Uniform Semi-classical Estimates for the propagation of Heisenberg Observables

A. Bouzouina[1]

School of Mathematics, University of Cardiff (Wales)
23, Senghennydd Road, CF2 4YH Cardiff, Great Britain.
E-mail: Abdelkader.Bouzouina@univ-reims.fr

D. Robert

cnrs, umr 6629.
Département de Mathématiques, Faculté des Sciences de Nantes,
2, rue de la Houssinière, 44072 Nantes cedex 03, France.
E-mail: robert@math.univ-nantes.fr

Abstract

We prove here that the semi-classical asymptotic expansion for the propagation of quantum Heisenberg 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 Heisenberg observable is a semi-classical observable of index Gevrey 2 (3/2 if the Hamiltonian is purely classical, without lower terms in $\hbar$).

1 Introduction-Assumptions-Results

According to the Bohr's correspondance principle, the quantum evolution of one observable is close to its classical evolution as the Planck constant $\hbar$ is small. In the mathematical litterature 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.

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 Heisenberg observable. The main goal of this paper is to 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

[1]Permanent address: Département de Mathématiques, Université de Reims, BP 1039, F-51687 Reims Cedex 2.

time dependent Heisenberg 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 is $Z = X \times X$, a symplectic linear space equipped with the symplectic form σ defined through the restriction to $\mathbb{R}^n$ of the Hermitian scalar product $< \cdot, \cdot >$ on $\mathbb{C}^n$

$$\sigma(p, q; p', q') = \langle p, q' \rangle - \langle p', q \rangle, \quad q, q' \in X, \ p, p' \in X^*. \tag{1}$$

A classical Hamiltonian is a smooth real function $H : Z \mapsto \mathbb{R}$. Our basic example will be $H(q,p) = \frac{\|p\|^2}{2m} + V(q)$ $(m > 0)$ where $\|p\|^2 =< p, p >$. The motion of the classical system is determined by the system of Hamilton's equations

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}(q,p), \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}(q,p). \tag{2}$$

The equations (2) 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

$$\frac{d}{dt}A(\Phi^t(z)) = \{H, A\}(\Phi^t(z)), \quad z = (q,p) \tag{3}$$

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

$$\{H, A\} = \partial_q H \cdot \partial_p A - \partial_p H \cdot \partial_q A. \tag{4}$$

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

$$\frac{d\hat{A}(t)}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}], \tag{5}$$

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 $\psi \in \mathcal{S}(X)$,

$$\hat{A}\psi(x) = (2\pi\hbar)^{-n} \iint_Z A\left(\frac{x+y}{2}, p\right) \mathrm{e}^{i\hbar^{-1}\langle x-y, p\rangle}\psi(y)dydp \tag{6}$$

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 $Z \overset{A}{\to} \mathbb{C}$ 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

$$\sup_Z \langle z\rangle^{-m} \left|\partial_z^\gamma \left(A(\hbar, z) - \sum_{0\leq j\leq N} \hbar^j A_j(z)\right)\right| \leq C_N \hbar^{N+1}. \tag{7}$$

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 (7), 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 :*

$$|\partial_z^\gamma H_j(z)| \leq C_{\gamma j}, \text{ for } |\gamma| + j \geq 2 \tag{8}$$

$$\hbar^{-2}(H - H_0 - \hbar H_1) \in \mathcal{O}_{sc}(0), \tag{9}$$

$$|\partial_z^\gamma A(z)| \leq C_\gamma, \text{ for } |\gamma| \geq 1. \tag{10}$$

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

$$A_0(t, z) = A(\Phi^t(z)), \tag{11}$$

$$A_1(t, z) = \int_0^t \{A(\Phi^\tau), H_1\}\Phi^{t-\tau}(z)d\tau \tag{12}$$

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

$$A_j(t, z) = \sum_{\substack{|(\alpha,\beta)|+k+\ell=j+1\\ 0\leq\ell\leq j-1}} \Gamma(\alpha, \beta) \int_0^t [(\partial_p^\alpha \partial_q^\beta H_k)(\partial_p^\alpha \partial_q^\beta A_\ell)(\Phi^\tau)](\Phi^{t-\tau}(z))d\tau, \tag{13}$$

