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PROPAGATION OF COHERENT STATES IN QUANTUM MECHANICS AND APPLICATIONS

by

Didier Robert

Abstract. — This paper present a synthesis concerning applications of Gaussian coherent states in semi-classical analysis for Schrödinger type equations, time dependent or time independent. We have tried to be self-contained and elementary as far as possible.

In the first half of the paper we present the basic properties of the coherent states and explain in details the construction of asymptotic solutions for Schrödinger equations. We put emphasis on accurate estimates of these asymptotic solutions: large time, analytic or Gevrey estimates. In the second half of the paper we give several applications: propagation of frequency sets, semi-classical asymptotics for bound states and for the scattering operator for the short range scattering.

Résumé **(Propagation d'états cohérents en mécanique quantique et applications)**

Cet article présente une synthèse concernant les applications des états cohérents gaussiens à l'analyse semi-classique des équations du type de Schrödinger, dépendant du temps ou stationnaires. Nous avons tenté de faire un travail aussi détaillé et élémentaire que possible.

Dans la première partie nous présentons les propriétés fondamentales des états cohérents et nous exposons en détails la construction de solutions asymptotiques de l'équation de Schrödinger. Nous mettons l'accent sur des estimations précises : temps grands, estimations du type analytique ou Gevrey. Dans la dernière partie de ce travail nous donnons plusieurs applications : propagation des ensembles de fréquences, asymptotiques semi-classiques pour les états bornés et leurs énergies ainsi que pour l'opérateur de diffusion dans le cas de la diffusion à courte portée.

Introduction

Coherent states analysis is a very well known tool in physics, in particular in quantum optics and in quantum mechanics. The name "coherent states" was first used by R. Glauber, Nobel prize in physics (2005), for his works in quantum optics

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and electrodynamics. In the book [**27**], the reader can get an idea of the fields of applications of coherent states in physics and in mathematical-physics.

A general mathematical theory of coherent states is detailed in the book [**33**]. Let us recall here the general setting of the theory.

G is a locally compact Lie group, with its Haar left invariant measure dg and R is an irreducible unitary representation of G in the Hilbert space $\mathcal{H}$. Suppose that there exists $\varphi \in \mathcal{H}$, $\|\varphi\| = 1$, such that

$$0 < \int_G |\langle \varphi, R(g)\varphi\rangle|^2 \, dg < +\infty \tag{1}$$

(R is said to be square integrable).

Let us define the coherent state family $\varphi_g = R(g)\varphi$. For $\psi \in \mathcal{H}$, we can define, in the weak sense, the operator $\mathcal{I}\psi = \int_G \langle \psi, \varphi_g\rangle \varphi_g dg$. $\mathcal{I}$ commute with R, so we have $\mathcal{I} = c\mathbb{1}$, with $c \neq 0$, where $\mathbb{1}$ is the identity on $\mathcal{H}$. Then, after renormalisation of the Haar measure, we have a resolution of identity on $\mathcal{H}$ in the following sense:

$$\psi = \int_G \langle \psi, \varphi_g\rangle \varphi_g \, dg, \quad \forall \psi \in \mathcal{H}. \tag{2}$$

(2) is surely one of the main properties of coherent states and is a starting point for a sharp analysis in the Hilbert space $\mathcal{H}$ (see [**33**]).

Our aim in this paper is to use coherent states to analyze solutions of time dependent Schrödinger equations in the semi-classical regime ($\hbar \searrow 0$).

$$i\hbar \frac{\partial \psi(t)}{\partial t} = \widehat{H}(t)\psi(t), \quad \psi(t = t_0) = f, \tag{3}$$

where f is an initial state, $\widehat{H(t)}$ is a quantum Hamiltonian defined as a continuous family of self-adjoint operators in the Hilbert space $L^2(\mathbb{R}^d)$, depending on time t and on the Planck constant $\hbar > 0$, which plays the role of a small parameter in the system of units considered in this paper. $\hat{H}(t)$ is supposed to be the $\hbar$-Weyl-quantization of a classical observable $H(t, x, \xi)$, $x, \xi \in \mathbb{R}^d$ (cf [**37**] for more details concerning Weyl quantization).

The canonical coherent states in $L^2(\mathbb{R}^d)$ are usually built from an irreducible representation of the Heisenberg group $\mathbb{H}_{2d+1}$(see for example [**15**]). After identification of elements in $\mathbb{H}_{2d+1}$ giving the same coherent states, we get a family of states $\{\varphi_z\}_{z\in\mathcal{Z}}$ satisfying (2) where $\mathcal{Z}$ is the phase space $\mathbb{R}^d \times \mathbb{R}^d$. More precisely,

$$\varphi_0(x) = (\pi\hbar)^{-d/4} \exp\left(\frac{x^2}{2\hbar}\right), \tag{4}$$

$$\varphi_z = \mathcal{T}_\hbar(z)\varphi_0 \tag{5}$$

where $\mathcal{T}_\hbar(z)$ is the Weyl operator

$$\mathcal{T}_\hbar(z) = \exp\left(\frac{i}{\hbar}(p\cdot x - q\cdot \hbar D_x)\right) \tag{6}$$

where $D_x = -i\frac{\partial}{\partial x}$ and $z = (q, p) \in \mathbb{R}^d \times \mathbb{R}^d$.

We have $\|\varphi_z\| = 1$, for the L^2 norm. If the initial state f is a coherent state φ_z, a natural ansatz to check asymptotic solutions modulo $O(\hbar^{(N+1)/2})$ for equation (3), for some $N \in \mathbb{N}$, is the following

$$\psi_z^{(N)}(t,x) = \mathrm{e}^{i\frac{\delta_t}{\hbar}} \sum_{0\le j\le N} \hbar^{j/2}\pi_j(t, \frac{x-q_t}{\sqrt{\hbar}})\varphi_{z_t}^{\Gamma_t}(x) \tag{7}$$

where $z_t = (q_t, p_t)$ is the classical path in the phase space $\mathbb{R}^{2d}$ such that $z_{t_0} = z$ and satisfying

$$\begin{cases} \dot{q}_t = \dfrac{\partial H}{\partial p}(t, q_t, p_t) \\ \dot{p}_t = -\dfrac{\partial H}{\partial p}(t, q_t, p_t), \quad q_{t_0} = q,\ p_{t_0} = p \end{cases} \tag{8}$$

and

$$\varphi_{z_t}^{\Gamma_t} = \mathcal{T}_\hbar(z_t)\varphi^{\Gamma_t}. \tag{9}$$

φ^{Γ_t} is the Gaussian state:

$$\varphi^{\Gamma_t}(x) = (\pi\hbar)^{-d/4} a(t) \exp\left(\frac{i}{2\hbar}\Gamma_t x.x\right). \tag{10}$$

Γ_t is a family of $d \times d$ symmetric complex matrices with positive non-degenerate imaginary part, δ_t is a real function, $a(t)$ is a complex function, $\pi_j(t,x)$ is a polynomial in x (of degree $\le 3j$) with time dependent coefficients.

More precisely Γ_t is given by the Jacobi stability matrix of the Hamiltonian flow $z \mapsto z_t$. If we denote

$$A_t = \frac{\partial q_t}{\partial q}, \quad B_t = \frac{\partial p_t}{\partial q}, \quad C_t = \frac{\partial q_t}{\partial p}, \quad D_t = \frac{\partial p_t}{\partial p} \tag{11}$$

then we have

$$\Gamma_t = (C_t + iD_t)(A_t + iB_t)^{-1}, \ \ \Gamma_{t_0} = \mathbb{1}, \tag{12}$$

$$\delta_t = \int_{t_0}^t (p_s \cdot \dot{q}_s - H(s, z_s))\, ds - \frac{q_t p_t - q_{t_0} p_{t_0}}{2}, \tag{13}$$

$$a(t) = [\det(A_t + iB_t)]^{-1/2}, \tag{14}$$

where the complex square root is computed by continuity from $t = t_0$.

In this paper we want to discuss conditions on the Hamiltonian $H(t,X)$ ($X = (x,\xi) \in \mathbb{R}^d \times \mathbb{R}^d$) so that $\psi_z^{(N)}(t,x)$ is an approximate solution with an accurate control of the remainder term in $\hbar$, t and N, which is defined by

$$R_z^{(N)}(t,x) = i\hbar\frac{\partial}{\partial t}\psi_z^{(N)}(t,x) - \widehat{H}(t)\psi_z^{(N)}(t,x). \tag{15}$$

The first following result is rather crude and holds for finite times t and N fixed. We shall improve later this result.

Theorem 0.1. — *Assume that $H(t,X)$ is continuous in time for t in the interval $I_T = [t_0 - T, t_0 + T]$, C^∞ in $X \in \mathbb{R}^{2d}$ and real.*

Assume that the solution z_t of the Hamilton system (8) exists for $t \in I_T$.

Assume that $H(t,X)$ satisfies one of the following global estimate in X

1. *$H(t,x,\xi) = \frac{\xi^2}{2} + V(t,x)$ and there exists $\mu \in \mathbb{R}$ and, for every multiindex α there exists C_α, such that*

$$|\partial_x{}^\alpha V(t,x)| \leq C_\alpha \mathrm{e}^{\mu x^2}; \tag{16}$$

2. *for every multiindex α there exist $C_\alpha > 0$ and $M_{|\alpha|} \in \mathbb{R}$ such that*

$$|\partial_X^\alpha H(t,X)| \leq C_\alpha (1 + |X|)^{M_{|\alpha|}}, \quad \textit{for } t \in I_T \textit{ and } X \in \mathbb{R}^{2d}.$$

Then for every $N \in \mathbb{N}$, there exists $C(I_T, z, N) < +\infty$ such that we have, for the L^2-norm in $\mathbb{R}^d_x$,

$$\sup_{t \in I_T} \|R_Z^{(N)}(t, \bullet)\| \leq C(I_T, z, N)\hbar^{\frac{N+3}{2}}, \quad \forall \hbar \in]0, \hbar_0],\ \hbar_0 > 0. \tag{17}$$

Moreover, if for every $t_0 \in \mathbb{R}$, the equation (3) has a unique solution $\psi(t) = U(t,t_0)f$ where $U(t,s)$ is family of unitary operators in $L^2\mathbb{R}^d)$ such that $U(t,s) = U(s,t)$, then we have, for every $t \in I_T$,

$$\|U(t,t_0)\varphi_z - \psi_z^{(N)}(t)\| \leq |t - t_0| C(I_T, z, N)\hbar^{\frac{N+1}{2}}. \tag{18}$$

In particular this condition is satisfied if H is time independent.

The first mathematical proof of results like this, for the Schrödinger Hamiltonian $\xi^2 + V(x)$, is due to G. Hagedorn [**18**].

There exist many results about constructions of asymptotic solutions for partial differential equations, in particular in the high frequency regime. In [**35**] J. Ralston constructs Gaussian beams for hyperbolic systems which is very close to construction of coherent states. This kind of construction is an alternative to the very well known WKB method and its modern version: the Fourier integral operator theory. It seems that coherent states approach is more elementary and easier to use to control estimates. In [**8**] the authors have extended Hagedorn's results [**18**] to more general Hamiltonians proving in particular that the remainder term can be estimated by $\rho(I_T, z, N) \leq K(z,N)\mathrm{e}^{\gamma T}$ with some $K(z,N) > 0$ and $\gamma > 0$ is related with Lyapounov exponents of the classical system.

It is well known that the main difficulty of real WKB methods comes from the occurring of caustics (the WKB approximation blows up at finite times). To get rid of the caustics we can replace the real phases of the WKB method by complex valued phases. This point of view is worked out for example in [**41**] (FBI transform theory, see also [**29**]). The coherent state approach is not far from FBI transform and can be seen as a particular case of it, but it seems more explicit, and more closely related with the physical intuition.

One of our main goal in this paper is to give alternative proofs of Hagedorn-Joye results [**20**] concerning large N and large time behaviour of the remainder term $R_N(t,x)$. Moreover our proofs are valid for large classes of smooth classical Hamiltonians. Our method was sketched in [**38**]. Here we shall give detailed proofs of the estimates announced in [**38**]. We shall also consider the short range scattering case, giving uniform estimates in time for $U_t\varphi_z$, with short range potential $V(x) = \mathcal{O}(|x|^{-\rho)}$ with $\rho > 1$. We shall show, through several applications, efficiency of coherent states: propagation of analytic frequency set, construction of quasi-modes, spectral asymptotics for bounded states and semi-classical estimates for the scattering operator.

1. Coherent states and quadratic Hamiltonians

1.1. Gaussians Coherent States. — We shall see in the next section that the core of our method to build asymptotic solutions of the Schrödinger equation, (3) for $f = \varphi_z$, it to rescale the problem by putting $\hbar$ at the scale 1 such that we get a regular perturbation problem, for a time dependent quadratic Hamiltonian.

For quadratic Hamiltonians, using the dilation operator $\Lambda_\hbar f(x) = \hbar^{-d/4} f(\hbar^{-1/2}x)$, it is enough to consider the case $\hbar = 1$. We shall denote g_z the coherent state φ_z for $\hbar = 1$ ($\varphi_z = \Lambda_\hbar g_{\hbar^{-1/2}z}$).

