. For $|\gamma| = k \geq 2$, let us assume that (36) holds for $|\gamma| < k$. Computing derivatives in z of (37) and applying Faà de Bruno formula, we get

$$\frac{d}{dt}\partial_z^\gamma(\Phi^t z) = \gamma! \sum_{|\alpha|=1} \partial^\alpha (J\nabla_z H_0)(\Phi^t z)(\partial_z^\gamma \Phi^t z)^\alpha + Y(t). \tag{38}$$

Using induction assumption, there exists $C > 0$ such that

$$\forall t \in \mathbb{R},\ \ \|Y(t)\| \leq C \exp(\Gamma|\gamma||t|). \tag{39}$$

To complete the proof of the lemma, we need some standard properties of linear differential equations which are recalled in the following lemma.

Lemma 2.3 *Let us consider the linear differential equation*

$$\frac{d}{dt}X(t) = M(t)X(t) + Y(t), \tag{40}$$

where $M(t)$ is a smooth family of $d \times d$ matrices defined on $\mathbb{R}$ such that $\Gamma = \sup_{t\in\mathbb{R}} \|M(t)\| < +\infty$. Let $R(t,s)$ be the resolvent of the homogeneous system i.e such that

$$\frac{\partial R(t,s)}{\partial t} = M(t)R(t,s),\quad R(s,s) = \mathbb{1}. \tag{41}$$

Then we have

$$X(t) = R(t,0)X(0) + \int_0^t R(t,s)Y(s)ds,\ \text{ and} \tag{42}$$

$$\|R(t,s)\| \leq \exp(\Gamma|t-s|),\ \ \forall t,s \in \mathbb{R}. \tag{43}$$

In particular, if $\|Y(t)\| \leq C\mathrm{e}^{K|t|}$ with $K \geq \Gamma$, then there exists $C' > 0$ such that

$$\|X(t)\| \leq C'\mathrm{e}^{K|t|}\ \ \forall t \in \mathbb{R}. \tag{44}$$

Using the inequality (36) and the Faà de Bruno formula again, we get easily the next lemma.

Lemma 2.4 *For every multi-index $\gamma \neq 0$, there exists $C_{0,\gamma} > 0$ such that*

$$\forall t \in \mathbb{R}, \forall z \in Z,\quad |\partial_z^\gamma A_0(t,z)| \leq C_{0,\gamma} \exp(\Gamma|\gamma||t|) \tag{45}$$

Now using the induction formula (14), the Leibniz formula and again the Faà de Bruno formula, we get estimates for $A_j(t)$.

Lemma 2.5 *For every $j \geq 1$ and every multi-index γ, there exists $C_{j,\gamma} > 0$ such that for every $z \in Z$ and every $t \in \mathbb{R}$, we have*

$$|\partial_z^\gamma A_j(t,z)| \leq C_{j,\gamma} \exp(\Gamma(2j-1+|\gamma|)|t|). \tag{46}$$

Now we want to estimate the error term in the propagation of observables. Let us define

$$A^{(N)}(t) := \sum_{0 \leq j \leq N} \hbar^j A_j(t). \tag{47}$$

Recall that the Moyal bracket, $\{K,B\}^*$ of two observables K, B is defined as the Weyl symbol of $\frac{i}{\hbar}[\hat{K},\hat{B}]$ which admits the following formal $\hbar$-expansion

$$\{K,B\}^* \asymp \sum_{j \geq 0} \hbar^j \{K,B\}_{j+1}.$$

Using the rule product (see Appendix), we can expand $\{H,B\}^*$ in a power serie in $\hbar$,

$$\begin{aligned} \{H,B\}^* = \{H_0,B\}_1 + \hbar(\{H_0,B\}_2 + \{H_1,B\}_1) + \cdots + \\ \hbar^{k-1}(\{H_0,B\}_k + \{H_1,B\}_{k-1}) + \hbar^k(\delta^k_{H_0,B} + \delta^{k-1}_{H_1,B}) + \cdots \end{aligned} \tag{48}$$

where $\{H_0,B\}_1$ is the usual Poisson bracket (see (5)). The remainder term is given by the remainder term in the product rule, with notations defined in Appendix,

$$\delta^k_{H,B} = i\hbar^{-k-1}(R_k(H,B) - R_k(B,H)). \tag{49}$$

The algorithm used to construct the A_j's is such that we have

$$\frac{d}{dt}A^{(N)}(t) = \{H, A^{(N)}(t)\}^* + \hbar^{N+1} R^{(N+1)}(t), \tag{50}$$

where

$$R^{(N+1)}(t) = \delta^{N+1}_{H_0,A_0} + \cdots + \delta^1_{H_0,A_N} + \delta^N_{H_1,A_0} + \cdots + \delta^0_{H_1,A_N}. \tag{51}$$

The following lemma gives the error in L^2-operator norm.

Lemma 2.6 *For every $N \in \mathbb{N}$ and every $t \in \mathbb{R}$, we have*

$$\|\hat{A}(t) - \hat{A}^{(N)}(t)\|_{L^2} \leq \hbar^{N+1}|t| \sup_{|s| \leq |t|} \|\hat{R}^{(N+1)}(s)\|_{L^2}. \tag{52}$$

Proof : Let us denote $E(t) = \hat{A}(t) - \hat{A}^{(N)}(t)$ and compute (15)

$$\frac{d}{ds}U(-s)E(t-s)U(s) = U(-s)\left\{\frac{i}{\hbar}[\hat{H}, E(t-s)] - \frac{d}{dt}E(t-s)\right\}U(s). \tag{53}$$

After integration in s and using $E(0) = 0$, we get the lemma. ∎

End of the proof of Theorem 1.4 : Using Appendix, we can estimate L^∞-norms of the derivatives of $\delta^{N+1-j}_{H_i,A_j(t)}$ and then conclude using the Calderon-Vaillancourt Theorem, with

the recent improvement by A. Boulkhemair ([Bo]). The statement is the following. There exists γ_n such that for all $B \in \mathcal{O}(0)$, we have :

$$\|\hat{B}\|_{L^2} \leq \gamma_n \sup_{\substack{|\alpha|,|\beta| \leq [n/2]+1 \\ z \in Z}} |\partial_z^{\alpha,\beta} B(z)|. \tag{54}$$

∎

By revisiting the proof, we can easily see that the conclusions of Theorem 1.4 are still valid if the following conditions on the Hamiltonian H and the observable A are fulfilled. For simplicity we assume that H is classical. We relax growth assumptions on H but we reinforce assumptions on the observable A.