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

$$\frac{d}{ds}U(-s)\widehat{A_0}(t-s)U(s) = U(-s)\left\{\frac{i}{\hbar}[\hat{H}, \widehat{A_0}(t-s)] - \widehat{\{H, A_0\}}(\Phi^{t-s})\right\}U(s), \tag{14}$$

where $A_0(t) = A(\Phi^t)$. But, from the product rule formula (see Appendix), the principal symbol of $\frac{i}{\hbar}[\hat{H}, \hat{A}_0(t-s)] - \widehat{\{H, A_0\}}(\Phi^{t-s})$ vanishes. So, in the first step, we get the error term

$$U(-t)\hat{A}U(t) - \widehat{A_0}(t) = \int_0^t U(-s)\left(\frac{i}{\hbar}[\hat{H}, \widehat{A_0}(t-s)] - \widehat{\{H, A_0\}}\Phi^{t-s}\right)U(s)ds. \tag{15}$$

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 (because $U(t)$ is a metaplectic transformation).*

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*

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

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

$$|\partial_z^\gamma A_j(t,z)| \leq C_{j,\gamma} \exp(\Gamma(2j - 1 + |\gamma|)|t|). \tag{16}$$

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

$$\|\hat{A}(t) - \sum_{0 \leq j \leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq C_N \hbar^{N+1} \exp(\Gamma(2N + 5n + 3)|t|). \tag{17}$$

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

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*

$$\|\hat{A}(t) - \sum_{0\leq j\leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq C_N \hbar^{\varepsilon N+1}\hbar^{\frac{\varepsilon-1}{2}(5n+3)}. \tag{18}$$

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 (16) becomes $\exp(\Gamma(3j/2 + |\gamma|)|t|)$. *In the remainder estimate (17) 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*

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

We remember that some times ago, S. Debièvre suggested that the Ehrenfest time could be greater that $\frac{1}{2\Gamma}\log\hbar^{-1}$. The above results confirm this guess.

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 1.6 *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 $C > 0$,*

$$\forall\gamma \in \mathbb{N}^{2n},\ \forall j \in \mathbb{N},\ \forall z \in Z, \text{ we have } |\partial_z^\gamma A_j(z)| \leq C^{|\gamma|+j+1}(|\gamma| + j)!^\sigma \tag{20}$$

$$\left|\partial_z^\gamma\left(A(\hbar, z) - \sum_{0\leq j\leq N}\hbar^j A_j(z)\right)\right| \leq \hbar^{N+1}C^{|\gamma|+N+2}(|\gamma| + N + 1)!^\sigma. \tag{21}$$

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

Theorem 1.7 *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 $\Omega(\delta) := \{z \in \mathbb{C}^{2n}, |\Im z| < \delta\}$. Suppose moreover that $\nabla_z^{(2)}H_0$, $\nabla_z H_1$, $\nabla_z A$ are bounded and continuous in $\Omega(\delta)$. Then, if we define*

$$\Gamma := \sup_{z\in\Omega(\delta)} \|\nabla_z^{(2)}H_0(z)\|.$$

we have the following improvement of Theorem 1.4, saying that $\hbar^{-1}(A(t,z) - A \circ \Phi^t)$ is a semi-classical observable with Gevrey index 2, with control in time. More explicitely, there exist constants $M > 0, K > 0$ such that

$$|\partial_z^\gamma A_j(t,z)| \leq M(j+|\gamma|)!^2 K^{j+|\gamma|} \exp(\Gamma(2j+|\gamma|)|t|) \tag{22}$$

$$\left|\partial_z^\gamma A(t,z)[\hbar] - \sum_{0\leq j\leq N} \hbar^j A_j(t,z)\right| \leq \hbar^{N+1}|t| M K^{N+1+|\gamma|}(N+1)!^2 \gamma! \tag{23}$$

$$\times \exp(|t|\Gamma(2N+4n+1)).$$

Furthermore we have the following estimate in L^2 operator-norm of the remainder term :

$$\|\hat{A}(t) - \sum_{0\leq j\leq N} \hbar^j \hat{A}_j(t)\|_{L^2} \leq M(N+1)!^2 K^{N+1} \hbar^{N+1} \exp(\Gamma(2N+5n+3)|t|). \tag{24}$$

We can deduce from Theorem 1.7 a semi-classical approximation of $A(t)$ with an exponentially small error in $\hbar$, for long time intervals.