For every $u \in L^2(\mathbb{R}^n)$ we have the following consequence of the Plancherel formula for the Fourier transform.

$$\int_{\mathbb{R}^d} |u(x)|^2\, dx = (2\pi)^{-d} \int_{\mathbb{R}^{2d}} |\langle u, g_z\rangle|^2\, dz. \tag{19}$$

Let $\hat{L}$ be some continuous linear operator from $\mathcal{S}(\mathbb{R}^d)$ into $\mathcal{S}'(\mathbb{R}^d)$ and K_L its Schwartz distribution kernel. By an easy computation, we get the following representation formula for K_L:

$$K_L(x,y) = (2\pi)^{-d} \int_{\mathbb{R}^{2d}} (\hat{L} g_z)(x)\overline{g_z(y)}\, dz. \tag{20}$$

In other words we have the following continuous resolution of the identity

$$\delta(x-y) = (2\pi)^{-n} \int_{\mathbb{R}^{2d}} g_z(x)\overline{g_z(y)}\, dz.$$

Let us denote by $\mathcal{O}^m$, $m \in \mathbb{R}$, the space of smooth (classical) obervables L (usually called symbols) such that for every $\gamma \in \mathbb{N}^{2d}$, there exists C_γ such that,

$$|\partial_X^\gamma L(X)| \le C_\gamma < X >^m, \quad \forall X \in \mathcal{Z}.$$

So if $L \in \mathcal{O}^m$, we can define the Weyl quantization of L, $\hat{L}u(x) = Op_\hbar^w[L]u(x)$ where

$$Op_\hbar^w[L]u(x) = (2\pi\hbar)^{-d} \iint_{\mathbb{R}^d\times\mathbb{R}^d} \exp\{i\hbar^{-1}(x-y)\cdot\xi\} L\left(\frac{x+y}{2}, \xi\right) u(y)\, dy\, d\xi \tag{21}$$

for every u in the Schwartz space $\mathcal{S}(\mathbb{R}^d)$. L is called the $\hbar$-Weyl symbol of $\hat{L}$. We have used the notation $x\cdot\xi = x_1\xi_1 + \cdots + x_d\xi_d$, for $x = (x_1, \cdots, x_d)$ and $\xi = (\xi_1, \cdots, \xi_d)$.

In (21) the integral is a usual Lebesgue integral if $m < -d$. For $m \geq -d$ it is an oscillating integral (see for example [**11**, **25**, **37**] for more details).

There are useful relationships between the Schwartz kernel K, the $\hbar$-Weyl symbol L and action on coherent states, for any given operator $\hat{L}$ from $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}'(\mathbb{R}^d)$.

$$K(x,y) = (2\pi\hbar)^{-d}\int_{\mathbb{R}^d} \mathrm{e}^{\frac{i}{\hbar}(x-y)\xi} L(\frac{x+y}{2},\xi)\, d\xi \tag{22}$$

$$L(x,\xi) = \int_{\mathbb{R}^d} \mathrm{e}^{-\frac{i}{\hbar}u\xi} K(x+\frac{u}{2}, x-\frac{u}{2})\, du \tag{23}$$

$$L(x,\xi) = (2\pi\hbar)^{-d}\int_{\mathcal{Z}\times\mathbb{R}^d} \mathrm{e}^{-\frac{i}{\hbar}u\xi} (\hat{L}\varphi_z)(x+\frac{u}{2})\overline{\varphi_z(x-\frac{u}{2})}\, dz\, du. \tag{24}$$

Let us remark that if $K \in \mathcal{S}(\mathbb{R}^d\times\mathbb{R}^d)$ these formulas are satisfied in a naïve sense. For more general $\hat{L}$ the meaning of these three equalities is in the sense of distributions in the variables (x,y) or (x,ξ).

We shall recall in section 3 and 4 more properties of the Weyl quantization. In this section we shall use the following elementary properties.

Proposition 1.1. — *Let be $L \in \mathcal{O}^m$. Then we have*

$$(\mathrm{Op}_\hbar^w(L))^\star = \mathrm{Op}_\hbar^w(\bar{L}) \tag{25}$$

where $(\bullet)^\star$ is the adjoint of operator $(\bullet)$.

For every linear form Q on $\mathcal{Z}$ we have

$$(\mathrm{Op}_\hbar^w Q)(\mathrm{Op}_\hbar^w L) = \mathrm{Op}_\hbar^w[Q \circledast L] \tag{26}$$

where $Q\circledast L = QL + \frac{\hbar}{2i}\{Q,L\}$, $\{Q,L\} = \sigma(J\nabla Q, \nabla L)$ (Poisson bracket) where σ is the symplectic bilinear form on the phase space $\mathbb{R}^{2d}$, defined by $\sigma(z,z') = \xi\cdot x' - x\cdot\xi'$ if $z = (x,\xi)$, $z' = (x',\xi')$.

For every quadratic polynomial Q on $\mathcal{Z}$ we have

$$i[\hat{Q},\hat{L}] = \hbar\widehat{\{Q,L\}} \tag{27}$$

where $[\hat{Q},\hat{L}] = \hat{Q}.\hat{L} - \hat{L}.\hat{Q}$ is the commutator of $\hat{Q}$ and $\hat{L}$.

Proof. — Properties (25) and (26) are straightforward.

It is enough to check (27) for $Q = Q_1Q_2$, where Q_1, Q_2 are linear forms. We have $\hat{Q} = \hat{Q}_1\hat{Q}_2 + c$ where c is a real number, so we have

$$[\hat{Q},\hat{L}] = \hat{Q}_1[\hat{Q}_2,\hat{L}] + [\hat{Q}_1,\hat{L}]\hat{Q}_2.$$

Then we easily get (27) from (26). □

The Wigner function $W_{u,v}$ of a pair (u, v) of states in $L^2(\mathbb{R}^d)$ is the $\hbar$-Weyl symbol, of the projection $\psi \mapsto \langle\psi, v\rangle u$. Therefore we have

$$\langle Op_\hbar^w L u, v\rangle = (2\pi\hbar)^{-d} \int_{\mathbb{R}^{2d}} L(X) W_{u,v}(X)\, dX. \tag{28}$$

The Wigner function of Gaussian coherent states can be explicitly computed by Fourier analysis. The result will be used later. Let us introduce the Wigner function $W_{z,z'}$ for the pair $(\varphi_{z'}, \varphi_z)$. Using computations on Fourier transform of Gaussians [**25**], we can prove the following formula:

$$W_{z,z'}(X) = 2^{2d} \exp\left(-\frac{1}{\hbar}\left|X - \frac{z+z'}{2}\right|^2 + \frac{i}{\hbar}\sigma(X - \frac{1}{2}z', z - z')\right). \tag{29}$$

It will be convenient to introduce what we shall call the Fourier-Bargmann transform, defined by $\mathcal{F}_\hbar^{\mathcal{B}}[u](z) = (2\pi\hbar)^{-d/2}\langle u, \varphi_z\rangle$. It is an isometry from $L^2(\mathbb{R}^d)$ into $L^2(\mathbb{R}^{2d})$. Its range consists of $F \in L^2(\mathbb{R}^{2d})$ such that $\exp\big(\frac{p^2}{2} - i\frac{q\cdot p}{2}\big)F(q,p)$ is holomorphic in $\mathbb{C}^d$ in the variable $q - ip$. (see [**29**]). Moreover we have the inversion formula

$$u(x) = \int_{\mathbb{R}^{2d}} \mathcal{F}_\hbar^{\mathcal{B}}[u](z)\varphi_z(x)\, dz, \text{ in the } L^2\text{-sense}, \tag{30}$$

where $\langle\cdot,\cdot\rangle$ is the scalar product in $L^2(\mathbb{R}^d)$.

In [**15**] (see also [**28**]) the Fourier-Bargmann transform is called wave packet transform and is very close to the Bargmann transform and FBI transform [**29**]. We shall denote $\mathcal{F}_1^{\mathcal{B}} = \mathcal{F}^{\mathcal{B}}$.

If L is a Weyl symbol as above and $u \in \mathcal{S}(\mathbb{R}^d)$ then we get

$$\mathcal{F}^{\mathcal{B}}[(Op^w L)u](z) = \int_{\mathbb{R}^{2d}} \mathcal{F}_\hbar^{\mathcal{B}}[u](z')\langle Op^w L\varphi_{z'}, \varphi_z\rangle\, dz'. \tag{31}$$

So, on the Fourier-Bargmann side, $Op^w L$ is transformed into an integral operator with the Schwartz kernel

$$K_L{}^{\mathcal{B}}(z, z') = (2\pi)^{-d}\int_{\mathbb{R}^{2d}} L(X) W_{z',z}(X)\, dX.$$

We shall also need the following localization properties of smooth quantized observables on a coherent state

Lemma 1.2. — *Assume that $L \in \mathcal{O}^m$. Then for every $N \geq 1$, we have*

$$\widehat{L}\varphi_z = \sum_{|\gamma|\leq N} \hbar^{\frac{|\gamma|}{2}} \frac{\partial^\gamma L(z)}{\gamma!}\Psi_{\gamma,z} + \mathcal{O}(\hbar^{(N+1)/2}) \tag{32}$$

in $L^2(\mathbb{R}^d)$, the estimate of the remainder is uniform for z in every bound set of the phase space.

The notations used are: $\gamma \in \mathbb{N}^{2d}$, $|\gamma| = \sum_1^{2d}$, $\gamma! = \prod_1^{2d}\gamma_j!$ and

$$\Psi_{\gamma,z} = \mathcal{T}(z)\Lambda_\hbar Op_1^w(z^\gamma)g. \tag{33}$$

where $Op_1^w(z^\gamma)$ *is the 1-Weyl quantization of the monomial:* $(x,\xi)^\gamma = x^{\gamma'}\xi^{\gamma''}$, $\gamma = (\gamma', \gamma'') \in \mathbb{N}^{2d}$. *In particular* $Op_1^w(z^\gamma)g = P_\gamma g$ *where* P_γ *is a polynomial of the same parity as* $|\gamma|$.

Proof. — Let us write

$$\hat{L}\varphi_z = \hat{L}\Lambda_\hbar\mathcal{T}(z)g = \Lambda_\hbar\mathcal{T}(z)(\Lambda_\hbar\mathcal{T}(z))^{-1}\hat{L}\Lambda\hbar\mathcal{T}(z)g$$

and remark that $(\Lambda_\hbar\mathcal{T}(z))^{-1}\hat{L}\Lambda_\hbar\mathcal{T}(z) = Op_1^w[L_{\hbar,z}]$ where $L_{\hbar,z}(X) = L(\sqrt{\hbar}X + z)$. So we prove the lemma by expanding $L_{\hbar,z}$ in X, around z, with the Taylor formula with integral remainder term to estimate the error term. □

Lemma 1.3. — *Let be* L *a smooth observable with compact support in* $\mathcal{Z}$. *Then there exists* $R > 0$ *and for all* $N \geq 1$ *there exists* C_N *such that*

$$\|\hat{L}\varphi_z\| \leq C_N\hbar^N\langle z\rangle^{-N}, \ \ \textit{for} \ \ |z| \geq R. \tag{34}$$

Proof. — It is convenient here to work on Fourier-Bargmann side. So we estimate

$$\langle\hat{L}\varphi_z, \varphi_X\rangle = \int_{\mathcal{Z}} L(Y)W_{z,X}(Y)\,dY. \tag{35}$$

The integral is a Fourier type integral:

$$\begin{aligned}&\int_{\mathcal{Z}} L(Y)W_{z,X}(Y)\,dY = \\ &2^{2d}\int_{\mathcal{Z}} \exp\left(-\frac{1}{\hbar}\left|Y - \frac{z+X}{2}\right|^2 + \frac{i}{\hbar}\sigma(Y - \frac{1}{2}X, z - X)\right)L(Y)\,dY.\end{aligned} \tag{36}$$

Let us consider the phase function $\Psi(Y) = -|Y - \frac{z+X}{2}|^2 + i\sigma(Y - \frac{1}{2}X, z - X)$ and its Y-derivative $\partial_Y\Psi = -2(Y - \frac{z+X}{2} - iJ(z - X))$. For z large enough we have $\partial_Y\Psi \neq 0$ and we can integrate by parts with the differential operator $\frac{\overline{\partial_Y\Psi}}{|\partial_Y\Psi|^2}\partial_Y$. Thefore we get easily the estimate using that the Fourier-Bargmann transform is an isometry. □

1.2. Quadratic time dependent Hamiltonians. — Let us consider now a quadratic time-dependent Hamiltonian: $H_t(z) = \sum_{1\leq j,k\leq 2d} c_{j,k}(t)z_jz_k$, with real and continuous coefficients $c_{j,k}(t)$, defined on the whole real line for simplicity. Let us introduce the symmetric $2d \times 2d$ matrix, S_t, for the quadratic form $H_t(z) = \frac{1}{2}S_tz\cdot z$. It is also convenient to consider the canonical symplectic splitting $z = (q,p) \in \mathbb{R}^d \times \mathbb{R}^d$ and to write down S_t as

$$S_t = \begin{pmatrix} G_t & L_t^T \\ L_t & K_t \end{pmatrix} \tag{37}$$

where G_t and K_t are real symmetric $d \times d$ matrices and L^T is the transposed matrix of L. The classical motion driven by the Hamiltonian $H(t)$ in the phase space $\mathcal{Z}$ is given by the Hamilton equation: $\dot{z}_t = JS_tz_t$. This equation defines a linear flow of symplectic transformations, $F(t,t_0)$ such that $F(t_0,t_0) = \mathbb{1}$. For simplicity we shall also use the notation $F_t = F(t,t_0)$.