- (C.4) there exists $M > 0$ such that for every $\gamma \in \mathbb{N}^{2n}$ there exists C_γ such that

$$|\partial_z^\gamma H(z)| \leq C_\gamma (1 + |z|)^M, \quad \forall z \in \mathbb{R}^{2n}, \tag{55}$$

- (C.5) Let A a smooth observable such that $\mathrm{supp}(A) \subset \Omega$ where $\bar{\Omega}$ is a compact, Φ^t-invariant set of Z, $\forall t \geq 0$. Let us introduce the real number

$$\Gamma := \sup_{z \in \Omega} |||J \nabla_z^{(2)} H(z)|||.$$

Proposition 2.7 *Let us assume that H and A satisfy the conditions* (C.4), (C.5). *Then the following estimates holds, for every $t \geq 0$ and $j \geq 0$,*

$$|\partial_z^\gamma A_j(t,z)| \leq C_{j,\gamma} \exp(\Gamma(3j/2 + |\gamma|)|t|). \tag{56}$$

Furthermore we have the following estimates in L^2 operator-norm of the remainder term. For every $N \in \mathbb{N}$ there exists C_N such that we have

$$\|\hat{A}(t) - \sum_{0 \leq j \leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq C_N \hbar^{N+1} \exp(\Gamma(3N/2 + \delta_n)|t|). \tag{57}$$

As we shall see later in more details for integrable sytems, when the classical system is stable it is expected that the quantum motion stays localized in the phase space for much larger time interval. This can be easily proved for periodic systems as we shall see now. Let us consider a classical Hamiltonian H and an observable A satisfying the assumptions (C.4), (C.5) with $\bar{\Omega}$ is a connected component of the compact set $H^{-1}([E_1, E_2])$ where $E_1 < E_2$. Let us introduce the following periodicity property :

- (Per) (i) For every $\lambda \in [E_1, E_2]$, $H^{-1}(\lambda) \cap \bar{\Omega}$ is a compact connected component of $H^{-1}(\lambda)$.
  (ii) $\nabla H(z) \neq 0$ for every $z \in \bar{\Omega}$.
  (iii) The Hamiltonian flow Φ_H^t defined by H is periodic with period $T(z)$ in Ω where T is a smooth function in Ω.

Proposition 2.8 *Let us assume that A and H satisfy the above assumptions, in particular* (Per). *Then for any N there exists $C_N > 0$ such that for any time $t \in \mathbb{R}$,*

$$\|\hat{A}(t) - \sum_{0 \leq j \leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq C_N \hbar^{N+1} |t| (1 + |t|)^{2N+\delta_n}. \tag{58}$$

where δ_n is a universal constant. In particular the semiclassical regime is still valid in time interval $[-\hbar^{\epsilon-1/2}, \hbar^{\epsilon-1/2}]$ for every $\epsilon > 0$, and the quantum particle stays localized close to the classical trajectory in this time interval.

Proof : We have to revisit the proof of Theorem 1.4 in this particular case. The proof of Proposition 2.8 is clear if we can choose the period $T(z)$ constant in Ω. Indeed, under this stronger assumption, for any multi-index $\gamma \in \mathbb{N}^{2n}$, there exists $C_\gamma > 0$, such that for all $z \in \Omega$ and all $t \in \mathbb{R}$, we have the uniform control in time : $|\partial_z^\gamma A(\Phi^t z)| \leq C_\gamma$. This is easily proved using conservation of the energy and the periodicity of the flow. Using the induction formula (14), the derivatives of the A_j's are also uniformly controled in time for the same reasons. To get the conclusion, we follow again the same method as in the C^∞-case (see proof of Theorem 1.4).
When the period is not constant but is smoothly varying, we can replace the Hamiltonian H by a new one, $\widetilde{H} = f(H)$, such that the Hamiltonian flow for $\widetilde{H}$ has a constant period in Ω. For a detailed construction of f we refer for exemple to [DS]. In particular we have $f'(E) \neq 0$ for $E \in [E_1, E_2]$ and

$$\Phi_H^t(z) = \Phi_{\tilde{H}}^{t/f'(H(z))}(z), \quad \forall z \in \Omega.$$

We get from that $|\partial_z^\gamma A(\Phi^t z)| \leq C_\gamma (1 + |t|)^{|\gamma|}$. We then finish the proof using the same method as for Theorem 1.4. ∎

3 The analytic case

To prove Theorem 1.8, we shall use the same strategy as for Theorem 1.4. For simplicity, we assume that $H = H_0 + \hbar H_1$. The general case is not more difficult. Let us point out that we will use in this section the same notation to define the Hermitian norm on $\mathbb{C}^n$ and on $\mathbb{C}^{2n}$; that is $\|\cdot\|$. First of all, we estimate the classical flow in complex domains (similar estimates are considered in [BGP]). That is under the assumptions of Theorem 1.8, we have

Lemma 3.1 *Φ^t is holomorphic in $\Omega(\delta e^{-|t|\ \Gamma})$ and the following estimate holds*

$$\|\partial_z^\gamma \Phi^t z\| \leq \gamma! \delta^{1-|\gamma|} \exp(|\gamma||t|\ \Gamma), \quad \forall \gamma \in \mathbb{N}^{2n},\ |\gamma| \geq 1,\ \forall z \in Z. \tag{59}$$

Moreover if $0 \leq s \leq t$ or if $t \leq s \leq 0$, for $\tau \in [0,1]$, we have

$$\|\Im z\| \leq \tau\delta e^{-|t|\Gamma} \Rightarrow \|\Im(\Phi^{t-s} z)\| \leq \tau\delta e^{-|s|\Gamma}. \tag{60}$$

Proof : We can assume that $t > 0$. Let us consider the differential equation

$$\frac{d}{dt}\Phi^t z = F(\Phi^t z),\ \Phi^0 z = z \tag{61}$$

where $F(z) := J\nabla_z H_0(z)$. $F(\cdot)$ is then holomorphic in $\Omega(\delta)$. Using Lemma 2.3 on linear differential, we get easily

$$\|\Im\Phi^s z\| < \delta,\ \forall s \in [0,t'] \Rightarrow \|\nabla_z \Phi^s z\| < \mathrm{e}^{s\Gamma},\ \ \forall s \in [0,t']. \tag{62}$$