Corollary 1.8 *Under the assumptions of Theorem 1.7, for every $\varepsilon > 0, C > 0$, such that $\varepsilon + C < 1/2$, there exists a constant K such that for $|t| \leq C\log(\hbar^{-1})$ we have*

$$\|\hat{A}(t) - \sum_{0\leq j\leq \hbar^{-\varepsilon}} \hbar^j \hat{A}_j(t)\|_{L^2} \leq K \exp\left(-\frac{1}{\hbar^\varepsilon}\right) \tag{25}$$

Remark 1.9 *Estimates (17) and (24) improve [BGP] in two ways. In the C^∞ case we get similar results without analyticity assumptions. In the analytic case we get better estimates with respect to N (see (24)). Note that in [BGP] the $A_j(t)$'s are not defined through the algorithm (13).*

Similar exponential estimates were recently proved in [HJ] for propagation of Gaussian coherent states.

Remark 1.10 *If the expansion of H in $\hbar$ is even then the estimates given in Theorem 1.7 hold with Gevrey index equal to $3/2$ and the $2N$ in the exponential term becomes $3N/2$.*

Example 1.11 *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.*

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*

$$\begin{aligned}
\partial^\alpha(f\circ g) &= \sum_{\gamma\neq 0, \gamma\leq\alpha} (\partial^\gamma f)\circ g \cdot \mathcal{B}_{\alpha,\gamma}[\partial^\beta g], \text{ where} \qquad (26)\\
\mathcal{B}_{\alpha,\gamma}[\partial^\beta g] &= \alpha! \sum_{\substack{\sum_\beta \beta=\gamma \\ \sum_\beta \beta|a_\beta|=\alpha}} \prod_{0\neq\beta\in\mathbb{N}^d} \frac{1}{a_\beta!}\left(\frac{\partial^\beta g}{\beta!}\right)^{a_\beta}.
\end{aligned}$$

In formula (26), 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

$$\left(\frac{\partial^\beta g}{\beta!}\right)^{a_\beta} = \left(\frac{\partial^\beta g_1}{\beta!}\right)^{a_{\beta,1}} \cdots \left(\frac{\partial^\beta g_d}{\beta!}\right)^{a_{\beta,d}}. \qquad (27)$$

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*

$$\forall t \in \mathbb{R},\ \forall z \in Z,\ \ \|\partial_z^\gamma \Phi^t z\| \leq C_\gamma \exp(|\gamma||t|\Gamma) \qquad (28)$$

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

$$\frac{d}{dt}\nabla_z\Phi^t(z) = J\nabla_z^{(2)}H_0(\Phi^t z)\nabla_z\Phi^t z. \qquad (29)$$

Using the definition of Γ and the Gronwall inequality, we get (28) for $|\gamma| = 1$ with $C_\gamma = 1$. For $|\gamma| = k \geq 2$, let us assume that (28) holds for $|\gamma| < k$. Computing derivatives in z of (29) and applying Faà de Bruno formula, we get

$$\frac{d}{dt}\partial_z^\gamma\Phi^t z = \gamma! \sum_{|\alpha|=1} \partial^\alpha(J\nabla_z^{(2)}H_0)(\Phi^t z)(\partial_z^\gamma\Phi^t z)^\alpha + Y(t). \qquad (30)$$

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

$$\forall t \in \mathbb{R},\ \ \|Y(t)\| \leq C\exp(\Gamma|\gamma||t|). \qquad (31)$$

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*

$$\frac{d}{dt}X(t) = M(t)X(t) + Y(t), \qquad (32)$$

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

$$\frac{\partial R(t,s)}{\partial t} = M(t)R(t,s), \quad R(s,s) = \mathbb{1}. \tag{33}$$

Then we have

$$X(t) = R(t,0)X(0) + \int_0^t R(t,s)Y(s)ds, \quad \text{and} \tag{34}$$

$$\|R(t,s)\| \leq \exp(\Gamma|t-s|), \quad \forall t,s \in \mathbb{R} \tag{35}$$

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

$$\|X(t)\| \leq C'\mathrm{e}^{K|t|} \quad \forall t \in \mathbb{R}. \tag{36}$$

Using the inequality (28) 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*

$$\forall t \in \mathbb{R}, \forall z \in Z, \quad |\partial_z^\gamma A_0(t,z)| \leq C_{0,\gamma} \exp(\Gamma|\gamma||t|) \tag{37}$$