On the quantum side, $\widehat{H_t} = Op_1^w[H(t)]$ is a family of self-adjoint operators on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d)$. The quantum evolution follows the Schrödinger equation, starting with an initial state $\varphi \in \mathcal{H}$.

$$i\frac{\partial \psi_t}{\partial t} = \widehat{H_t}\psi_t, \quad \psi_{t_0} = \varphi. \tag{38}$$

This equation defines a quantum flow $U(t, t_0)$ in $L^2(\mathbb{R}^d)$ and we also denote $U_t = U(t, t_0)$.

F_t is a $2d \times 2d$ matrix which can be written as four $d \times d$ blocks:

$$F_t = \begin{pmatrix} A_t & B_t \\ C_t & D_t \end{pmatrix}. \tag{39}$$

Let us introduce the squeezed states g^Γ defined as follows.

$$g^\Gamma(x) = a_\Gamma \exp\left(\frac{i}{2\hbar}\Gamma x \cdot x\right) \tag{40}$$

where $\Gamma \in \Sigma_d^+$, Σ_d^+ is the Siegel space of complex, symmetric matrices Γ such that $\Im(\Gamma)$ is positive and non-degenerate and $a_\Gamma \in \mathbb{C}$ is such that the L^2-norm of g^Γ is one. We also denote $g_z^\Gamma = \mathcal{T}(z)g^\Gamma$.

For $\Gamma = i\mathbb{1}$, we have $g = g^{i\mathbb{1}}$.

The following explicit formula will be our starting point to build asymptotic solutions for general Schrödinger (3).

Theorem 1.4. — *For every $x \in \mathbb{R}^d$ and $z \in \mathbb{R}^{2d}$, we have*

$$U_t\varphi^\Gamma(x) = g^{\Gamma_t}(x) \tag{41}$$

$$U_t\varphi_z^\Gamma(x) = \mathcal{T}(F_t z)g^{\Gamma_t}(x) \tag{42}$$

where $\Gamma_t = (C_t + D_t\Gamma)(A_t + B_t\Gamma)^{-1}$ and $a_{\Gamma_t} = a_\Gamma \left(\det(A_t + B_t\Gamma)\right)^{-1/2}$.

For the reader convenience, let us recall here the proof of this result, given with more details in [**9**] (see also [**15**]).

Proof. — The first formula will be proven by the Ansatz

$$U_t g(x) = a(t) \exp\left(\frac{i}{2}\Gamma_t x \cdot x\right)$$

where $\Gamma_t \in \Sigma_d$ and $a(t)$ is a complex values time dependent function. We find that Γ_t must satisfy a Riccati equation and $a(t)$ a linear differential equation.

The second formula is easy to prove from the first, using the Weyl translation operators and the following well known property saying that for quadratic Hamiltonians quantum propagation is exactly given by the classical motion:

$$U_t\mathcal{T}(z)U_t^* = \mathcal{T}(F_t z). \quad \square$$

Let us now give more details for the proof of (42). We need to compute the action of a quadratic Hamiltonian on a Gaussian. A straightforward computation gives:

Lemma 1.5

$$Lx\cdot D_x \mathrm{e}^{\frac{i}{2}\Gamma x\cdot x} = (L^T x\cdot\Gamma x - \frac{i}{2}\mathrm{Tr}L)\mathrm{e}^{\frac{i}{2}\Gamma x\cdot x}$$
$$(GD_x\cdot D_x)\mathrm{e}^{\frac{i}{2}\Gamma x\cdot x} = (G\Gamma x\cdot\Gamma x - i\mathrm{Tr}(G\Gamma))\,\mathrm{e}^{\frac{i}{2}\Gamma x\cdot x}.$$

Using this Lemma, We try to solve the equation

$$i\frac{\partial}{\partial t}\psi = \hat{H}\psi \tag{43}$$

with $\psi|_{t=0}(x) = g^{\Gamma}(x)$ with the Ansatz

$$\psi(t,x) = a(t)e^{\frac{i}{2}\Gamma_t x\cdot x}. \tag{44}$$

We get the following equations.

$$\dot{\Gamma}_t = -K - 2\Gamma_t^T L - \Gamma_t G\Gamma_t \tag{45}$$

$$\dot{a}(t) = -\frac{1}{2}\left(\mathrm{Tr}(L + G\Gamma_t)\right)a(t) \tag{46}$$

with the initial conditions

$$\Gamma_{t_0} = \Gamma,\quad a(t_0) = a_\gamma.$$

$\Gamma^T L$ and $L\Gamma$ determine the same quadratic forms. So the first equation is a Ricatti equation and can be written as

$$\dot{\Gamma}_t = -K - \Gamma_t L^T - L\Gamma_t - \Gamma_t G\Gamma_t. \tag{47}$$

We shall now see that equation (47) can be solved using Hamilton equation

$$\dot{F}_t = J\begin{pmatrix} K & L\\ L^T & G\end{pmatrix}F_t \tag{48}$$

$$F_{t_0} = \mathbb{1}. \tag{49}$$

We know that

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

is a symplectic matrix. So we have, $\det(A_t + iB_t) \neq 0$ (see below and Appendix). Let us denote

$$M_t = A_t + iB_t,\quad N_t = C_t + iD_t. \tag{50}$$

We shall prove that $\Gamma_t = N_t M_t^{-1}$. By an easy computation, we get

$$\begin{aligned}\dot{M}_t &= L^T M_t + GN_t\\ \dot{N}_t &= -KM_t - LN_t\end{aligned} \tag{51}$$

Now, compute

$$\begin{aligned} \frac{d}{dt}(N_tM_t^{-1}) &= \dot{N}M^{-1} - NM^{-1}\dot{M}M^{-1} \\ &= -K - LNM^{-1} - NM^{-1}(L^TM + GN)M^{-1} \\ &= -K - LNM^{-1} - NM^{-1}L^T - NM^{-1}GNM^{-1} \end{aligned} \tag{52}$$

which is exactly equation (47).

Now we compute $a(t)$. We have the following equalites,

$$\mathrm{Tr}\left(L^T + G(C+iD)(A+iB)^{-1}\right) = \mathrm{Tr}(\dot{M})M^{-1} = \mathrm{Tr}\left(L + G\Gamma_t\right).$$

Applying the Liouville formula

$$\frac{d}{dt}\log(\det M_t) = \mathrm{Tr}(\dot{M}_tM_t^{-1}) \tag{53}$$

we get

$$a(t) = a_\gamma\left(\det(A_t + B_t\Gamma)\right)^{-1/2}. \tag{54}$$

To complete the proof of Theorem (1.4) we apply the following lemma which is proved in [**9**], [**15**] and the appendix A of this paper.

Lemma 1.6. — *Let S be a symplectic matrix,*

$$S = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

is a symplectic matrix and $\Gamma \in \Sigma_d^+$ then $A + B\Gamma$ and $C + D\Gamma$ are non-singular and $\Sigma_S(\Gamma) := (C + D\Gamma)(A + B\Gamma)^{-1} \in \Sigma_d^+$.

Remark 1.7. — It can be proved (see [**15**]) that $\Sigma_{S_1}\Sigma_{S_2} = \Sigma_{S_1S_2}$ for every $S_1, S_2 \in \mathrm{Sp}(2d)$ and that for every $\Gamma \in \Sigma_d^+$ there exists $S \in \mathrm{Sp}(2d)$, such that $\Sigma_S(Z) = i\mathbb{1}$. In particular $S \mapsto \Sigma_S$ is a transitive projective representation of the symplectic group in the Siegel space.

A consequence of our computation of exact solutions for (43) is that the propagator $U(t,t_0)$ extends to a unitary operator in $L^2(\mathbb{R}^d)$. This is proved using the resolution of identity property.

Because $U(t,t_0)$ depends only on the linear flow $F(t,t_0)$, we can denote $U(t,t_0) = \mathcal{M}[F(t,t_0] = \mathcal{M}[F_t]$, where $\mathcal{M}$ denotes a realization of the metaplectic representation of the symplectic group $\mathrm{Sp}(2d)$. Let us recall now the main property of $\mathcal{M}$ (symplectic invariance).

Proposition 1.8. — *For every $L \in \mathcal{O}^m$, $m \in \mathbb{R}$, we have the equation*

$$\mathcal{M}[F_t]^{-1}Op_1^w[L]\mathcal{M}[F_t] = Op_1^w[L \circ F_t]. \tag{55}$$

Proof. — With the notation $U(t,s)$ for the propagator of $\hat{H}(t)$ we have to prove that for every $t,s \in \mathbb{R}$ and every smooth observable L we have:

$$U(s,t)\widehat{L \circ F(s,t)}U(t,s) = \hat{L}. \tag{56}$$

Let us compute the derivative in t. Let us remark that $U(s,t) = U(t,s)^{-1}$ and $i\partial_t U(t,s) = \hat{H}(t)U(t,s)$. So we have

$$i\partial_t(U(s,t)\widehat{L \circ F(s,t)}U(t,s) = U(s,t)\Big([\widehat{L \circ F(s,t)}, \hat{H}] + i\frac{d}{dt}\widehat{L \circ F(s,t)}\Big)U(t,s). \tag{57}$$

So, using (27) we have to prove

$$\{H(t), L \circ F(s,t)\} + \frac{d}{dt}(L \circ F(s,t)). \tag{58}$$

Using the change of variable $z = F(t,s)X$ and symplectic invariance of the Poisson bracket , (58) is easily proved. □

Remark 1.9. — It was remarked in [**9**] that we can establish many properties of the metaplectic representation, including Maslov index, from theorem (1.4). In particular the metaplectic representation $\mathcal{M}$ is well defined up to $\pm\mathbb{1}$ (projective representation).

Let us recall the definition of generalized squeezed coherent states:

$g^{\Gamma}(x) = a_{\gamma}\mathrm{e}^{i2\Gamma x\cdot x}$, where Γ is supposed to be a complex symmetric matrix in the Siegel space Σ_d^+. We know that there exists a symplectic matrix S such that $\Gamma = \varSigma_S(i\mathbb{1})$ (see [**15**] and remark (1.7). We have seen that $g^{\Gamma} = \mathcal{M}(S)g$ where $\mathcal{M}(S)$ is a metaplectic transformation. So we have, if

$$S = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

$\Gamma = (C + iD)(A + iB)^{-1}$ and $\Im(\Gamma)^{-1} = A \cdot A^T + B \cdot B^T$.

As already said in the introduction, we get a resolution of identity in $L^2(\mathbb{R}^d)$ with $g_z^{\Gamma} = \mathcal{T}(z)g^{\Gamma}$ (here $\hbar = 1$).

2. Polynomial estimates

In this section we are interested in semi-classical asymptotic expansion with error estimates in $O(\hbar^N)$ for arbitrary large N.

Let us now consider the general time dependent Schrödinger equation (3). We assume that $\hat{H}(t)$ is defined as the $\hbar$-Weyl-quantization of a smooth classical observable $H(t,x,\xi)$, $x,\xi \in \mathbb{R}^d$, so we have $\widehat{H}(t) = Op_{\hbar}^w[H(t)]$.

In this section we shall give first a proof of Theorem (0.1). Then we shall give a control of remainder estimates for large time and we shall remark that we can extend the results to vectorial Hamiltonians and systems with spin such that in the Dirac equation.

In what follows partial derivatives will be denoted indifferently $\partial_x = \frac{\partial}{\partial x}$ and for a mutilindex $\alpha \in \mathbb{N}^m$, $x = (x_1, \cdots, x_m) \in \mathbb{R}^m$, $\partial_x^\alpha = \partial_{x_1}^{\alpha_1} \cdot \cdots . \partial_{x_m}^{\alpha_m}$.

2.1. Proof of theorem (0.1). — We want to solve the Cauchy problem

$$i\hbar \frac{\partial \psi(t)}{\partial t} = \widehat{H}(t)\psi(t), \quad \psi(t_0) = \varphi_z, \tag{59}$$

where φ_z is a coherent state localized at a point $z \in \mathbb{R}^{2d}$. Our first step is to transform the problem with suitable unitary transformations such that the singular perturbation problem in $\hbar$ becomes a regular perturbation problem.