We also have

$$\|\Im\Phi^s z\| \leq \|\Phi^s z - \Phi^s(\Re z)\| \leq \|\Im z\| \sup_{\|y\| \leq \|\Im z\|} \|\nabla_z \Phi^s(\Re z + iy)\|. \tag{63}$$

Let us assume now that $\|\Im z\| < \delta \mathrm{e}^{-t\Gamma}$ and define

$$t' = \sup\{t'' > 0,\ \|\Im\Phi^s\zeta\| < \delta, \forall\zeta,\ \|\Im\zeta\| \leq \|\Im z\|,\ \forall s \in [0,t'']\}.$$

Using (62) and (63), we get

$$\|\Im\Phi^{t'}\zeta\| \leq \mathrm{e}^{(t'-t)\Gamma},\ \forall\zeta,\ \|\Im\zeta\| \leq \|\Im z\|. \tag{64}$$

So that for $\varepsilon > 0$, we have $\|\Im\Phi^{t'+\varepsilon}\zeta\| < \delta$ which contradicts the assumption on t' and proves that $t' = t$. This proves (60) for $s = 0$. To prove it for all $s \in [0,t]$, we use the same method but taking $\tau\delta\mathrm{e}^{-s\Gamma}$ as a new δ and $t - s$ as a new t. Finally, using smoothness for solutions of differential equations, we get that Φ^t is holomorphic in $\Omega(\delta\mathrm{e}^{-t\Gamma})$. Then using Cauchy inequalities, we get (59). ∎

From the above lemma and Cauchy inequalities, we get also the following estimates.

Lemma 3.2 *There exists a constant $M > 0$ such that for every $\gamma \in \mathbb{N}^{2n}$, $|\gamma| \geq 1$, $z \in \Omega(\delta\mathrm{e}^{-\Gamma|t|})$, we have*

$$|\partial_z^\gamma [A(\Phi^t(z))]| \leq M\gamma!\delta^{1-|\gamma|}\mathrm{e}^{\Gamma|\gamma||t|}. \tag{65}$$

To prove Theorem 1.8, the analyticity assumptions on H and A will also be used through the following lemma (see also [Tr]).

Lemma 3.3 *Let $f : \Omega(\delta) \to \mathbb{C}$ be an holomorphic function, where $\Omega(\delta) = \{z \in \mathbb{C}^d, \|\Im z\| < \delta\}$. For $\tau \in]0,1[$, let us define*

$$\|f\|_\tau = \sup_{z \in \Omega(\tau\delta)} |f(z)|.$$

And assume that there exist $M > 0, a \geq 0$ such that

$$\|f\|_\tau \leq M\left(\frac{e}{1-\tau}\right)^a,\ \forall\tau \in]0,1[. \tag{66}$$

Then $\forall\gamma \in \mathbb{N}^d$, $\forall\tau \in]0,1[$, we have

$$\|\partial_z^\gamma f\|_\tau \leq M\delta^{-|\gamma|}(a+1)\cdots(a+|\gamma|)\left(\frac{e}{1-\tau}\right)^{a+|\gamma|}. \tag{67}$$

Proof : Let us start with $|\gamma| = 1$. Using the Cauchy inequality, we have that $\forall \tau' \in]0, \tau[$,

$$\|\frac{\partial f}{\partial z_j}\|_{\tau'} \leq \frac{\delta^{-1}}{\tau - \tau'} \|f\|_{\tau}. \tag{68}$$

Using now (66) with $\tau = \tau' + \frac{1-\tau'}{1+a}$ and the elementary inequality $\left(\frac{1+a}{a}\right)^a \leq e$, we get

$$\|\frac{\partial f}{\partial z_j}\|_{\tau'} \leq M \delta^{-1} (a+1) \left(\frac{e}{1-\tau'}\right)^{a+1}. \tag{69}$$

Then coming back to the notation $\tau' = \tau$, we prove easily the lemma by induction on $|\gamma|$. ∎

The proof of Theorem 1.8 is based on the following estimate.

Proposition 3.4 *Let A and H satisfying the assumptions of Theorem 1.8. Then there exist two constant K_0 and K_1 such that for all $j \geq 1$, $t \in \mathbb{R}$, $\tau \in]0, 1[$ we have*

$$\sup_{z \in \Omega(\tau\delta \mathrm{e}^{-|t|\Gamma})} |A_j(t,z)| \leq K_0 \left\{ \left(\frac{\mathrm{e}}{1-\tau}\right)^{j-1} \mathrm{e}^{(2j-1)|t|\Gamma} \right\} \sum_{1 \leq m \leq j} \frac{(j+m)!}{m!} |t|^m \begin{pmatrix} j-1 \\ m-1 \end{pmatrix} K_1^{j+m} \tag{70}$$

where $\begin{pmatrix} j-1 \\ m-1 \end{pmatrix} = \dfrac{(j-1)!}{(m-1)!(j-m)!}$.

Proof : We shall prove (70) by induction on j using the three previous lemmas. The estimate is clearly satisfied for $j = 1$. Indeed, according to Lemma 3.1 and formula (13), $A_1(t, \cdot)$ is holomorphic in the domain $\Omega(\tau\delta \mathrm{e}^{-|t|\Gamma})$. And then, from Lemma 3.2, there exists $K_0 > 0$ such that for any $z \in \Omega(\tau\delta \mathrm{e}^{-|t|\Gamma})$,

$$|A_1(t,z)| \leq K_0 \left(\frac{\mathrm{e}}{1-\tau}\right)^0 \mathrm{e}^{|t|\Gamma} |t|. \tag{71}$$

Note that by application of Lemma 3.3,

$$\sup_{z \in \Omega(\tau\delta \mathrm{e}^{-|t|\Gamma})} |\partial_z^\gamma A_1(t,z)| \leq K_0 \gamma! \left(\frac{\mathrm{e}}{1-\tau}\right)^{|\gamma|} \mathrm{e}^{(1+|\gamma|)|t|\Gamma} |t|. \tag{72}$$