Now using the induction formula (13), 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*

$$|\partial_z^\gamma A_j(t,z)| \leq C_{j,\gamma} \exp(\Gamma(2j - 1 + |\gamma|)|t|). \tag{38}$$

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

$$A^{(N)}(t) := \sum_{0\leq j\leq N} \hbar^j A_j(t). \tag{39}$$

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 $\hbar$,

$$\begin{aligned}\{H,B\}^* = \{H_0,B\}_1 + \hbar(\{H_0,B\}_2 + \{H_1,B\}_1) + \cdots + \\ \hbar^{k-1}(\{H_0,B\}_k + \{H_1,B\}_{k-1} + \hbar^k(\delta^k_{H_0,B} + \delta^{k-1}_{H_1,B}),\end{aligned} \tag{40}$$

where $\{H_0,B\}_1$ is the usual Poisson bracket (see (4)). The remainder term is given by the remainder term in the product rule, with notations defined in Appendix,

$$\delta^k_{H,B} = i\hbar^{-k-1}(R_k(H,B) - R_k(B,H)). \tag{41}$$

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

$$\frac{d}{dt}A^{(N)}(t) = \{H, A^{(N)}(t)\}^* + \hbar^{N+1}R^{(N+1)}(t), \tag{42}$$

where

$$R^{(N+1)}(t) = \delta^{N+1}_{H_0,A_0} + \cdots + \delta^{1}_{H_0,A_N} + \delta^{N}_{H_1,A_0} + \cdots + \delta^{0}_{H_1,A_N}. \tag{43}$$

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*

$$\|\hat{A}(t) - \hat{A}^{(N)}(t)\|_{L^2} \leq \hbar^{N+1}|t| \sup_{|s|\leq|t|} \|\hat{R}^{(N+1)}(t)\|_{L^2}. \tag{44}$$

Proof: Let us denote $E(t) = \hat{A}(t) - \hat{A}^{(N)}(t)$ and compute (14)

$$\frac{d}{ds}U(-s)E(t-s)U(s) = U(-s)\left\{\frac{i}{\hbar}[\hat{H}, E(t-s)] - \frac{d}{dt}E(t-s)\right\}U(s). \tag{45}$$

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 derivatives for $\delta^{N+1-j}_{H_i,A_j(t)}$ and then we 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 :

$$\|\hat{B}\|_{L^2} \leq \gamma_n \sup_{\substack{|\alpha|,|\beta|\leq[n/2]+1 \\ z\in Z}} |\partial_z^{\alpha,\beta}B(z)|. \tag{46}$$

∎

3 The Analytic case

To prove Theorem 1.7, 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 were considered in [BGP]). That is under the assumptions of Theorem 1.7, we have

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

$$\|\partial_z^\gamma \Phi^t z\| \leq \gamma!\delta^{1-|\gamma|}\exp(|\gamma||t|\ \Gamma), \quad \forall\gamma\in\mathbb{N}^{2n},\ |\gamma|\geq 1,\ \forall z\in Z. \tag{47}$$

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

$$\|\Im z\| \leq \tau\delta\mathrm{e}^{-|t|\Gamma} \Rightarrow \|\Im(\Phi^{t-s}z)\| \leq \tau\delta\mathrm{e}^{-|s|\Gamma}. \tag{48}$$

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

$$\frac{d}{dt}\Phi^t z = F(\Phi^t z),\ \Phi^0 z = z \tag{49}$$

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

$$\|\Im\Phi^s z\| < \delta,\ \forall s \in [0, t'] \Rightarrow \|\nabla_z \Phi^s z\| < \mathrm{e}^{s\Gamma},\ \ \forall s \in [0, t']. \tag{50}$$

We also have

$$\|\Im\Phi^s z\| \le \|\Phi^s z - \Phi^s(\Re z)\| \le \|\Im z\| \sup_{\|y\| \le \|\Im z\|} \|\nabla_z \Phi^s(\Re z + iy)\|. \tag{51}$$