Let us define f_t by $\psi_t = \mathcal{T}(z_t)\Lambda_\hbar f_t$. Then f_t satisfies the following equation.

$$i\hbar\partial_t f_t = \Lambda_\hbar^{-1}\mathcal{T}(z_t)^{-1}\left(\widehat{H}(t)\mathcal{T}(z_t) - i\hbar\partial_t\mathcal{T}(z_t)\right)\Lambda_\hbar f_t \tag{60}$$

with the initial condition $f_{t=t_0} = g$. We have easily the formula

$$\Lambda_\hbar^{-1}\mathcal{T}(z_t)^{-1}\widehat{H}(t)\mathcal{T}(z_t)\Lambda_\hbar = Op_1^w H(t, \sqrt{\hbar}x + q_t, \sqrt{\hbar}\xi + p_t). \tag{61}$$

Using the Taylor formula we get the formal expansion

$$\begin{aligned} H(t, \sqrt{\hbar}x + q_t, \sqrt{\hbar}\xi + p_t) &= H(t, z_t) + \sqrt{\hbar}\partial_q H(t, z_t)x \\ &+ \sqrt{\hbar}\partial_p H(t, z_t)\xi + \hbar K_2(t; x, \xi) + \hbar \sum_{j\geq 3} \hbar^{j/2-1} K_j(t; x, \xi), \end{aligned} \tag{62}$$

where $K_j(t)$ is the homogeneous Taylor polynomial of degree j in $X = (x, \xi) \in \mathbb{R}^{2d}$.

$$K_j(t; X) = \sum_{|\gamma|=j} \frac{1}{\gamma!}\partial_X^\gamma H(t; z_t)X^\gamma.$$

We shall use the following notation for the remainder term of order $k \geq 1$,

$$R_k(t; X) = \hbar^{-1}\left(H(t, z_t + \sqrt{\hbar}X) - \sum_{j<k} \hbar^{j/2} K_j(t; X)\right). \tag{63}$$

It is clearly a term of order $\hbar^{k/2-1}$ from the Taylor formula. By a straightforward computation, the new function $f_t{}^\# = \exp\left(-i\frac{\delta_t}{\hbar}\right) f_t$ satisfies the following equation

$$i\partial_t f_t^\# = Op_1^w[K_2(t)]f^\# + Op_1^w[R_H^{(3)}(t)]f^\#, \quad f_{t=t_0}^\# = g. \tag{64}$$

In the r.h.s of equation (64) the second term is a (formal) perturbation series in $\sqrt{\hbar}$. We change again the unknown function $f_t^\#$ by $b(t)g$ such that $f_t^\# = \mathcal{M}[F_t]b(t)g$. Let us recall that the metaplectic transformation $\mathcal{M}[F_t]$ is the quantum propagator associated with the Hamiltonian $K_2(t)$ (see section 1). The new unknown function $b(t, x)$ satisfies the following regular perturbation differential equation in $\hbar$,

$$\begin{aligned} i\partial_t b(t, x)g(x) &= Op_1^w[R_H^{(3)}(t, F_t(x, \xi)](b(t)g)(x) \\ b(t_0) &= 1. \end{aligned} \tag{65}$$

Now we can solve equation (65) semiclassically by the ansatz

$$b(t,x) = \sum_{j\geq 0} \hbar^{j/2} b_j(t,x).$$

Let us identify powers of $\hbar^{1/2}$, denoting

$$K_j^{\#}(t,X) = K_j(t, F_t(X)), \quad X \in \mathbb{R}^{2d},$$

we thus get that the $b_j(t,x)$ are uniquely defined by the following induction formula for $j \geq 1$, starting with $b_0(t,x) \equiv 1$,

$$\partial_t b_j(t,x) g(x) = \sum_{k+\ell=j+2,\ \ell\geq 3} Op_1^w[K_\ell^{\#}(t)](b_k(t,\cdot)g)(x) \tag{66}$$

$$b_j(t_0,x) = 0. \tag{67}$$

Let us remark that $Op_1^w[K_\ell^{\#}(t)]$ is a differential operator with polynomial symbols of degree ℓ in (x,ξ). So it is not difficult to see, by induction on j, that $b_j(t)$ is a polynomial of degree $\leq 3j$ in variable $x \in \mathbb{R}^d$ with complex time dependent coefficient depending on the center z of the Gaussian in the phase space. Moreover, coming back to the Schrödinger equation, using our construction of the $b_j(t,x)$, we easily get for every $N \geq 0$,

$$i\hbar\partial_t \psi_z^N = \widehat{H}(t)\psi^N + R_z^{(N)}(t,x) \tag{68}$$

where

$$\psi_z^{(N)}(t,x) = \mathrm{e}^{i\delta_t/\hbar}\mathcal{T}(z_t)\Lambda_\hbar \mathcal{M}[F_t]\left(\sum_{0\leq j\leq N} \hbar^{j/2} b_j(t) g\right) \tag{69}$$

and

$$R_z^N(t,x) = \mathrm{e}^{i\delta_t/\hbar}\left(\hbar^{j/2} \sum_{\substack{j+k=N+2\\ k\geq 3}} \mathcal{T}(z_t)\Lambda_\hbar \mathcal{M}[F_t] Op_1^w[R_k(t)\circ F_t](b_j(t)g)\right). \tag{70}$$

Then we have an algorithm to build approximate solutions $\psi_z^{(N)}(t,x)$ of the Schrödinger equation (3) modulo the error term $R_z^{(N)}(t,x)$. Of course the real mathematical work is to estimate accurately this error term.

Let us start with a first estimate which is proved using only elementary properties of the Weyl quantization. This estimate was first proved by Hagedorn in 1980 for the Schrödinger Hamiltonian $-\hbar^2\triangle + V$, using a different method.

Proposition 2.1. — *Under assumption (1) or (2) of theorem (0.1), we have*

$$\sup_{t\in I_T} \|R_z^{(N)}(t,\bullet)\| \leq C(I_T, z, N)\hbar^{\frac{N+3}{2}} \tag{71}$$

for some constant $C(I_T,z,N) < +\infty$.

Proof. — Let us apply the integral formula for the remainder term $R_k(t, X)$ in the Taylor expansion formula.

$$R_k(t,X) = \frac{\hbar^{k/2-1}}{k!} \sum_{|\gamma|=k} \int_0^1 \partial_X^\gamma H(t, z_t + \theta\sqrt{\hbar}X) X^\gamma (1-\theta)^{k-1}\, d\theta. \tag{72}$$

So we have to show that $Op_1^w[R_k(t)](\pi(t)g^{\Gamma_t})$ is in $L^2(\mathbb{R}^d)$, for every $k \geq 3$, where $g^{\Gamma_t} = \varphi^{\Gamma_t}$, $\pi(t)$ is a polynomial with smooth coefficient in t.

If $H(t)$ satisfies condition 2 then we get the result by using the following lemma easy to prove by repeated integrations by parts (left to the reader).

Lemma 2.2. — *For every integers k', k'', ℓ', ℓ'' such that $k'-k'' > d/2$ and $\ell'-\ell'' > d/2$ there exists a constant C such that for every symbol $L \in C^\infty(\mathbb{R}^{2d})$ and state $f \in \mathcal{S}(\mathbb{R}^d)$ we have*

$$\begin{aligned} \|Op_1^w[L]f\| \leq C &\left(\int_{\mathbb{R}^d} (1+y^2)^{k'+k''} |f(y)| dy\right) \\ &\sup_{x,\xi} \left[(1+x^2)^{-k''}(1+\xi^2)^{-\ell''}\right] |(1-\triangle_\xi)^{k'}(1-\triangle_x)^{\ell'} L(x,\xi)|, \end{aligned} \tag{73}$$

where $\triangle_\xi$ is the Laplace operator in the variable ξ.

If $H(t)$ satisfies assumption 1, we have for $X = (x, \xi)$,

$$R_k(t,X) = \frac{\hbar^{k/2-1}}{k!} \sum_{|\gamma|=k} \int_0^1 \partial_x^\gamma V(t, q_t + \theta\sqrt{\hbar}x) X^\gamma (1-\theta)^{k-1}\, d\theta. \tag{74}$$

Then we have to estimate the L^2-norm of

$$k(x) := \mathrm{e}^{(q_t+\theta\sqrt{\hbar}x)^2} x^\gamma \pi_j(t,x) |\det(\Im\Gamma_t)|^{-1/4} \mathrm{e}^{-\Im\Gamma_t x\cdot x}.$$

But for ε small enough, we clearly have $\sup_{0<\hbar\leq\varepsilon} \|k\|_2 < +\infty$. □

Using the Duhamel principle, we get now the following result.

Theorem 2.3. — *Let us assume the conditions of theorem (0.1) are satisfied for every time ($I_T = \mathbb{R}$) and that the quantum propagator $U(t,t_0)$ for $\widehat{H(t)}$ exists for every $t, t_0 \in \mathbb{R}$).*

For every $T > 0$, there exists $C(N,z,T) < +\infty$ such that for every $\hbar \in]0,1]$ and every $t \in [t_0 - T, t_0 + T]$, we have

$$\|\Psi_z^{(N)}(t) - U(t,t_0)\varphi_z\| \leq C(N,z,T)\hbar^{(N+1)/2}. \tag{75}$$

Proof. — The Duhamel principle gives the formula

$$U(t,t_0)\varphi_z - \psi_z^{(N)}(t) = \frac{i}{\hbar}\int_{t_0}^t U(t,s) R_z^{(N)}(s)\, ds. \tag{76}$$

So (75) follows from (76) and (71). □

Remark 2.4. — Proofs of Theorems 2.3 and 2.3 extend easily for more general profiles $g \in \mathcal{S}(\mathbb{R}^d)$. But explicit formulae are known only for Gaussian g^Γ (see [**8**]).

To get results in the long time régime (control of $C(N, z, T)$ for large T) it is convenient to use the Fourier-Bargmann transform. We need some basic estimates which are given in the following subsection.

2.2. Weight estimates and Fourier-Bargmann transform. — We restrict here our study to properties we need later. For other interesting properties of the Fourier-Bargmann transform the reader can see the book [**29**].

Let us begin with the following formulae, easy to prove by integration by parts. With the notations $X = (q, p) \in \mathbb{R}^{2d}$, $x \in \mathbb{R}^d$ and $u \in \mathcal{S}(\mathbb{R}^d)$, we have

$$\mathcal{F}_\mathcal{B}(xu)(X) = i(\partial_p - \frac{i}{2}q)\mathcal{F}_\mathcal{B}(u)(X) \tag{77}$$

$$\mathcal{F}_\mathcal{B}(\partial_x u)(X) = i(p - \partial_p)\mathcal{F}_\mathcal{B}(u)(X). \tag{78}$$

So, let us introduce the weight Sobolev spaces, denoted $\mathcal{K}_m(d)$, $m \in \mathbb{N}$. $u \in \mathcal{K}_m(d)$ means that $u \in L^2(\mathbb{R}^d)$ and $x^\alpha \partial_x^\beta u \in L^2(\mathbb{R}^d)$ for every multiindex α, β such that $|\alpha + \beta| \le m$, with its natural norm. Then we have easily

Proposition 2.5. — *The Fourier-Bargmann is a linear continuous application from $\mathcal{K}_m(d)$ into $\mathcal{K}_m(2d)$ for every $m \in \mathbb{N}$.*

Now we shall give an estimate in exponential weight Lebesgue spaces.

Proposition 2.6. — *For every $p \in [1, +\infty]$, for every $a \ge 0$ and every $b > a\sqrt{2}$ there exists $C > 0$ such that for all $u \in \mathcal{S}(\mathbb{R}^d)$ we have,*

$$\|\mathrm{e}^{a|x|}u(x)\|_{L^p(\mathbb{R}^d_x)} \le C\|\mathrm{e}^{b|X|}\mathcal{F}^\mathcal{B}u(X)\|_{L^2(\mathbb{R}^{2d}_X)}. \tag{79}$$

More generally, for every $a \ge 0$ and every $b > a\frac{\sqrt{2}}{|S|}$ there exists $C > 0$ such that for all $u \in \mathcal{S}(\mathbb{R}^d)$ and all $S \in \mathrm{Sp}(2d)$ we have

$$\|\mathrm{e}^{a|x|}\left[\mathcal{M}(S)u\right](x)\|_{L^p(\mathbb{R}^d_x)} \le C\left\|\mathrm{e}^{b|X|}\mathcal{F}^\mathcal{B}u(X)\right\|_{L^2(\mathbb{R}^{2d}_X)}. \tag{80}$$

Proof. — Using the inversion formula and Cauchy-Schwarz inequality, we get

$$|u(x)|^2 \le (2\pi)^{-d}\|\mathrm{e}^{b|X|}\mathcal{F}^\mathcal{B}u(X)\|_{L^2(\mathbb{R}^{2d}_X)}\left(\int_{\mathbb{R}^d}\mathrm{e}^{-b\sqrt{2}|q|-|x-q|^2}\,dq\right).$$

We easily estimate the last integral by a splitting in q according $|q| \le \varepsilon|x|$ or $|q| \ge \varepsilon|x|$, with $\varepsilon > 0$ small enough hence we get (79).

Let us denote $\tilde{u} = \mathcal{F}_\mathcal{B}u$. We have

$$\mathcal{M}(S)u(x) = (2\pi)^{-d}\int_{R^{2d}}\tilde{u}(X)\left[\mathcal{M}(S)g_X)\right](x)\,dX$$

and $\mathcal{M}g_X(S)(x) = \hat{T}(SX)g^{\Gamma(S)}(x)$ where $\Gamma(S) = (C + iD)(A + iB)^{-1}$. But we have $\Im(\Gamma(S) = (A \cdot A^T + B \cdot B^T)^{-1}$ and $|(A \cdot A^T + B \cdot B^T)| \le |2S|^2$. Here $|\cdot|$ denote the matrix norm on Euclidean spaces et A^T is the transposed of the matrix A. So we get easily

$$(81)\quad \begin{aligned}|\mathcal{M}(S)u(x)|^2 \leq (2\pi)^{-d}\|\mathrm{e}^{b|X|}\mathcal{F}_{\mathcal{B}}u(X)\|_{L^2(\mathbb{R}^{2d}_X)}\cdot\\ \int_{\mathbb{R}^{2d}} \exp\left(-2b|X| - \frac{1}{|S|^2}|x - Aq + Bp|^2\right) dq\,dp.\end{aligned}$$

As above, the last integral is estimated by splitting the integration in X, according $|X| \leq \delta|x|$ and $|X| \geq \delta|x|$ and choosing $\delta = \frac{1}{|S|} + \varepsilon$ with $\varepsilon > 0$ small enough. □

We need to control the norms of Hermite functions in some weight Lebesgue spaces. Let us recall the definition of Hermite polynomials in one variable $x \in \mathbb{R}$, $k \in \mathbb{N}$, $H_k(x) = (-1)^k \mathrm{e}^{x^2}\partial_x^k(\mathrm{e}^{-x^2})$ and in $x \in \mathbb{R}^m$, $\beta \in \mathbb{N}^m$,

$$(82)\quad H_\beta(x) = (-1)^{|\beta|}\mathrm{e}^{x^2}\partial_x^\beta(\mathrm{e}^{-x^2}) = H_{\beta_1}(x_1).\cdots.H_{\beta_m}(x_m)$$

for $\beta = (\beta_1, \cdots, \beta_m)$ and $x = (x_1, \cdots, x_m)$. The Hermite functions are defined as $h_\beta(x) = \mathrm{e}^{-x^2/2}H_\beta(x)$. $\{h_\beta\}_{\beta\in\mathbb{N}^m}$ is an orthogonal basis of $L^2(\mathbb{R}^m)$ and we have for the L^2-norm, by a standard computation,

$$(83)\quad \|h_\beta\|_2^2 = 2^{|\beta|}\beta!\pi^{m/2}.$$

We shall need later more accurate estimates. Let be μ a C^∞-smooth and positive function on $\mathbb{R}^m$ such that

$$(84)\quad \lim_{|x|\to+\infty}\mu(x) = +\infty$$

$$(85)\quad |\partial^\gamma\mu(x)| \leq \theta|x|^2, \quad \forall x \in \mathbb{R}^m,\ |x| \geq R_\gamma,$$

for some $R_\gamma > 0$ and $\theta < 1$.