Assume now that (70) is satisfied for $0 \leq \ell \leq j-1$. So that according to Lemmas 3.1 and 3.3, for $\|\Im z\| \leq \tau\delta \mathrm{e}^{-|t|\Gamma}$,

$$|\partial_z^\gamma A_\ell(t,z)| \leq M \left(\frac{\mathrm{e}}{1-\tau}\right)^{\ell-1+|\gamma|} \mathrm{e}^{(2\ell-1+|\gamma|)|t|\Gamma} \delta^{-|\gamma|} \gamma! \sum_{1 \leq m \leq \ell} \frac{(\ell+m)!}{m!} |t|^m \begin{pmatrix} \ell-1 \\ m-1 \end{pmatrix} K^{\ell+m}. \tag{73}$$

We apply now (14) and (73) to estimate each term in the sum given A_j . In particular we use the identity :

$$\begin{pmatrix} j-1 \\ m \end{pmatrix} = \sum_{m \leq k \leq j-1} \begin{pmatrix} k-1 \\ m-1 \end{pmatrix} \tag{74}$$

and the elementary inequality

$$\gamma! \leq |\gamma|! \leq 2^{|\gamma|}\gamma!. \tag{75}$$

So we can prove easily, using standard estimates, that (70) is satisfied. ∎

We then deduce the following result on the A_j's.

Corollary 3.5 *There exist $K_1 > 0$ and $K_2 > 0$ such that for every $\gamma \in \mathbb{N}^{2n}$, $j \in \mathbb{N}$ satisfying $|\gamma| + j \geq 1$, $t \in \mathbb{R}$ we have*

$$\sup_{z \in Z} |\partial_z^\gamma A_j(t,z)| \leq K_1(j+|\gamma|)!K_2^{j+|\gamma|}(1+|t|)^j \mathrm{e}^{(2j-1+|\gamma|)|t|_\Gamma}. \tag{76}$$

Proof : According to Lemma 3.3 and Proposition 3.4, the formula (73) is valid for any $j \geq 1$ in the domain $\Omega(\tau\delta \mathrm{e}^{-|t|_\Gamma})$ where τ is arbitrary small and $\delta > 1$. Note first that using (75), for $0 \leq m \leq j$,

$$\frac{(j+m)!}{m!} \leq \frac{(2j)!}{j!} \leq 4^j j!.$$

Thus for $\|\Im z\| \leq \tau\delta \mathrm{e}^{-|t|_\Gamma}$,

$$\begin{aligned} |\partial_z^\gamma A_j(t,z)| &\leq C_0 \left(\frac{\mathrm{e}}{1-\tau}\right)^{j-1+|\gamma|} \mathrm{e}^{(2j-1+|\gamma|)|t|_\Gamma}(j+|\gamma|)!(4C_1)^j \sum_{0 \leq m \leq j} \binom{j}{m} (|t|C_1)^m \\ &\leq C_0 \left(\frac{\mathrm{e}}{1-\tau}\right)^{j-1+|\gamma|} \mathrm{e}^{(2j-1+|\gamma|)|t|_\Gamma}(j+|\gamma|)!(4K)^j(1+C_1|t|)^j. \end{aligned}$$

The results follows by restriction to the real Euclidean space Z (taking τ small enough). ∎

End of the proof of Theorem 1.8 :
We follow the same method as in the C^∞-case, with the above estimates on A_j by using the Appendix and Lemma 2.6. We left the details to the reader. ∎

4 The Gevrey case

The proofs of the Gevrey estimates in Theorem 1.11 and Theorem 1.13 use the following more or less well known lemma :

Lemma 4.1 *Let us consider a real analytic map f from Ω_1 to Ω_2 where Ω_j is an open set in $\mathbb{R}^{n_j}$ and u a Gevrey s function from Ω_2 into the complex plane $\mathbb{C}$. Then $u \circ f$ is Gevrey s in Ω_1. More precisely there exist universal positive constants δ, δ_1 such that if there exist constants C_0, C_1, K_0, K_1 and*

$$|\partial_x^\alpha f(x)| \leq \alpha! K_0 K_1^{|\alpha|}, \qquad |\partial_z^\beta u(z)| \leq C_0 C_1^{|\beta|}\beta!^s, \tag{77}$$

then we have, for every real number r such that $0 < r \leq \frac{1}{2K_1}$ and $r \leq \frac{1}{2\delta K_0 K_1 C_1}$,

$$|\partial_x^\alpha (u \circ f)(x)| \leq \delta_1 C_0 r^{-|\alpha|}\alpha!^s. \tag{78}$$

Proof : As in L. Hörmander, Vol.1, [Ho], we fix $x \in \mathbb{R}^{n_1}$ and consider the Taylor expansion for u in $f(x)$, at order $k = |\alpha|$,

$$F(y) = \sum_{|\beta| \leq k} \frac{\partial_z^\beta u(f(x))}{\beta!}(f(y) - f(x))^\beta. \tag{79}$$

Note that $\partial_x^\alpha u \circ f(x) = \partial_y^\alpha F(y)|_{y=x}$. The lemma is then proved by applying the Cauchy integral formula to F. ∎

Theorem 1.11 is proved by induction on j, using several times Lemma 4.1. The main step to prove Theorem 1.13 is the following result :

Proposition 4.2 *There exist $K_0 > 0$, $K_1 > 0$ such that for all $t \in \mathbb{R}$, $j \in \mathbb{N}$, $z \in Z$, $\gamma \in \mathbb{N}^{2n}$ we have*

$$|\partial_z^\gamma A_j(t,z)| \leq K_0 K_1^{|\gamma|+3j/2}(1+|t|)^{|\gamma|+2j}(|\gamma|+3j/2)!^s (j/2)!^{-1} \tag{80}$$

Let us recall that $A_j = 0$ for j odd because here H has no lower order terms.
It is convenient to prove estimates first in action-angle variables and afterwards to use Lemma 4.1 to get estimates in position-momentum coordinates. So let us consider the new classical observables $\tilde{A}_j(t, I, \varphi) = A_j(t, \chi(I, \varphi + t\omega(I))$.