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

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

Using (50) and (51), we get

$$\|\Im\Phi^{t'}\zeta\| \le \mathrm{e}^{(t'-t)\Gamma},\ \forall\zeta,\ \|\Im\zeta\| \le \|\Im z\|. \tag{52}$$

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 (48) 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 (47). ∎

¿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 $\gamma \in \mathbb{N}^{2n}$, $|\gamma| \ge 1$, $z \in \Omega(\delta\mathrm{e}^{-\Gamma|t|})$, we have*

$$|\partial_z^\gamma[A(\Phi^t(z))]| \le M\gamma!\delta^{1-|\gamma|}\mathrm{e}^{\Gamma|\gamma||t|}. \tag{53}$$

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 $M > 0, a > 0$ such that

$$\|f\|_\tau \le M\left(\frac{e}{1-\tau}\right)^a,\ \forall\tau \in]0, 1[. \tag{54}$$

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

$$\|\partial_z^\gamma f\|_\tau \le M\delta^{-|\gamma|}(a+1)\cdots(a+|\gamma|)\left(\frac{e}{1-\tau}\right)^{a+|\gamma|}. \tag{55}$$

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

$$\|\frac{\partial f}{\partial z_j}\|_{\tau'} \leq \frac{\delta^{-1}}{\tau - \tau'}\|f\|_{\tau}. \tag{56}$$

Using now (54) with $\tau = \tau' + \frac{1-\tau'}{1+a}$ and the elementary inequality $\left(\frac{1+a}{a}\right)^a \leq e$, we get

$$\|\frac{\partial f}{\partial z_j}\|_{\tau'} \leq M\delta^{-1}(a+1)\left(\frac{e}{1-\tau'}\right)^{a+1}. \tag{57}$$

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

The proof of Theorem 1.7 is based on the following estimate.

Proposition 3.4 *There exists a constant C_1 large enough, depending only on n, A, H, such that for all $j \geq 1$, $t \in \mathbb{R}$, we have*

$$\sup_{z\in\Omega(\tau\delta \mathrm{e}^{-|t|\Gamma})} |A_j(t,z)| \leq Mj!^2 C_1^j \left(\frac{\mathrm{e}}{1-\tau}\right)^{2j-1} \mathrm{e}^{(2j-1)|t|\Gamma}. \tag{58}$$

Proof: Let us assume for simplicity that $t > 0$. We shall prove (58) by induction on j. From Lemma 3.2, the estimate is clearly satisfied for $j = 1$. Let us assume that (58) is satisfied for $\ell \leq j-1$. Then using Lemma 3.3, we get, for $\|\Im z\| \leq \tau\delta\mathrm{e}^{-t\Gamma}$,

$$\begin{aligned}|\partial_z^\gamma A_\ell(s, \Phi^{t-s}z| \leq M\ell!^2 \left(\frac{\mathrm{e}}{1-\tau}\right)^{2\ell-1+|\gamma|} \delta^{-|\gamma|}\mathrm{e}^{(2\ell-1+|\gamma|)s\Gamma} \\ \times 2\ell(2\ell+1)\cdots(2\ell-1+|\gamma|).\end{aligned} \tag{59}$$

In the induction formula (13), we have $|\gamma| + \ell = j+1$ and $\ell \leq j-1$. So we shall use the two following elementary inequalities

$$2\ell(2\ell+1)\cdots(2j-1+) \leq 4^{j-\ell}\frac{j!^2}{\ell!^2}, \tag{60}$$

$$\sum_{|\gamma|=j-\ell+1} 1 = (2n)^{j-\ell+1}. \tag{61}$$

¿From the assumptions on H, taking a smaller $\delta > 0$ if necessary, there exists $C_0 > 0$ such that for $|\gamma| + k \geq 2$, we have

$$\sup_{\Omega(\delta)} |\partial_z^\gamma H_k| \leq \gamma! C_0^{|\gamma|+1}. \tag{62}$$

Then, it follows from (13) that the following estimate holds

$$\begin{aligned}\sup_{z\in\Omega(\tau\delta\mathrm{e}^{-|t|\Gamma})} |A_j(t,z)| \leq Mj!^2 C_1^j \left(\frac{\mathrm{e}}{1-\tau}\right)^{2j-1} \mathrm{e}^{(2j-1)|t|\Gamma} \\ \times\frac{4nMC_0^2}{\delta\Gamma}\sum_{0\leq\ell\leq j-1}\left(\frac{4nC_0}{\delta C_1}\right)^{j-\ell}.\end{aligned} \tag{63}$$