Lemma 2.7. — *For every real $p \in [1, +\infty]$, for every $\ell \in \mathbb{N}$, there exists $C > 0$ such that for every $\alpha, \beta \in \mathbb{N}^m$ we have:*

$$(86)\quad \|\mathrm{e}^{\mu(x)}x^\alpha\partial_x^\beta(\mathrm{e}^{-|x|^2})\|_{\ell,p} \leq C^{|\alpha+\beta|+1}\Gamma\left(\frac{|\alpha+\beta|}{2}\right)$$

where $\|\bullet\|_{\ell,p}$ is the norm on the Sobolev space $W^{\ell,p}$, Γ is the Euler gamma function.

More generally, for every real $p \in [1, +\infty]$, for every $\ell \in \mathbb{N}$, there exists $C > 0$ there exists $C > 0$ such that

$$(87)\quad \|\mathrm{e}^{\mu(\Im(\Gamma)^{-1/2}x)}x^\alpha\partial^\beta(\mathrm{e}^{-|x|^2})\|_{\ell,p} \leq C^{|\alpha+\beta|+1}(|\Im(\Gamma)^{1/2}| + |\Im(\Gamma)^{-1/2}|\Gamma\left(\frac{|\alpha+\beta|}{2}\right).$$

Proof. — We start with $p = 1$ and $\ell = 0$. By the Cauchy-Schwarz inequality, we have

$$\|\mathrm{e}^{\mu(x)}x^\alpha\partial^\beta(\mathrm{e}^{-x^2})\|_1 \leq \|\mathrm{e}^{\mu(x)}x^\alpha\mathrm{e}^{-x^2/2}\|_2\|h_\beta\|_2$$

But we have, $\forall a > 0$, $\int_0^\infty t^{2k}\mathrm{e}^{-t^2/a}dt = a^{2k+1}\Gamma(k + 1/2)$ so using (83) we get easily (86) for $\ell = 0$ and $p = 1$.

It is not difficult, using the same inequalities, to prove (86) for $p = 1$ and every $\ell \geq 1$. Then, using the Sobolev embedding $W^{\ell+m,1} \subset W^{\ell,+\infty}$ we get (86) for $p = +\infty$

and every $\ell \in \mathbb{N}$. Finally, by interpolation, we get (86) in the general case. We get a proof of (87) by the change of variable $y = \Im(\Gamma)^{1/2}x$. □

2.3. Large time estimates and Fourier-Bargmann analysis. — In this section we try to control the semi-classical error term in theorem 0.1 for large time. It is convenient to analyze this error term in the Fourier-Bargmann representation. This is also a preparation to control the remainder of order N in N for analytic or Gevrey Hamiltonians in the following section.

Let us introduce the Fourier-Bargmann transform of $b_j(t)g, B_j(t,X) = \mathcal{F}^{\mathcal{B}}[b_j(t)g](X) = \langle b_j(t)g, g_X\rangle$, for $X \in \mathbb{R}^{2d}$.

The induction equation (193) becomes for $j \geq 1$,

$$\partial_t B_j(t,X) = \int_{\mathbb{R}^{2d}} \left(\sum_{\substack{k+\ell=j+2\\ \ell\geq 3}} < Op_1^w[K_\ell^{\#}(t)]g_{X'}, g_X > \right) B_k(t,X')\, dX'. \tag{88}$$

With initial condition $B_j(t_0,X) = 0$ and with $B_0(t,X) = \exp\big(-\frac{|X|^2}{4}\big)$.

We have seen in the section 1 that we have

$$\big\langle Op_1^w[K_\ell^\sharp(t)]g_{X'}, g_X\big\rangle = (2\pi)^{-d}\int_{\mathbb{R}^{2d}} K_\ell^\sharp(t,Y)W_{X,X'}(Y)\, dY, \tag{89}$$

where $W_{X,X'}$ is the Wigner function of the pair $(g_{X'}, g_X)$. Let us now compute the remainder term in the Fourier-Bargmann representation. Using that $\mathcal{F}_{\mathcal{B}}$ is an isometry we get

$$\mathcal{F}^{\mathcal{B}}[Op_1^w[R_\ell(t)\circ F_{t,t_0}](b_j(t)g)](X) = \int_{\mathbb{R}^{2d}} B_j(t,X')\langle Op_1^w[R_\ell(t)\circ F_{t,t_0}]g_{X'}, g_X\rangle\, dX' \tag{90}$$

where $R_\ell(t)$ is given by the integral (72). We shall use (90) to estimate the remainder term $R_z^{(N)}$, using estimates (79) and (80).

Now we shall consider long time estimates for the $B_j(t,X)$.

Lemma 2.8. — *For every $j \geq 0$, every ℓ, p, there exists $C(j,\alpha,\beta)$ such that for $|t - t_0| \leq T$, we have*

$$\left\| e^{\mu(X/4)} X^\alpha \partial_X^\beta B_j(t,X)\right\|_{\ell,p} \leq C(j,\alpha,\beta)|F|_T|^{3j}(1+T)^j M_j(T,z) \tag{91}$$

where $M_j(T,z)$ is a continuous function of $\sup_{\substack{|t-t_0|\leq T\\ |\gamma|\leq j}} |\partial_X^\gamma H(t,z_t)|$ and $|F|_T = \sup_{|t-t_0|\leq T} |F_t|$.

Proof. — We proceed by induction on j. For $j = 0$ (91) results from (86).

Let us assume inequality proved up to $j-1$. We have the induction formula ($j \geq 1$)

$$\partial_t B_j(t,X) = \sum_{\substack{k+\ell=j+2\\ \ell\geq 3}} \int_{\mathbb{R}^{2d}} K_\ell(t,X,X')B_k(t,X')\, dX' \tag{92}$$

where

$$K_\ell(t,X,X') = \sum_{|\gamma|=\ell} \frac{1}{\gamma!}\partial_X^\gamma H(t,z_t)\langle Op_1^w(F_tY)^\gamma g_{X'}, g_X\rangle, \quad \text{and} \tag{93}$$

$$\langle Op_1^w(F_tY)^\gamma g_{X'}, g_X\rangle = 2^{2d}\int_{\mathbb{R}^{2d}} (F_tY)^\gamma W_{X,X'}(Y)\,dY. \tag{94}$$

By a Fourier transform computation on Gaussian functions (see Appendix), we get the following more explicit expression

$$\begin{aligned}\langle Op_1^w(F_tY)^\gamma g_{X'}, g_X\rangle = \sum_{\beta\le\gamma} C_\beta^\gamma 2^{-|\beta|}\left(F_t\left(\frac{X+X'}{2}\right)\right)^{\gamma-\alpha}\cdot\\ \cdot H_\beta\left(F_t\left(\frac{J(X-X')}{2}\right)\right)\mathrm{e}^{-|X-X'|^2/4}\mathrm{e}^{-(i/2)\sigma(X',X)}.\end{aligned} \tag{95}$$

We shall apply (95), with the following expansion

$$(F_tX)^\gamma = \sum_{|\alpha|=|\gamma|} X^\alpha q_\alpha(F_t) \tag{96}$$

where q_α is an homogeneous polynomial of degree $|\gamma|$ in the entries of F_t. Using multinomials expansions and combinatorics, we find that we have the following estimate

$$|q_\alpha(F_t)| \le (2d)^{|\gamma|}|F_t|^{|\gamma|}. \tag{97}$$

So, we have to consider the following integral kernels:

$$\begin{aligned}K^{(\gamma)}(t,X,X') = \sum_{\beta\le\gamma} C_\beta^\gamma 2^{-|\beta|}\left(F_t\frac{X+X'}{2}\right)^{\gamma-\beta}\cdot\\ \cdot H_\beta\cdot\left(F_t\frac{J(X-X')}{2}\right)\mathrm{e}^{-|X-X'|^2/4}\mathrm{e}^{-i/2\sigma(X',X)}.\end{aligned} \tag{98}$$

Let us assume that the lemma is proved for $k\le j-1$. To prove it for $k=j$ we have to estimate, for every $k\le j-1$,

$$E(X) := X^\alpha\partial_X^\beta\left(\int_{\mathbb{R}^{2d}} K^{(\gamma)}(X,X')B_k(t,X')\,dX'\right).$$

Let us denote

$$F_\beta(X,X') = H_\beta\left(\frac{J(X-X')}{2}\right)\mathrm{e}^{-|X-X'|^2/4}\mathrm{e}^{-i/2\sigma(X',X)}.$$

By expanding $X^\alpha = (X-X'+X')^\alpha$ with the multinomial formula and using integration by parts, we find that $E(X)$ is a sum of terms like

$$D_P(X) = \int_{\mathbb{R}^{2d}} (X')^{\alpha'}\partial_{X'}^{\beta'}B_k(t,X')P(X-X')\mathrm{e}^{-|X-X'|^2/4}\,dX'$$

where P is a polynomial.

We can now easily conclude the induction argument by noticing that the kernel

$$(X,X') \longmapsto P(X-X')\mathrm{e}^{-|X-X'|^2/4}\mathrm{e}^{\mu(X)-\mu(X')}$$

defines a linear bounded operator on every Sobolev spaces $W^{\ell,p}(\mathbb{R}^{2d})$. □

Now we have to estimate the remainder term. Let us assume that the following condition is satisfied:

$(AS1)$ There exists $\nu \in \mathbb{R}$ such that for every multiindex α there exist $C_\alpha > 0$ such that

$$|\partial_X^\alpha H(t,X)| \leq C_\alpha (1+|X|)^\nu, \quad \forall t \in \mathbb{R} \text{ and } \forall X \in \mathbb{R}^{2d}.$$

Let us compute the Fourier-Bargmann transform:

$$\begin{aligned}\tilde{R_z}^{(N+1)}(t,X) &= \mathcal{F}_{\mathcal{B}}\left[\sum_{\substack{j+k=N+2\\k\geq 3}} Op_1^w[R_k)(t)\circ F_t](b_j(t)g)\right](X)\\ &= \sum_{\substack{j+k=N+2\\k\geq 3}} \int_{\mathbb{R}^{2d}} B_j(t,X')\langle Op_1^w[R_k(t)\circ F_t]g_{X'}, g_X\rangle\, dX'.\end{aligned} \tag{99}$$

We shall prove the following estimates

Lemma 2.9. — *If condition $(AS1)$ is satisfied, then for every $\kappa > 0$, for every $\ell \in \mathbb{N}$, $s \geq 0$, $r \geq 1$, there exists C_ℓ and N_ℓ such that for all T and t, $|t-t_0| \leq T$, we have*

$$\left\|X^\alpha \partial_X^\beta \widetilde{R}_z^{(N+1)}(t,X)\right\|_{s,r} \leq C_{N,\ell} M_{N,\ell}(T,z) ||F|_T^{3N+3}(1+T)^{N+1} \tag{100}$$

for $\sqrt{\hbar}|F|_T \leq \kappa$, $|\alpha|+|\beta| \leq \ell$, where $M_{N,\ell}(T,z)$ is a continuous function of $\sup_{\substack{|t-t_0|\leq T\\ 3\leq|\gamma|\leq N_\ell}} |\partial_X^\gamma H(t,z_t)|$.

Proof. — As above for estimation of the $B_j(t,X)$, let us consider the integral kernels

$$N_k(t,X,X') = \langle Op_1^w[R_k(t)\circ F_t]g_{X'}, g_X\rangle. \tag{101}$$

We have

$$\begin{aligned}N_k(t,X,X') &= \hbar^{(k+1)/2}\sum_{|\gamma|=k+1}\frac{1}{k!}\int_0^1(1-\theta)^k.\\ &\times\left(\int_{\mathbb{R}^{2d}}\partial_Y^\gamma H(t,z_t+\theta\sqrt{\hbar}F_tY)(F_tY)^\gamma.W_{X',X}(Y)dY\right)d\theta.\end{aligned} \tag{102}$$

Let us denote by $N_{k,t}$ the operator with the kernel $N_k(t,X,X')$. Using the change of variable $Z = Y - \frac{X+X'}{2}$ and integrations by parts in X as above, we can estimate $N_{k,t}[B_j(t,\bullet)](X)$. □

Now, it is not difficult to convert these results in the configuration space, using (79). Let us define $\lambda_{\hbar,t}(x) = \left(\frac{|x-q_t|^2+1}{\hbar|F_t|^2}\right)^{1/2}$.