Lemma 4.3 *There exist $K_0 > 0$, $K_1 > 0$, $K_2 > 0$, such that for all $t \in \mathbb{R}$, $j \in \mathbb{N}$, $z \in Z$, $\gamma \in \mathbb{N}^{2n}$, we have*

$$|\partial_I^\alpha \partial_\varphi^\beta \tilde{A}_0(t, I, \varphi)| \leq K_0 K_1^{|\alpha|+|\beta|}(|\alpha|+|\beta|)!^s (1+|t|)^{|\alpha|} \tag{81}$$

and for $j \geq 2$,

$$|\partial_I^\alpha \partial_\varphi^\beta \tilde{A}_j(t, I, \varphi)| \leq K_0 K_1^{|\alpha|+|\beta|+3j/2}(|\alpha|+|\beta|+3j/2)!^{s-1}(1+|t|)^{|\alpha|+3j/2} \sum_{1 \leq m \leq j/2} (|\alpha|+|\beta|+j+m)! \frac{|t|^m}{m!} \binom{j/2-1}{m-1} K_2^m \tag{82}$$

Proof : For $j = 0$ we have $\tilde{A}_0(t, I, \varphi) = \tilde{A}(I, \varphi + t\omega(I))$ where $\tilde{A} := A \circ \chi^{-1}$. We know that $\tilde{A}$ is Gevrey s and ω is analytic so we get easily (81) from Lemma 4.1.
For $j \geq 2$, with some tedious but not very difficult computations, we can prove (82) by induction on j as we have done in the analytic case (see section 3). ∎

End of proof of Proposition 4.2 : It results easily using estimates (82) and systematic use of Lemma 4.1. ∎

End of proof of Theorem 1.13 : We get control of the remainder terms with the same method as in section 2, using Lemma 2.6, the Appendix and the Calderon-Vaillancourt Theorem. ∎

Remarks concerning Hamiltonians with singularities
For the statement of Theorems 1.11 and 1.13, smoothness of the Hamiltonian H is required

only on a flow invariant domain of Z containing the support of the observable A. These results can then be extended, as briefly explained below, in the case of local Hamiltonians of the form :

$$H(x,\xi) = \sum_{|\alpha|\leq m} a_\alpha(x)\xi^\alpha$$

satisfying for every α, $|\alpha| \leq m$:

- (H.1) $\partial_x^\beta a_\alpha \in L^1_{\ell oc}(\mathbb{R}^n)$, $\forall\ |\beta| \leq |\alpha|$.
- (H.2) There exists a compact $K \subset \mathbb{R}^n$ and $\rho > 0$ such that a_α is analytic in $I_K := \{\|\Im x\| < \rho,\ \Re x \notin K\}$ and satisfies in I_K, for some $C > 0$ and $M > 0$,

  $$|a_\alpha(x)| \leq C(1+|x|)^M.$$

  Moreover $\hat{H}$ is supposed to be self-adjoint in $L^2(\mathbb{R}^n)$.

As an example of such H, we can consider the following Coulomb like Hamiltonian on $\mathbb{R}^3$:

$$H(x,\xi) = \|\xi\|^2 + \sum_{j=1}^{L} \frac{c_j}{\|x - x^{(j)}\|} + W(x)$$

where $c_j \in \mathbb{R}$, $x^{(j)} \in \mathbb{R}^3$ and W satisfies (H.2) with $K = \emptyset$. Of course, one needs to adapt to this case the previous assumptions (C.1) and (C.2) concerning the observable A :

- (C'.1) Let Ω be a bounded open subset of Z such that $\bar{\Omega}$ is Φ^t-invariant for every $t \in \mathbb{R}$ and $\bar{\Omega} \subset \mathbb{R}^{2n} \setminus (K \times \mathbb{R}^n)$. The observable A is such that $supp(A) \subset \Omega$.
- (C'.2) A is Gevrey $s > 1$.

Under the assumptions (H.1), (H.2), (C'.1), (C'.2), we can prove that the singular region contributes in the Egorov Theorem by an error term which is of the same order as in the smooth case. This fact can be seen by standard commutator arguments and integrations by parts. We give here the main steps of the proof without going to the details.
Let us introduce two C^∞ cutoff functions χ and ζ where ζ is supported in a small neighborood of K such that $\zeta = 1$ on K and $\chi = 1$ on $supp(\zeta)$. The distance between the supports of ζ and $1-\chi$ is then positive. Write the commutator $[\hat{H}, \hat{A^{(N)}}(t)]$ as follows :

$$[\hat{H}, \hat{A^{(N)}}(t)] = [\hat{H}, \hat{A^{(N)}}(t)]\chi + \hat{H}\zeta\hat{A^{(N)}}(t)(1-\chi) + [\hat{H}(1-\zeta), \hat{A^{(N)}}(t)](1-\chi) \qquad (83)$$

In the last term of the r.h.s of (83) each operator has a smooth symbol so that we can use the same computations as in the C^∞ case with $\hbar$-pseudodifferential operators. We explain now how the first two terms give negligible contributions. We suppose here, to fix ideas, that the system is integrable in Ω so that the Gevrey estimates on $A_j(t)$ established in Theorem 1.13 are still valid under the above assumptions. Using now integration by parts, taking into account of the support of the involved symbols, we can estimate the integral kernel of operators $[\hat{H}, \hat{A_j}(t)]\chi$ and $\hat{H}\zeta\hat{A_j}(t)(1-\chi)$ to get the L^2 estimate :

$$\|[\hat{H}, \hat{B}]\chi\|_{L^2} + \|\hat{H}\zeta\hat{B}(1-\chi)\|_{L^2} \leq K_0 K_1^N N!^{(3s-1)/2}(1+|t|)^{2N}\hbar^N. \qquad (84)$$

By combination of (83) and (84), we then obtain the same L^2 estimate for $\hat{A(t)} - \hat{A^{(N)}}(t)$ as in Theorem 1.13. ∎

5 Propagation of coherent states and Ehrenfest time

Let us consider a usual Gaussian coherent state ϕ_{z_0} concentrated around the point $z_0 = (q_0, p_0)$ of the phase space, defined as follows :

$$\phi_{z_0} := W(z_0)\eta$$

where $\eta(x) = (\pi\hbar)^{-\frac{n}{4}} e^{-\frac{|x|^2}{2\hbar}}$ is the ground state of the n-dimensionnal harmonic oscillator $K_0 = \frac{1}{2}(P^2 + Q^2)$ and $W(z_0) = e^{-\frac{i}{\hbar}(q_0 P - p_0 Q)}$ is the unitary translation operator in the phase space. Here $P = -i\hbar\partial_x$ and $Q\psi(x) = x\psi(x)$. Note that $W(0,0) = Id$ so that η is concentrated at the origine (see [CR] for a more complete description of the Gaussian coherent states and [PU1] for a more general class). Here, we study the semiclassical limit of a quantum observable $\hat{A}(t)$ along the coherent state ϕ_{z_0} through the quantity $\langle \hat{A}(t)\phi_{z_0}, \phi_{z_0}\rangle$. In other words, we study the average on A of the quantum evolution $U(t)\phi_{z_0}$ of a well localized wave paquet ϕ_{z_0}. It is well known that $U(t)\phi_{z_0}$ stays concentrated around the classical trajectory $\Phi^t(z_0)$ (see Remark 5.2 below). Here we give an estimate of the duration $T_\hbar$, such that for $|t| \leq T_\hbar$, $\langle \hat{A}(t)\phi_{z_0}, \phi_{z_0}\rangle$ goes to its classical limit $A(\Phi^t(z_0))$ when $\hbar$ goes to zero. The following result can be interpreted as a weak version of Theorem 1.4.