Taking now C_1 large enough, we get the conclusion. ∎

Using Cauchy inequalities, we deduce the following result on the A_j's

Corollary 3.5 *For every $\gamma \in N^{2n}$ and $j \in \mathbb{N}$ such that $|\gamma| + j \geq 1$, we have*

$$\sup_{z \in Z} |\partial_z^\gamma A_j(t,z)| \leq M j!^2 \gamma! C_1^j \delta^{-|\gamma|} \mathrm{e}^{(2j-1+|\gamma|)|t|\Gamma}. \tag{64}$$

End of the proof of Theorem 1.7

We follow the same method as in the C^∞-case, with the above estimates on A_j by using the Appendix and (69). We left the details to the reader. ∎

Acknowledgement: The authors thank S.Graffi, for discussions about long time semi-classical approximation, P. Bolley, B. Grébert and JP. Guillement for discussions concerning the Faà de Bruno formula.

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]

$$C(q,p) = \exp\left(\frac{i\hbar}{2}\sigma(D_q, D_p; D_{q'}, D_{p'})\right) A(q,p)B(q',p')|_{(q,p)=(q',p')}, \tag{65}$$

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

$$C(q,p) = \sum_{j\geq 0} \frac{\hbar^j}{j!}(\frac{i}{2}\sigma(D_q, D_p; D_{q'}, D_{p'}))^j A(q,p)B(q',p')|_{(q,p)=(q',p')}. \tag{66}$$

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

$$C_j(q,p) = \frac{1}{2^j} \sum_{|\alpha+\beta|=j} \frac{(-1)^{|\beta|}}{\alpha!\beta!}(D_q^\beta \partial_p^\alpha A).(D_q^\alpha \partial_p^\beta B)(q,p). \tag{67}$$

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 $N \geq 1$,

$$A\#B(z) - \sum_{0\leq j\leq N} \hbar^j C_j(z) =: R_N(A, B; z; \hbar). \tag{68}$$

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 $z \in Z$,*

$$\begin{aligned}|\partial_z^\gamma \left(A\#B(z) - \sum_{0\leq j\leq N} \hbar^j C_j(z)\right)| &\leq \hbar^{N+1}\rho_{n,m,s}K_n^{N+|\gamma|}(N!)^{-1}\cdots \\ &\times \sup_{(*)}\left[(1+u^2+v^2)^{(s-m)/2}|\partial_u^{(\alpha,\beta)+\mu}A(u+z)||\partial_v^{(\beta,\alpha)+\nu}B(v+z)|\right]\end{aligned} \tag{69}$$

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

$$\begin{aligned}R_N(A, B; z; \hbar) &= \frac{1}{N!}\left(\frac{i\hbar}{2}\right)^{N+1} \int_0^1 (1-t)^N R_{N,t}(z;\hbar)dt \quad \text{where} \quad R_{N,t}(z;\hbar) = \\ &(2\pi\hbar t)^{-2n} \int\int_{Z\times Z} \exp(-\frac{i}{2t\hbar}\sigma(u,v))\sigma^{N+1}(D_u, D_v)A(u+z)B(v+z)dudv.\end{aligned} \tag{70}$$

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*

$$I(\lambda) = \lambda^{2n} \int\int_{Z\times Z} \exp[-i\lambda\sigma(u,v)]F(u,v)dudv. \tag{71}$$

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

$$|I(\lambda)| \leq \kappa(n,s,m) \sup_{\substack{u,v\in Z,\\ |\mu|+|\nu|\leq m}} (1+u^2+v^2)^{s-m/2}|\partial_u^\mu \partial_v^\nu F(u,v)|. \tag{72}$$

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

$$I_0(\lambda) = \lambda^{2n} \iint_{Z\times Z} \exp[-i\lambda\sigma(u,v), \chi_0(\lambda(u^2+v^2))F(u,v)dudv, \tag{73}$$

$$I_1(\lambda) = \lambda^{2n} \iint_{Z\times Z} \exp[-i\lambda\sigma(u,v)](1-\chi_0(u^2+v^2))\chi_0(\lambda(u^2+v^2))F(u,v)dudv, \tag{74}$$

$$I_2(\lambda) = \lambda^{2n} \iint_{Z\times Z} \exp[-i\lambda\sigma(u,v)](1-\chi_0(u^2+v^2))F(u,v)dudv. \tag{75}$$