Theorem 2.10. — *Let us assume that all the assumptions of Theorem (0.1) are satisfied. Then we have for the reminder term,*

$$R_z^{(N)}(t,x) = i\hbar\frac{\partial}{\partial t}{\psi_z}^{(N)}(t,x) - \widehat{H}(t)\psi(t,x),$$

the following estimate. For every $\kappa > 0$, for every $\ell, M \in \mathbb{N}$, $r \geq 1$ there exist $C_{N,M,\ell}$ and N_ℓ such that for all T and t, $|t - t_0| \leq T$, we have:

$$\left\| \lambda_{\hbar,t}^M R_z^{(N)}(t) \right\|_{\ell,r} \leq C_{N,\ell} \hbar^{(N+3-|\alpha+\beta|)/2} M_{N,\ell}(T,z) |F|_T^{3N+3} (1+T)^{N+1} \tag{103}$$

for every $\hbar \in]0,1]$, $\sqrt{\hbar}|F_t| \leq \kappa$.

Moreover, as in theorem (0.1) if $\hat{H}(t)$ admits a unitary propagator, then under the same conditions as above, we have

$$\|U_t \varphi_z - \psi_z^{(N)}(t)\|_2 \leq C_{N,\ell} \hbar^{(N+1)/2} |F|_T^{3N+3} (1+T)^{N+2}. \tag{104}$$

Proof. — Using the inverse Fourier-Bargmann transform, we have

$$R_z^{(N)}(t,x) = \mathcal{T}(z_t) \Lambda_\hbar \left(\int_{\mathbb{R}^{2d}} (\mathcal{M}[F_t] \varphi_X)(x) \widetilde{R}_z^{(N+1)}(t,X)\, dX \right)$$

Let us remark that using estimates on the $b_j(t,x)$, we can assume that N is arbitrary large. We can apply previous result on the Fourier-Bargmann estimates to get (103). The second part is a consequence of the first part and of the Duhamel principle. □

***Corollary 2.11* (Ehrenfest time).** — *Let us assume that $|F_t| \leq e^{\gamma|t|}$, for some $\gamma > 0$, and that for all $|\alpha| \geq 3$, $\sup_{t \in \mathbb{R}} |\partial^\alpha H(t, z_t)| < +\infty$. Then for every $\varepsilon > 0$ and every $N \geq 1$, there exists $C > 0$ such that every t such that $|t| \leq \frac{1-\varepsilon}{6\gamma} |\log \hbar|$ we have, for $\hbar$ small enough,*

$$\|U_t \varphi_z - \psi_z^{(N)}(t)\|_2 \leq C \hbar^{\varepsilon(N+1)/2} |\log \hbar|^{N+2}.$$

In other words the semi-classical is valid for times smaller that the Ehrenfest time $T_E := \frac{1}{6\gamma} |\log \hbar|$.

***Remark 2.12*.** — Theorem 2.10 shows that, for $T > 0$ fixed the quantum evolution stays close of the classical evolution, with a probability very close to one, in the following sense

$$\int_{[|x-q_t| \geq \sqrt{\hbar}]} |\psi_z(t,x)|^2\, dx = O(\hbar^\infty). \tag{105}$$

From the corollary, we see that The estimate (105) is still true as long as t satisfies $|t| \leq \frac{1-\varepsilon}{6\gamma}$. We shall improve this result in the analytic and Gevrey cases in a following section.

***Remark 2.13*.** — Propagation of coherent states can be used to recover a lot of semi-classical results like the Gutzwiller trace formula [**7**], the Van Vleck formula [**3**], the Ahronov-Bohm effect [**3**]. We shall see later in this paper applications to the Bohr-Sommerfeld quantization rules and to semiclassical approximation for the scattering operator.

3. Systems with Spin

Until now we have assumed that the classical Hamiltonian $H(t)$ does not depend on $\hbar$. In many applications we have to consider classical Hamiltonians depending on $\hbar$. It is the case in quantum mechanics for particles with spin or particle in magnetic fields. To include these interesting examples in our setting, we shall consider in this section more general classical Hamiltonians $H(t, X)$, taking their values in the space of $m \times m$ complex Hermitean matrices. We shall denote by $\mathrm{Mat}(m)$ the space of of $m \times m$ complex matrices and $\mathrm{Mat}_h(m)$ the space of $m \times m$ complex Hermitean matrices. $|\bullet|$ denotes a matrix norm on $\mathrm{Mat}(m)$. Let us introduce a suitable class of matrix observables of size m.

Definition 3.1. — We say that $L \in \mathcal{O}^{\nu}_{m})$, $\nu \in \mathbb{R}$, if and only if L is a C^∞-smooth function on $\mathcal{Z}$ with values in $\mathrm{Mat}(m)$ such that for every multiindex γ there exists $C > 0$ such that

$$|\partial_X^\gamma L(X)| \leq C\langle X\rangle^\nu, \quad \forall X \in \mathcal{Z}.$$

Let us denote $\mathcal{O}^{+\infty)}_m = \bigcup_\nu \mathcal{O}^{(}_m\nu)$. We have obviously $\bigcap_\nu \mathcal{O}^\nu_m = \mathcal{S}(Z, \mathrm{Mat}(m))$ (the Schwartz space for matrix values functions).

For every $L \in \mathcal{O}^\nu_m$ and $\psi \in \mathcal{S}(Z, \mathbb{C}^m)$ we can define $\widehat{L}\psi = (Op^w_\hbar L)\psi$ by the same formula as for the scalar case ($m = 1$), where $L(\frac{x+y}{2}, \xi)\psi(y)$ means the action of the matrix $L(\frac{x+y}{2}, \xi)$ on the vector $\psi(y)$. Most of general properties already seen in the scalar can be extended easily in the matrix case:

1. $\widehat{L}$ is a linear continuous mapping on $\mathcal{S}(Z, \mathrm{Mat}(m))$;
2. $\widehat{L^\star} = \widehat{L}^\star$ and $\widehat{L}$ is a linear continuous mapping on $\mathcal{S}'(X, \mathrm{Mat}(m))$.

We have an operational calculus defined by the *product rule for quantum observables.* Let be $L, K \in \mathcal{S}(\mathcal{Z}, \mathrm{Mat}(m))$. We look for a classical observable M such that $\widehat{K} \cdot \widehat{L} = \widehat{M}$. Some computations with the Fourier transform give the following formula (see [**25**])

$$M(x, \xi) = \exp\Big(\frac{i\hbar}{2}\sigma(D_x, D_\xi; D_y, D_\eta)\Big)K(x, \xi)L(y, \eta)|_{(x,\xi)=(y,\eta)}, \tag{106}$$

where σ is the symplectic bilinear form introduced above. By expanding the exponent we get a formal series in $\hbar$:

$$M(x, \xi) = \sum_{j\geq 0} \frac{\hbar^j}{j!}\Big(\frac{i}{2}\sigma(D_x, D_\xi; D_y, D_\eta)\Big)^j a_1(x, \xi)a_2(y, \eta)|_{(x,\xi)=(y,\eta)}. \tag{107}$$

We can easily see that in general M is not a classical observable because of the $\hbar$ dependence. It can be proved that it is a *semi-classical observable* in the following sense. We say that L is a semi-classical observable of weight ν and size m if there exists $L_j \in \mathcal{O}^m(\nu)$, $j \in \mathbb{N}$, so that L is a map from $]0, \hbar_0]$ into $\mathcal{O}^m(\nu)$ satisfying the following asymptotic condition: for every $N \in \mathbb{N}$ and every $\gamma \in \mathbb{N}^{2d}$ there exists $C_N > 0$ such that for all $\hbar \in]0,1[$ we have

$$\sup_Z \langle X\rangle^{-\nu} \left| \frac{\partial^\gamma}{\partial X^\gamma}\left(L(\hbar, X) - \sum_{0\leq j\leq N} \hbar^j L_j(X)\right)\right| \leq C_N \hbar^{N+1}, \tag{108}$$

L_0 is called the principal symbol, L_1 the sub-principal symbol of $\hat{L}$.

The set of semi-classical observables of weight ν and size m is denoted by $\mathcal{O}^\nu_{m,sc}$. Now we can state the product rule

Theorem 3.2. — *For every $K \in \mathcal{O}^\nu_m$ and $L \in \mathcal{O}^\mu_m$, there exists a unique $M \in \mathcal{O}^{\nu+\mu}_{m,sc}$ such that $\widehat{K} \cdot \widehat{L} = \widehat{M}$ with $M \asymp \sum_{j\geq 0} \hbar^j M_j$. We have the computation rule*

$$M_j(x,\xi) = \frac{1}{2^j} \sum_{|\alpha+\beta|=j} \frac{(-1)^{|\beta|}}{\alpha!\beta!} (D^\beta_x \partial^\alpha_\xi K).(D^\alpha_x \partial^\beta_\xi L)(x,\xi), \tag{109}$$

where $D_x = i^{-1}\partial_x$.

In particular we have

$$M_0 = K_0 L_0, \quad M_1 = K_0 L_1 + K_1 L_0 + \frac{1}{2i}\{K_0, L_0\} \tag{110}$$

where $\{R, S\}$ is the Poisson bracket of the matricial observables $R = R_{j,k}$ and $S = S_{j,k}$ defined by the matrices equality

$$\{R,S\} = (\{R,S\}_{j,k})_{j,k}, \quad \{R,S\}_{j,k} = \sum_{1\leq \ell\leq m} \{R_{j,\ell}, S_{\ell,k}\}.$$

Let us recall that the Poisson bracket of two scalar observables F, G is defined by $\{F,G\} = \partial_\xi F \cdot \partial_x G - \partial_x F \cdot \partial_\xi G$.

A proof of this theorem in the scalar case, with an accurate remainder estimate, is given in the Appendix of [**4**]. This proof can be easily extented to the matricial case considered here. This is an exercise left to the reader.

Let us recall also some other useful properties concerning Weyl quantization of observables. Detailed proofs can be found in [**25**] and [**37**] for the scalar and the extension to the matricial case is easy.

- if $L \in \mathcal{O}^0$ then $\widehat{L}$ is bounded in $L^2(\mathcal{Z}, \mathbb{C}^m)$ (Calderon-Vaillancourt theorem).
- if $L \in L^2(Z, \mathrm{Mat(m)})$ then $\hat{L}$ is an Hilbert-Schmidt operator in $L^2(X, \mathbb{C}^m)$ and its Hilbert-Schmidt norm is

$$\|\widehat{L}\|_{HS} = (2\pi\hbar)^{-d/2}\left(\int_{\mathcal{Z}} \|L(z)\|^2\, dz\right)^{1/2},$$

  where $\|L(z)\|$ is the Hilbert-Schmidt norm for matrices.
- if $L \in \mathcal{O}^m(\nu)$ with $\nu < -2d$ then $\widehat{L}$ is a trace-class operator. Moreover we have

$$\mathrm{tr}(\hat{L}) = (2\pi\hbar)^{-d} \int_Z \mathrm{tr}(L(z))\, dz. \tag{111}$$

– $K, L \in L^2(Z, \mathrm{Mat}(m))$ then $\hat{K} \cdot \hat{L}$ is a trace class operator in $L^2(X, \mathbb{C}^m)$ and

$$\mathrm{tr}(\hat{K} \cdot \hat{L}) = (2\pi\hbar)^{-n} \int_Z \mathrm{tr}(K(z)L(z))\, dz.$$

The extension to the matricial case of the propagation of coherent states may be difficult if the principal symbol $H_0(t, X)$ has crossing eigenvalues. We shall not consider this case here (accurate results have been obtained in [**19**] and in [**45**]). We shall consider here two cases: firstly the principal symbol $H_0(t, X)$ is scalar and we shall write $H_0(t, X) = H_0(t, X)\mathbb{1}_m$ where we have identify $H_0(t, X)$ with a scalar Hamiltonian; secondly $H_0(t, X)$ is a matrix with two distinct eigenvalues of constant multiplicity (like Dirac Hamiltonians). The general case of eigenvalues of constant multiplicities is no more difficult.

Our goal here is to construct asymptotic solutions for the Schrödinger system

$$(112) \qquad i\hbar \frac{\partial \psi(t)}{\partial t} = \widehat{H}(t)\psi(t), \quad \psi(t = t_0) = v\varphi_z,$$

where $v \in \mathbb{C}^m$ and $z \in \mathcal{Z}$.

Let us remark that the coherent states analysis of the scalar case can be easily extended to the matricial case, with an extra variable $s \in \{1, 2, \cdots, m\}$ which represent a spin variable in quantum mechanics. The Fourier-Bargmann is defined for $u \in L^2(\mathbb{R}^d, \mathbb{C}^m)$, $u = (u_1, \cdots, u_m)$, using the more convenient notation $u_s(x) = u(x, s)$, $s \in \{1, 2, \cdots, m\}$,

$$\mathcal{F}^{\mathcal{B}}[u](z, s) = (2\pi)^{-d/2}\langle u_s, g_z\rangle.$$

It is an isometry from $L^2(\mathbb{R}^d)$ into $L^2(\mathbb{R}^{2d})$. Moreover we have the inversion formula

$$(113) \qquad u_s(x) = \int_{\mathcal{Z}} \mathcal{F}_{\mathcal{B}}[u](z, s)\varphi_z(x)\, dz, \text{ in the } L^2\text{-sense},$$

where $\langle \cdot, \cdot \rangle$ is the scalar product in $L^2(\mathbb{R}^d, \mathbb{C}^m)$. It also convenient to define the coherent states on $\mathcal{Z} \times \{1, 2, \cdots, m\}$ by $\varphi_{z,s} = \varphi_z e_s$ where $\{e_1, \cdots, e_m\}$ is the canonical basis of $\mathbb{C}^m$. We shall also use the notation $\varphi_{z,v} = \varphi_z v$ for $(z, v) \in \mathcal{Z} \times \mathbb{C}^m$.