Proposition 5.1 *Under the hypotheses of the Theorem 1.4, for any $\epsilon > 0$, we have the following uniform (in time) limit.*

$$\lim_{\substack{\hbar \searrow 0 \\ |t| \leq \frac{1-\epsilon}{2\Gamma} \ln(\frac{1}{\hbar})}} \Big(\langle \hat{A}(t)\phi_{z_0}, \phi_{z_0}\rangle - A(\Phi^t(z_0)) \Big) = 0. \tag{85}$$

Proof : Using the Wigner function of ϕ_{z_0} and the Weyl $\hbar$-symbol $A_\hbar(t,z)$ of $\hat{A}(t)$, we get the following well known integral :

$$\langle \hat{A}(t)\phi_{z_0}, \phi_{z_0}\rangle = (\pi\hbar)^{-n} \int_{\mathbb{R}^{2n}} A_\hbar(t,z) e^{-\frac{|z-z_0|^2}{\hbar}} dz. \tag{86}$$

Then since we are interested in the limit as $\hbar$ goes to zero, according to Theorem 1.4, one can substitute $\hat{A}_0(t)$ to $\hat{A}(t)$ in (86). So that we have now to estimate the following expression :

$$\begin{aligned} \rho(t,\hbar) &= (\pi\hbar)^{-n} \int_{\mathbb{R}^{2n}} A(\Phi^t(z)) e^{-\frac{|z-z_0|^2}{\hbar}} dz - A(\Phi^t(z_0)) \\ &= (\pi\hbar)^{-n} \int_{\mathbb{R}^{2n}} (A(\Phi^t(z)) - A(\Phi^t(z_0))) e^{-\frac{|z-z_0|^2}{\hbar}} dz. \end{aligned}$$

Now using the estimate $|\nabla_z A(\Phi^t(z))| \leq Ce^{\Gamma|t|}$ for any $t \in \mathbb{R}$ (see Lemma 2.4) and the Taylor formula, we get

$$\begin{aligned} |\rho(t,\hbar)| &\leq C'\hbar^{-n} \left(\int_{\mathbb{R}^{2n}} |z - z_0| e^{-\frac{|z-z_0|^2}{\hbar}} dz \right) e^{\Gamma|t|} \\ &\leq C''\hbar^{\frac{1}{2}} e^{\Gamma|t|}, \end{aligned}$$

where C', C" are constant independent on t and $\hbar$. Hence for any t satisfying $|t| \leq \frac{1-\epsilon}{2\Gamma}\ln(\frac{1}{\hbar})$ with $\epsilon > 0$, we have $|\rho(t,\hbar)| \leq C''\hbar^\epsilon$. ∎

Remark 5.2 *(i) Since for any $A \in \mathcal{O}(0)$, we have that*

$$\|\hat{A} - \hat{A}^{aw}\|_{L^2} = \mathcal{O}(\hbar)$$

where $\hat{A}^{aw}$ is the anti-Wick quantization of A, we can replace $\hat{A}$ by $\hat{A}^{aw}$ in (85) (see [HMR] for definition and properties of anti-Wick quantization) and consider the semiclassical Husimi measures :

$$\mu_{t,\hbar,z_0} : A \longmapsto \langle \hat{A}^{aw} U(t)\phi_{z_0}, U(t)\phi_{z_0}\rangle.$$

Then, if we denote by δ_ζ the Dirac measure in $\zeta \in Z$, the Proposition 5.1 means that we have the following uniform (in time) weak limit of measures. For any $\epsilon > 0$ we have

$$\lim_{\substack{\hbar \searrow 0 \\ |t| \leq \frac{1-\epsilon}{2\Gamma} \ln(\frac{1}{\hbar})}} \left(\mu_{t,\hbar,z_0} - \delta_{\Phi^t(z_0)}\right) = 0. \tag{87}$$

(ii) A result similar to (87) has been already obtained for some specific quantized hyperbolic maps on the torus (hyperbolic automorphisms and Baker map) [BDB].
(iii) In [CR] a result similar to Proposition 5.1 and (87) was obtained as a consequence of propagation results for coherent states but for smaller times : $|t| \leq \frac{1-\epsilon}{6\Gamma} \ln(\frac{1}{\hbar})$. So by the method of this paper we have improved 1/6 by 1/2.
(iv) Now, a natural question is what happens for times $|t| \geq \frac{1}{2\Gamma} \ln(\frac{1}{\hbar})$? An answer is given in [BDB] for quantized hyperbolic maps on the torus. After the critical time $T_\hbar := \frac{1}{2\Gamma} \ln(\frac{1}{\hbar})$, appears a new regime, called "mixing regime", where the Dirac measure at $\Phi^t(z_0)$ is replaced by some absolutely continuous measure on some flow invariant set (delocalization phenomenon).
For Schrödinger operators, and more generally for classical Hamiltonians H, we have already seen that the semiclassical expansion for the quantum observable $\hat{A}(t)$ is valid for $|t| \leq \frac{2-\epsilon}{3\Gamma} \ln(\frac{1}{\hbar})$ for every $0 < \epsilon$. This result suggests that the mixing regime is also accessible for Schrödinger operators, at least for some examples. In [DBR] we shall consider this problem, in particular when the starting point z_0 is an hyperbolic fixed point of the flow.

6 Examples

The goal of this section is to check through two examples that the error bounds in Theorems 1.4 and 1.8 are in some sense optimal. To this end, we establish, for these examples, exponential lower bounds of the remainder term. We have already seen in previous sections that for some particular (but important) dynamical sytems that this phenomenon does not hold. We suppose in our examples that $t > 0$. For the complementary case $t < 0$ we have the same results.