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

$$|I_0(\lambda)| \leq \omega_{4n} \sup_{u^2+v^2\leq 1} |F(u,v)|, \tag{76}$$

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

$$L = \frac{i}{u^2+v^2}\left(Ju\frac{\partial}{\partial v} - Jv\frac{\partial}{\partial u}\right), \tag{77}$$

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

$$|I_1(\lambda)| \leq c_n \sup_{\substack{u^2+v^2\leq 1\\ |\mu|+|\nu|\leq 4n}} |\partial_u^\mu \partial_v^\nu F(u,v)|. \tag{78}$$

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

$$|I_2(\lambda)| \leq c_n \sup_{\substack{u,v\in Z\\ |\mu|+|\nu|\leq m}} (1+u^2+v^2)^{(s-m)/2}|\partial_u^\mu \partial_v^\nu F(u,v)|. \tag{79}$$

∎

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 $u = (x,\xi)$, $v = (y,\eta)$,

$$\begin{aligned}&|\sigma^N(\partial_x, \partial_\xi; \partial_y, \partial_\eta))F(x,\xi)G(y,\eta)| \leq \\ &(2n)^N \sup_{|\alpha|+|\beta|=N} |\partial_x^\alpha \partial_\xi^\beta A(x,\xi)\partial_y^\beta \partial_\eta^\alpha B(y,\eta)|.\end{aligned} \tag{80}$$

∎

Remark A.3 *We can easily extend the estimate (69) 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 (69) 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 $m - s \geq \mu_A + \mu_B$.*

References

[BGP] D. Bambusi, S. Graffi, T. Paul, *Long time semi-classical approximation of quantum flows: a proof of the Ehrenfest time*, (1998), Asymptotic Analysis (to appear).

[Be] R. Beals, *Propagation des singularités pour des opérateurs du type $D_t^2 - \Box_b$*, Conf. No.19, Colloque EDP Saint Jean de Monts (1980).

[Bo] A. Boulkhemair, *L^2-estimates for Weyl quantization*, preprint university of Nantes, (1998).

[BK] L. Boutet de Monvel, P. Kree, *Pseudodifferential operator and Gevrey classes.*, Ann. Inst. Fourier, Grenoble, 17, (1967) 295-323.

[Ce] L. Cesari, *Asymptotic Behavior and Stability Problems in Ordinary Differential Equations*, Springer (1963).

[Ch] B. Chirikov, *A universal instability of many dimensional oscillator systems*, Phys. Reports **52** (1979).

[CR] M. Combescure, D. Robert, *Semi-classical spreading of quantum wave packets and applications near unstable fixed points of the classical flow*, Asymptotic Analysis **14** (1997), 377-404.

[Co] L. Comtet, *Analyse combinatoire* Tome 1, Presses Universitaires de France (1970).

[DR] M. Dauge, D. Robert, *Weyl's formula for a class of pseudodifferential operators with negative order on $L^2(\mathbb{R}^n)$*. Lecture Notes in Math, n.1256, Springer-Verlag, (1986) 90-122.

[Eg] Y.V. Egorov, *On canonical transformations of pseudodifferential operators*, Upehi Mat. Nauk,25, 235-236, (1969).

[HJ] G.A. Hagedorn, A. Joye, *Semiclassical Dynamics with Exponentially Small Error Estimates*, (1998), Commun. Math. Phys. (to appear).

[HR] B. Helffer, D. Robert, *Calcul fonctionnel pour la transformée de Mellin*, J. Funct. Anal., **53** (1983), 246-268.

[Ho] L. Hörmander, *The Analysis of Linear Partial Differential Operators I to IV* Springer Verlag (1983-85).

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

[Tr] F. Trèves, *Introduction to pseudodifferential and Fourier integral operators.* Vol.2. Plenum Press, New-York, London (1980).

[Sj] J. Sjöstrand, *Singularités analytiques microlocales*, Astérique 95, SMF, (1982).

[Za] G. M. Zaslavski, *Stochasticity in quantum systems*, Phys. Reports **80** (1981), 157-250.