The mathematical results explained in this section are proved in the thesis [**2**]. We shall revisit this work here. Let us introduce the following assumptions.

(Σ_1) $H(t)$ is a semiclassical observable of weight ν and size m such that $\hat{H}(t)$ is essentially self-adjoint in $L^2(\mathbb{R}^d, \mathbb{C}^m)$ and such that the unitary propagator $U(t, t_0)$ exists for every $t, t_0 \in \mathbb{R}$. We also assume that the classical flow for $H_0(t, X)$ exists for every $t, t_0 \in \mathbb{R}$.

The main fact here is the contribution of the subprincipal term $H_1(t, X)$. This is not difficult to see. We perform exactly the same analysis as in section 2.1. Almost nothing is changed, except that $K_j(t, X)$ are polynomials in X, with time dependent matrices depending on the Taylor expansions of the matrices $H_j(t, X)$ around z_t, and more important, we have to add to the scalar Hamiltonian $\hbar K_2(t, X)\mathbb{1}_m$ the matrix $\hbar H_1(t, z_t)$. So the spin of the system will be modify along the time evolution according to the matrix $\mathcal{R}(t,t_0)$ solving the following differential equation

$$\partial_t\mathcal{R}(t,t_0) + iH_1(t,z_t) = 0, \quad \mathcal{R}(t_0,t_0) = \mathbb{1}_m. \tag{114}$$

The following lemma is easy to prove and is standard for differential equations.

Lemma 3.3. — *Let us denote respectively by $U_2(t,t_0)$ and $U_2{}'(t,t_0)$ the quantum propagators defined by the Hamiltonians $\widehat{K_2(t)}$ respectively $\widehat{K_2(t)} + \hbar H_1(t,z_t)$. Then we have*

$$U_2{}'(t,t_0) = \mathcal{R}(t,t_0)U_2(t,t_0). \tag{115}$$

Then, for every $N \geq 0$, we get an approximate solution $\psi_{z,v}^{(N)}(t,x)$ in the following way. First, we get polynomials $b_j(t,x)$ with coefficient in $\mathbb{C}^m$, uniquely defined by the following induction formula for $j \geq 1$, starting with $b_0(t,x) \equiv v$,

$$\partial_t b_j(t,x)g(x) = \sum_{k+\ell=j+2,\ \ell\geq 3} Op_1^w[K_\ell^\#(t)](b_k(t,\cdot)g)(x) \tag{116}$$

$$b_j(t_0,x) = 0. \tag{117}$$

Moreover, coming back to the Schrödinger equation, we get, in the same way as for the scalar case, for every $N \geq 0$,

$$i\hbar\partial_t\psi_{z,v}^{(N)}(t) = \widehat{H}(t)\psi_{z,v}^{(N)} + R_z^{(N)}(t) \tag{118}$$

where

$$\psi_{z,v}^{(N)}(t,x) = \mathrm{e}^{i\delta_t/\hbar}\mathcal{T}(z_t)\Lambda_\hbar\mathcal{R}(t,t_0)\mathcal{M}[F_t]\left(\sum_{0\leq j\leq N}\hbar^{j/2}b_j(t)g\right) \tag{119}$$

and

$$R_{z,v}^{(N)}(t,x) = \mathrm{e}^{i\delta_t/\hbar}\left(\hbar^{j/2}\sum_{\substack{j+k=N+2\\ k\geq 3}}\mathcal{T}(z_t)\Lambda_\hbar\mathcal{R}(t,t_0)\mathcal{M}[F_t]Op_1^w[R_k(t)\circ F_t](b_j(t)g)\right). \tag{120}$$

Theorem 3.4. — *Let us assume the assumptions (Σ_1) are satisfied. Then we have, for every $(z,v) \in \mathcal{Z}\times\mathbb{C}^m$, for every $t \in I_T = \{t,\ |t-t_0| \leq T\}$,*

$$\|U_t\varphi_{z,v} - \psi_{z,v}^{(N)}(t)\|_2 \leq C_{N,\ell}\hbar^{(N+1)/2}M_{N,\ell}(T,z)||F|_T^{3N+3}(1+T)^{N+2}. \tag{121}$$

Let us consider now the case where the principal part $H_0(t,X)$ has two distinct eigenvalues $\lambda_\pm(t,X)$ for $(t,X) \in I_T \times Z$, with constant multiplicities $m_\pm$. Let us denote by $\pi_\pm(t,X)$ the spectral projectors on $\ker(H_0(t,X) - \lambda_\pm(t,X)\mathbb{1}_m$. All these functions are smooth in (t,X) because we assume that $\lambda_+(t,X) \neq \lambda_-(t,X)$.

To construct asymptotic solutions of equation (112) we shall show that the evolution in $\mathbb{C}^m$ splits into two parts coming from each eigenvalues $\lambda_\pm$.

In a first step we work with formal series matrix symbols in $\hbar$. Let us denote by $\mathcal{O}_{m,sc}$ the set of formal serie $L = \sum_{j\geq 0} L_j\hbar^j$ where L_j is a C^∞-smooth application from the phase space $\mathcal{Z}$ in $\mathrm{Mat}(m)$. $\mathcal{O}_{m,sc}$ is an algebra for the Moyal product defined by $M = K \circledast L$ where $M = \sum_{j\geq 0} M_j \hbar^j$ with the notations used in (109). This product is associative but non-commutative. The commutator will be denoted $[L, M]_\circledast = L \circledast M - M \circledast L$ if $L, M \in \mathcal{O}_{m,sc}$.

A formal self-adjoint observable L is a $L \in \mathcal{O}_{m,sc}$ such that each L_j is an Hermitean matrix. L is a formal projection if L is self-adjoint and if $L \circledast L = L$.

***Theorem 3.5* (Formal diagonalisation)**. — *There exists a unique self-adjoint formal projections $\Pi^\pm(t)$, smooth in t, such that $\Pi_0^\pm(t, X) = \pi_\pm(t, X)$ and*

$$(i\hbar\partial_t - H(t))\Pi^\pm(t) = \Pi^\pm(t)(i\hbar\partial_t - H(t)). \tag{122}$$

There exist $H^\pm(t) \in \mathcal{O}_{sc}^m$ such that $H_0^\pm(t, X) = \lambda^\pm(t, X)\mathbb{1}_m$ and

$$\Pi^\pm(t)(i\hbar\partial_t - H(t)) = \Pi^\pm(t)(i\hbar\partial_t - H^\pm(t)). \tag{123}$$

Moreover, the subprincipal term, $H_1^+(t)$, of $H^+(t)$ is given by the formula

(124)
$$H_1^+(t) = \pi(t)H_1(t) - \frac{1}{2i}(\lambda_+(t) - \lambda_(t))\{\pi_+, \pi_+\} + i(\partial_t\pi_+(t) - \{\pi_+, \lambda_+\})(\pi_+ - \pi_-).$$

The proof of this Theorem is postpone in Appendix A. We shall see now that we can get asymptotic solutions for (112) applying Theorems (3.5) and (3.4).

To do that we have to transform formal asymptotic observables into semiclassical quantum observables. Let us introduce the following notations. $I_T = [t_0 - T, t_0 + T]$, Ω is a bounded open set in the phase space $\mathcal{Z}$ such that we have:

(Σ_2) $H(t)$ is a semiclassical observable of weight ν and size m such that $\hat{H}(t)$ is essentially self-adjoint in $L^2(\mathbb{R}^d, \mathbb{C}^m)$ and such that the unitary propagator $U(t, t_0)$ exists for every $t \in I_T$.

Let be $z \in \Omega$ and $z_t^\pm$ the solutions of Hamilton equations

$$\partial_t z_t^\pm = J\partial_X \lambda_\pm(t, X), \quad z_{t_0}^\pm = z. \tag{125}$$

We assume that $z_t^\pm$ exist for all $t \in I_T$ and $z_t^\pm \in \Omega$.

Let us define the following symbols

$$\widetilde{H^\pm}(t, X) = H^\pm(t, X)\chi_1(X), \quad \widetilde{\Pi^\pm}(t, X) = \Pi^\pm(t, X)\chi_1(X).$$

To the formal series $\widetilde{H^\pm}(t)$ and $\widetilde{\Pi^\pm}(t, X)$ correspond semi-classical observables of weight 0, by the Borel Theorem ([**25**], Theorem 1.2.6). So there exists corresponding quantum observables, $\widehat{\widetilde{H^\pm}}(t)$, $\widehat{\widetilde{\Pi^\pm}}(t, X)$. Because $\widehat{\widetilde{H^\pm}}(t)$ is a bounded observable, it defines a quantum propagator $U^\pm(t, t_0)$. So we can apply Theorem (3.4) to get

$$\|U^\pm(t, t_0)\varphi_{z,v} - \psi_{z,v}^{\pm,(N))}(t)\|_{L^2} \leq C_{N,T}\hbar^{(N+1)/2} \tag{126}$$

where $\psi^{\pm,(N)}_{z,v}(t)$ is defined in Theorem (3.4) (we add the superscript $\pm$ for the Hamiltonians with scalar principal parts $H^{\pm}$. Hence we have the following propagation result

Theorem 3.6. — *Let us assume that assumptions* (Σ_2) *are satisfied. Then, for every* $(z,v)\in Z\times\mathbb{C}^m$*, and every* $t\in I_T$*, there exists two families of polynomials* $\widetilde{b^{\pm}_j(t)}$*, of degree no more than* $3j$*, with coefficients in* $\mathbb{C}^m$ *depending on* t,z,v*, and for every* N *there exists* $C(N,T)$*, such that if*

$$\psi^{\pm,(N)}_{z,v}(t)=\mathrm{e}^{i\delta^{\pm}_t/\hbar}\mathcal{T}(z_t)\Lambda_\hbar\mathcal{R}^{\pm}(t,t_0)\mathcal{M}[F^{\pm}_t]\left(\sum_{0\le j\le N}\hbar^{j/2}\widetilde{b^{\pm}_j(t)}g\right)\tag{127}$$

we have

$$\|U(t,t_0)\varphi_{z,v}-\psi^{+,(N)}_{z,v}(t)-\psi^{-,(N)}_{z,v}(t)\|_2\le C(N,T)\hbar^{(N+1)/2}.\tag{128}$$

Moreover we have for the principal term,

$$\widetilde{b_0(t)}=\mathcal{R}^{+}(t,t_0)\pi_{+}(t_0,z)v+\mathcal{R}^{-}(t,t_0)\pi_{-}(t_0,z)v.\tag{129}$$

Proof. — Let us define

$$\psi^{(N)}_{z,v}=\widehat{\widetilde{\Pi^{+}}}(t)\psi^{+,(N)}_{z,v}(t)+\widehat{\widetilde{\Pi^{-}}}(t)\psi^{-,(N)}_{z,v}(t).$$

Let us simplifly the notations by erasing variables N,v,z and tilde accent.

We have

$$\psi(t)=\widehat{\Pi^{+}}(t)\psi^{+}(t)+\widehat{\Pi^{-}}(t)\psi^{-}(t).$$

Let us compute $i\hbar\partial_t\psi(t)$. Remember that $i\hbar\partial_t\Pi^{\pm}(t)=[H(t),\pi^{\pm}]_\star$, we get

$$i\hbar\partial_t\psi(t)=\widehat{H(t)}\psi(t)+\widehat{\Pi^{+}}(t)(i\hbar\partial_t\psi^{+}-\widehat{H^{+}}(t))\widehat{\Pi^{-}}(t)(i\hbar\partial_t\psi^{-}-\widehat{H^{-}}(t))+R(t)$$

where $R(t)$ is a remainder term depending on the cut-off functions χ_1, χ_2. We can see easily that $R(t)=\mathcal{O}(\hbar^N)$. So the error term in the Theorem follows from Theorem 3.4, using the following elementary lemma (proved using the Taylor formula). □

Lemma 3.7. — *If* $\pi(x)$ *is a polynomial of degree* M *and* L *an observable of order* ν*, then for every* N *we have the following equality in* $L^2(\mathbb{R}^d)$*,*

$$Op^w_1[L(\sqrt{\hbar}\bullet](\pi g)=\sum_{0\le j\le N}\hbar^{j/2}{\pi_j}^Lg+\mathcal{O}(\hbar^{(N+1)/2})$$

where ${\pi_j}^L$ *is a polynomial of degree* $\le M+j$*.*

Now let us prove the formula (129). Let us first remark that we have, modulo $\mathcal{O}(\hbar^\infty)$,

$$U(t,t_0)\varphi_{z,v}\asymp\widehat{\Pi^{+}}(t)U_{+}(t,t_0)\widehat{\Pi^{+}}(t_0)\varphi_{z,v}+\widehat{\Pi^{+}}(t)U_{+}(t,t_0)\widehat{\Pi^{+}}(t_0)\varphi_{z,v}.$$

Therefore it is enough to prove the following equalities

$$\pi_{\pm}(t,z^{\pm}_t)\mathcal{R}^{\pm}(t,t_0)\pi_{\pm}(t_0,z)=\mathcal{R}^{\pm}(t,t_0)\pi_{\pm}(t_0,z).$$

Let us denote $v(t) = \mathcal{R}^{\pm}(t,t_0)\pi_{\pm}(t_0,z)$. Computing derivatives in t of $v(t)$ and $\pi_{\pm}(t,z^{\pm}{}_t)v(t)$ we can see that they satisfy the same differential equation and we conclude that $v(t) = \pi_{\pm}(t,z^{\pm}{}_t)v(t)$ for every $t\in I_T$.