Example 1 :
Let us consider the semi-classical Hamiltonian

$$H = H_0 + \hbar H_1$$

where $H_0, H_1 : \mathbb{R}^2 \longrightarrow \mathbb{R}$ are defined as follows

$$H_0(q,p) = \frac{1}{2}(p^2 - q^2), \quad H_1(q,p) = \varepsilon q.$$

The linear Hamiltonian flow $\Phi^t : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$ associated to H_0 is given by

$$\Phi^t(q,p) = (q\cosh t + p\sinh t, q\sinh t + p\cosh t).$$

If we consider the observable $A(q,p) = q$, according to Theorem 1.4, we have that for any coherent states ϕ_z concentrated around the point $z = (q,p)$,

$$\lim_{\hbar\to 0} \frac{\langle \hat{A}(t)\phi_z, \phi_z\rangle - \langle \hat{A}_0(t)\phi_z, \phi_z\rangle}{\hbar} = A_1(t,z).$$

Using the formula (14), for any $z \in \mathbb{R}^2$ we have $A_1(t,z) = \varepsilon(\cosh t - 1)$. So that

$$\liminf_{\hbar\to 0} \frac{\|\hat{A}(t) - \hat{A}_0(t)\|_{L^2}}{\hbar} \geq \lim_{\hbar\to 0} \frac{\langle \hat{A}(t)\phi_z, \phi_z\rangle - \langle \hat{A}_0(t)\phi_z, \phi_z\rangle}{\hbar} = \varepsilon(\cosh t - 1). \tag{88}$$

Then, according to (88), we can assert that the remainder in Egorov's Theorem is exponentially large in time. Indeed, suppose that H and A are as above. More precisely there exists a function $M : \mathbb{R}^* \longrightarrow \mathbb{R}$ such that

$$\|\hat{A}(t) - \hat{A}_0(t)\|_{L^2} \leq \hbar M(t), \forall \hbar \in]0,1], \ \forall t > 0, \tag{89}$$

then there exists $C_\varepsilon > 0$ such that $M(t) \geq C_\varepsilon e^t$, $\forall t > 0$. ∎

Example 2 : (Non symmetric double well. Local phenomenon around an instable fixed point)
Let us consider the classical Hamiltonian H defined on $\mathbb{R}^2$ as follows :

$$H(q,p) = \frac{p^2}{2} + V(q)$$

where $V'(0) = 0$, $V''(0) = -1$ and $V^{(3)}(0) \neq 0$. The condition on the third derivative of V implies that the double well is non symmetric. It will ensure that the coefficient $A_2(t,0)$ in the formal expansion of the Heisenberg observable is not zero. Consider, for example, the following potential

$$V(q) = \frac{1}{4}(q^2-1)^2 - \frac{1}{4} + \frac{q^3}{3}\chi(q) \ \text{ where } \ \chi \in C_0^\infty(\mathbb{R}) \ \text{ and } \ \chi(0) \neq 0.$$

Note that the associated linearized flow at the equilibrium point is

$$\nabla_z \Phi^t(0,0) = \begin{pmatrix} \cosh t & \sinh t \\ \sinh t & \cosh t \end{pmatrix}.$$

According to the Theorem 1.4, if ϕ_0 is a coherent state concentrated around $(0,0)$, we have as in the previous example,

$$\lim_{\hbar\to 0} \frac{\langle \hat{A}(t)\phi_0, \phi_0\rangle - \langle \hat{A}_0(t)\phi_0, \phi_0\rangle}{\hbar^2} = A_2(t,0). \tag{90}$$

Suppose that A is a classical observable satisfying $A(q,p) := f(q)$ with $f'(0) = f''(0) = 0$ and $f^{(3)}(0) \neq 0$. According to the formula (14),

$$A_2(t,0) = \Gamma(0,3)V^{(3)}(0)f^{(3)}(0)\int_0^t (\sinh s)^3 ds.$$

Then, as in the previous example, we get the following inequality, for some $C > 0$

$$\liminf_{\hbar\to 0} \frac{\|\hat{A}(t) - \hat{A}_0(t)\|_{L^2}}{\hbar^2} \geq Ce^{3t},\ \forall t > 0.$$

Therefore, one concludes that if $M : \mathbb{R}^* \longrightarrow \mathbb{R}$ is a function satisfying

$$\forall t \geq 0, \forall \hbar \in]0,1],\quad \|\hat{A}(t) - \hat{A}_0(t)\|_{L^2} \leq \hbar^2 M(t), \tag{91}$$

then $M(t) \geq Ce^{3t}$, $\forall t > 0$. ∎

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A APPENDIX : Product of observables

Let us first recall the formal product rule for quantum observables with Weyl quantization. Let $A, B \in \mathcal{S}(Z)$. We look for a semi-classical observable C such that $\hat{A}\cdot\hat{B} = \hat{C}$. Some computations with the Fourier transform give the following formula [Ho]

$$C(q,p) = \exp\left(\frac{i\hbar}{2}\sigma(D_q, D_p; D_{q'}, D_{p'})\right) A(q,p)B(q',p')|_{(q,p)=(q',p')}, \tag{92}$$

where σ is the symplectic bilinear form (1) and $D = i^{-1}\nabla$. By expanding the exponential term, we get

$$C(q,p) = \sum_{j\geq 0} \frac{\hbar^j}{j!}(\frac{i}{2}\sigma(D_q, D_p; D_{q'}, D_{p'}))^j A(q,p)B(q',p')|_{(q,p)=(q',p')}. \tag{93}$$

So that $C(q,p)$ is a formal power serie in $\hbar$ with coefficients given by

$$C_j(q,p) = \frac{1}{2^j}\sum_{|\alpha+\beta|=j} \frac{(-1)^{|\beta|}}{\alpha!\beta!}(D_q^\beta \partial_p^\alpha A).(D_q^\alpha \partial_p^\beta B)(q,p). \tag{94}$$

It is well known that if A, B are observables with polynomial growth then C is a C^∞ semi-classical observable (see for example [Ho, Ro]). Here we need more accurate remainder estimates. Let us denote $A\#B = C$, $z = (q,p) \in Z$ and for every $N \geq 1$,

$$A\#B(z) - \sum_{0\leq j\leq N} \hbar^j C_j(z) =: R_N(A,B;z;\hbar). \tag{95}$$

The main result of this appendix is the following

Theorem A.1 *There exists $K_n > 0$ and for every $m \in \mathbb{N}$, $m \geq 4n$, for every $s > 4n$ there exists a constant $\rho_{n,m,s}$ such that for every $A, B \in \mathcal{S}(Z)$, for every $N \geq 1$, for every multi-index γ, the following estimate holds, for every $z \in Z$,*

$$|\partial_z^\gamma \left(A\#B(z) - \sum_{0 \leq j \leq N} \hbar^j C_j(z) \right)| \leq \hbar^{N+1} \rho_{n,m,s} K_n^{N+|\gamma|} (N!)^{-1} \cdots$$
$$\times \sup_{(*)} \left[(1+u^2+v^2)^{(s-m)/2} |\partial_u^{(\alpha,\beta)+\mu} A(u+z)| |\partial_v^{(\beta,\alpha)+\nu} B(v+z)| \right] \tag{96}$$

where $\sup_{(*)}$ *means that the supremum holds under the conditions* $u, v \in Z$, $|\mu| + |\nu| \leq m + |\gamma|$, $|\alpha| + |\beta| = N + 1$ *($\mu, \nu \in \mathbb{N}^{2n}$, $\alpha, \beta \in \mathbb{N}^n$).*

Proof : We follow [DR]. By Fourier transform computations and Taylor formula, we get the following formula

$$R_N(A, B; z; \hbar) = \frac{1}{N!} \left(\frac{i\hbar}{2} \right)^{N+1} \int_0^1 (1-t)^N R_{N,t}(z; \hbar) dt \quad \text{where} \quad R_{N,t}(z; \hbar) =$$
$$(2\pi\hbar t)^{-2n} \int \int_{Z \times Z} \exp(-\frac{i}{2t\hbar} \sigma(u, v)) \sigma^{N+1}(D_u, D_v) A(u+z) B(v+z) du dv. \tag{97}$$

We shall use the following lemma to estimate $R_{N,t}(z; \hbar)$.

Lemma A.2 *Let us consider $F \in \mathcal{S}(Z \times Z)$ and the integral*

$$I(\lambda) = \lambda^{2n} \int \int_{Z \times Z} \exp[-i\lambda\sigma(u, v)] F(u, v) du dv. \tag{98}$$

Then for every real number $s > 4n$ and every integer $m \geq 4n$ there exists $\kappa(n, s, m) > 0$ depending only on n, s, m (but independent of F) such that the following estimate holds

$$|I(\lambda)| \leq \kappa(n, s, m) \sup_{\substack{u,v \in Z, \\ |\mu|+|\nu| \leq m}} (1+u^2+v^2)^{s-m/2} |\partial_u^\mu \partial_v^\nu F(u, v)|. \tag{99}$$

Proof : This lemma is more or less standard (see [Ho]). For completeness, we give here a direct proof. Let us introduce a cut-off χ_0, C^∞ on $\mathbb{R}$, $\chi_0(x) = 1$ for $|x| \leq 1/2$ and $\chi_0(x) = 0$ for $|x| \geq 1$. We split $I(\lambda)$ into three pieces

$$I_0(\lambda) = \lambda^{2n} \iint_{Z \times Z} \exp[-i\lambda\sigma(u, v), \chi_0(\lambda(u^2+v^2)) F(u, v) du dv, \tag{100}$$

$$I_1(\lambda) = \lambda^{2n} \iint_{Z \times Z} \exp[-i\lambda\sigma(u, v)](1 - \chi_0(u^2+v^2)) \chi_0(\lambda(u^2+v^2)) F(u, v) du dv, \tag{101}$$

$$I_2(\lambda) = \lambda^{2n} \iint_{Z \times Z} \exp[-i\lambda\sigma(u, v)](1 - \chi_0(u^2+v^2)) F(u, v) du dv. \tag{102}$$

For $I_0(\lambda)$, we easily have

$$|I_0(\lambda)| \leq \omega_{4n} \sup_{u^2+v^2 \leq 1} |F(u, v)|, \tag{103}$$

where ω_{4n} is the volume of the unit ball in Z^2. For $I_1(\lambda)$ and $I_2(\lambda)$, we integrate by parts with the differential operator

$$L = \frac{i}{u^2+v^2}\left(Ju\frac{\partial}{\partial v} - Jv\frac{\partial}{\partial u}\right), \tag{104}$$

where J is the matrix associated to the symplectic form ($\sigma(u,v) =< Ju, v >$). Performing $4n$ integrations by parts, we can see that it exists a constant c_n such that

$$|I_1(\lambda)| \leq c_n \sup_{\substack{u^2+v^2\leq 1 \\ |\mu|+|\nu|\leq 4n}} |\partial_u^\mu \partial_v^\nu F(u,v)|. \tag{105}$$

Similarly, performing m integrations by parts, we get for a constant $c(n,s,m)$,

$$|I_2(\lambda)| \leq c_n \sup_{\substack{u,v\in Z \\ |\mu|+|\nu|\leq m}} (1+u^2+v^2)^{(s-m)/2} |\partial_u^\mu \partial_v^\nu F(u,v)|. \tag{106}$$

∎

Now we can complete the proof of the theorem by using Lemma A.2, the Leibniz formula and the following elementary estimate, using in Z the coordinates $u = (x,\xi)$, $v = (y,\eta)$,

$$\begin{aligned} &|\sigma^N(\partial_x, \partial_\xi; \partial_y, \partial_\eta))F(x,\xi)G(y,\eta)| \leq \\ &(2n)^N \sup_{|\alpha|+|\beta|=N} |\partial_x^\alpha \partial_\xi^\beta A(x,\xi) \partial_y^\beta \partial_\eta^\alpha B(y,\eta)|. \end{aligned} \tag{107}$$

∎

Remark A.3 *We can easily extend the estimate (96) for observables A, B with polynomial growth at infinity, by choosing m large enough to get a finite r.h.s. Let us assume that $A \in \mathcal{O}(\mu_A)$, $B \in \mathcal{O}(\mu_B)$, where $\mu_A, \mu_B \in \mathbb{R}$. Then we can apply (96) to $A_\varepsilon(u) = \mathrm{e}^{-\varepsilon u^2} A(u)$ and $B_\varepsilon(v) = \mathrm{e}^{-\varepsilon v^2} B(v)$ for $\varepsilon > 0$ and pass to the limit $\varepsilon \to 0$ with $m - s \geq \mu_A + \mu_B$.*

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