Remark 3.8. — It is not difficult to extend the proof of Theorem (3.6) to systems such that the principal term has any number of constant multiplicities eigenvalues. We left to the reader the study of the remainder term for large T (estimation of the Ehrenfest time) which can be obtained following the method already used for scalar Hamiltonians.

To finish this section let us apply the results to the Dirac operator.

Let us recall that the Dirac Hamiltonien is defined in the following way. Its symbol is

$$H(t,x,\xi) = c\sum_{j=1}^{3}\alpha_j\cdot(\xi_j - A_j(t,x)) + \beta mc^2 + V(t,x),$$

where $\{\alpha_j\}_{j=1}^3$ and β are the 4×4-matrices of Dirac satisfying the anti-commutation relations

$$\alpha_j\alpha_k + \alpha_k\alpha_j = 2\delta_{jk}I_4, \quad 1\le j,k\le 4,$$

($\alpha_4 = \beta$, $\mathbb{1}_4$ is the 4×4 identity matrix). $A = (A_1,A_2,A_3)$ is the magnetic vector potential and

$$V = \begin{pmatrix} V_+\mathbb{1}_2 & 0\\ 0 & V_-\mathbb{1}_2\end{pmatrix}$$

where $V_{\pm}$, is a scalar potential (1_2 is the identity matrix on $\mathbb{C}^2$). The physical constant m (mass) and c (velocity) are fixed so we can assume $m = c = 1$. We assume for simplicity that the potentials are C^∞ and there exists $\mu\in\mathbb{R}$ such that for very $k\in\mathbb{N}$, $\alpha\in\mathbb{N}^d$ there exists $C>0$ such that for all $(t,x)\in I_T\times\mathbb{R}^d$ we have

$$|\partial_t^k\partial_x^\alpha A(t,x)| + |\partial_t^k\partial_x^\alpha V(t,x) \le C < x >^{\mu} .$$

$H(t,X)$ has two eigenvalues $\lambda_{\pm} = \pm\sqrt{1+|\xi - A(t,x)|^2} + V_{\pm}(t,x)$. To apply our results it could be sufficient to assume that $V_+(t,x) - V_-(t,x) \ge -2+\delta$ for some $\delta>0$. But to make computations easier we shall assume $V_+ = V_- = V$. Then the spectral projections are given by the formula

$$\pi_{\pm}(t,x) = \frac{1}{2} \pm \frac{\alpha\cdot(\xi - A(t,x)) + \beta}{2\sqrt{1+|\xi - A(t,x)|^2}}. \tag{130}$$

Then we compute the subprincipal terms $H^{\pm}$ by the general formula (124). After a computation left to the reader, we get the following formula

$$H_1^{\pm}(t,x,\xi) = \frac{i}{2(1+|p|^2)}\left(p\mathbb{1}_4 - \alpha\cdot H(p)\right)\cdot(\partial_t A + \partial_x V) - \sum_{1\le j<k\le 3} B_{j,k}\Gamma_{j,k}, \tag{131}$$

where $p = \xi - A(t,x)$, $B_{j,k} = \partial_{x_j}A_k - \partial_{x_k}A_j$, $\Gamma_{j,k} = \frac{-i\alpha_j\alpha_k}{\sqrt{1+|p|^2}}$.

Remark 3.9. — For physical interpretation of this term we refer to the book [**43**].

Remark 3.10. — We can extend the domain of validity of our analysis by only assumming that $H_0(t, X)$ has an eigenvalue $\lambda_+(t, X)$ with a constant multiplicity in $I_T \times \Omega$. Keeping the same notations as above, we still have that $\Pi^+(t)\psi_{z,v}^{+(N)}(t)$ is an asymptotic solution of the full Schrödinger equation (with Hamiltonian $H(t)$), for an approximate initial condition, equal to $\pi_+(t_0, z)v\varphi_z + O(\sqrt{\hbar})$ for $t = t_0$. This can be proved using the semi-classical formal construction of the nice paper [**14**].

4. Analytic and Gevrey estimates

To get exponentially small estimates for asymptotic expansions in small $\hbar$ it is quite natural to assume that the classical Hamiltonian $H(t, X)$ is analytic in X, where $X = (x, \xi) \in \mathbb{R}^{2d}$. So, in what follows we introduce suitable assumptions on $H(t, X)$. As before we assume that $H(t, X)$ is continuous in time t and C^∞ in X and that the quantum and classical dynamics are well defined.

(A_0) The quantum propagator $U(t, s)$ defined by $\hat{H}(t)$ exist for $t, s \in I_T$ as well the classical flow $\Phi^{t,s}$ defined by the Hamiltonian vector field $J\partial_X H(t, X)$.

For simplicity we shall assume that $H(t)$ is a classical symbol but the proof could be easily adapted for suitable semiclassical observables ($H(t) \asymp \sum_{j\geq 0} \hbar^j H_j(t)$).

Let us define the complex neighborhood of $\mathbb{R}^{2d}$ in $\mathbb{C}^{2d}$,

$$\Omega_\rho = \{X \in \mathbb{C}^{2d}, |\Im X| < \rho\} \tag{132}$$

where $\Im X = (\Im X_1, \cdots, \Im X_{2d})$ and $|\cdot|$ is the Euclidean norm in $\mathbb{R}^{2d}$ or the Hermitean norm in $\mathbb{C}^{2d}$. Our main asumptions are the following.

(A_ω) (Analytic assumption) There exists $\rho > 0$, $T \in]0, +\infty]$, $C > 0$, $\nu \geq 0$, such that $H(t)$ is holomorphic in Ω_ρ and for $t \in I_T$, $X \in \Omega_\rho$, we have

$$|H(t, X)| \leq C\mathrm{e}^{\nu|X|}. \tag{133}$$

(A_{G_s}) (Gevrey assumption). Let be $s \geq 1$. $H(t)$ is C^∞ on $\mathbb{R}^{2d}$ and there exist $R > 0$, $\nu \geq 0$ such that for every $t \in I_T$, $X \in \mathbb{R}^{2d}$, $\gamma \in \mathbb{N}^{2d}$, we have

$$|\partial_X^\gamma H(t, X)| \leq R^{|\gamma|+1}(\gamma!)^s \mathrm{e}^{\nu|X|^{1/s}}. \tag{134}$$

For $s = 1$, the assumptions (A_ω) and (A_{G_1}) are clearly equivalent by Cauchy formula for complex analytic functions.

We begin by giving the results on the Fourier-Bargmann side. It is the main step and gives accurate microlocal estimates for the propagation of Gaussian coherent states. We have seen (section 1) that it is not difficult to transfer theses estimates in the configuration space to get approximations of the solution of the Schrödinger equation, by applying the inverse Fourier-Bargmann transform as we did in the C^∞ case (section 3).

4.1. Analytic type estimates

***Theorem 4.1* (Analytic).** — *Let us assume that conditions (A_0) and (A_ω) are satisfied. Then the following uniform estimates hold. For every $\lambda \geq 0$, $T > 0$, there exists $C_{\lambda,T} > 0$ such that for all $j \in \mathbb{N}$, $\alpha, \beta \in \mathbb{N}^{2d}$ and $t \in I_T$ we have:*

$$\begin{aligned}(135)\qquad &\left\| X^\alpha \partial_X^\beta B_j(t, X) \right\|_{L^2(\mathbb{R}^{2d}, \mathrm{e}^{\lambda|X|}dX)} \leq \\ &\quad C_{\lambda,T}^{3j+1+|\alpha|+|\beta|} |F|_T^{3j} (1 + |t - t_0|)^j j^{-j} (3j + |\alpha| + |\beta|)^{\frac{3j+|\alpha|+|\beta|}{2}}.\end{aligned}$$

Moreover if there exists $R > 0$ such that for all $\gamma \in \mathbb{N}^{2d}$, $|\gamma| \geq 3$, we have

$$(\star) \quad |\partial_X^\gamma H(t, z_t)| \leq R^\gamma \gamma!, \quad \forall t \in \mathbb{R},$$

then $\sup_{T>0} C_{\lambda,T} := C_\lambda < +\infty$. Concerning the remainder term estimate we have: for every $\lambda < \rho$ and $T > 0$ there exists $C'_{\lambda,T}$ such that for any $\alpha, \beta \in \mathbb{N}^{2d}$, $N \geq 1$, $\nu\sqrt{\hbar}||F|_T \leq 2(\rho - \lambda)$, we have

$$\begin{aligned}(136)\qquad &\left\| X^\alpha \partial_X^\beta \tilde{R}_z^{N+1}(t, X) \right\|_{L^2(\mathbb{R}^{2d}, \mathrm{e}^{\lambda|X|}dX)} \leq \hbar^{(N+3)/2} (1 + |t - t_0|)^{N+1} \\ &\quad |F|_T^{3N+3} (C'_\lambda)^{3N+3+|\alpha|+|\beta|} (N + 1)^{-N-1} (3N + 3 + |\alpha| + |\beta|)^{\frac{3N+3+|\alpha|+|\beta|}{2}}.\end{aligned}$$

and if the condition $(\star\star)$ is fulfilled, then $\sup_{T>0} C'_{\lambda,T} := C'_\lambda < +\infty$, where

$$(\star\star) \quad |\partial_X^\gamma H(t, z_t + Y)| \leq R^\gamma \gamma! \mathrm{e}^{\nu|Y|}, \quad \forall t \in \mathbb{R},\ Y \in \mathbb{R}^{2d}$$

***Remark 4.2*.** — Condition $(\star\star)$ is convenient to control long time behaviour and large N behaviour simultaneously. From the proof we could also analyze other global conditions.

Concerning exponential weighted estimates for the $B_j(t, z)$, it would be better to get estimates with the weight $\exp(\lambda|X|^2)$ for $\lambda > 0$ small enough. But it seems more difficult to check such estimates with our method.

From theorem 4.1 we get easily weight estimates for approximate solutions and remainder term for the time dependent Schrödinger equation. Let us introduce the Sobolev norms

$$\|u\|_{r,m,\hbar} = \left(\sum_{|\alpha| \leq m} \hbar^{|\alpha|/2} \int_{\mathbb{R}^n} |\partial_x^\alpha u(x)|^r dx \right)^{1/r}$$

and a function $\mu \in C^\infty(\mathbb{R}^n)$ such that $\mu(x) = |x|$ for $|x| \geq 1$.

***Proposition 4.3*.** — *For every $m \in \mathbb{N}$, $r \in [1, +\infty]$, $\lambda > 0$ and $\varepsilon \leq \min\{1, \frac{\lambda}{|F|_T}\}$, there exists $C_{r,m,\lambda,\varepsilon} > 0$ such that for every $j \geq 0$ and every $t \in I_T$ we have*

$$(137)\qquad \|\mathcal{M}[F_{t,t_0}] b_j(t) g \mathrm{e}^{\varepsilon\mu}\|_{r,m,1} \leq (C_{r,m,\lambda,\varepsilon})^{j+1} (1 + |F|_T)^{3j+2d} j^{j/2} (1 + |t - t_0|)^j.$$

For T large the estimate is uniform if the condition $(\star)$ of the theorem (4.1) is fulfilled.

Theorem 4.4. — *With the notations of subsection (2.1) and under the assumptions of Theorem 4.1,* $\psi_z^{(N)}(t,x)$ *satisfies the Schrödinger equation*

$$i\hbar\partial_t\psi_z^{(N)}(t,x) = \widehat{H}(t)\psi_z^{(N)}(t,x) + \hbar^{(N+3)/2}R_z^{(N+1)}(t,x), \tag{138}$$

$$\text{where } \psi_z^{(N)}(t,x) = \mathrm{e}^{i\delta_t/\hbar}\mathcal{T}(z_t)\Lambda_\hbar\mathcal{M}[F_{t,t_0}]\left(\sum_{0\leq j\leq N}\hbar^{j/2}b_j(t)g\right) \tag{139}$$

is estimated in proposition 4.3 and the remainder term is controlled with the following weight estimates:
for every $m\in\mathbb{N}$, $r\in[1,+\infty]$, *there exists* $m'\geq 0$ *such that for every* $\varepsilon<\min\{1,\frac{\rho}{|F|_T}\}$, *there exist* $C>0$ *and* $\kappa>0$ *such that we have*

$$\|\hbar^{(N+3)/2}R_z^{(N+1)}(t)\mathrm{e}^{\varepsilon\mu_{\hbar,t}}\|_{r,m,\hbar}\leq C^{N+1}(N+1)^{(N+1)/2}\left(\sqrt{\hbar}|F|_T^3\right)^{N+1}\hbar^{-m'}(1+|t-t_0|)^{N+1} \tag{140}$$

for all $N\geq 0$, $t\in I_T$ *and* $\hbar>0$ *with the condition* $\sqrt{\hbar}|F|_T\leq\kappa$. *The exponential weight is defined by* $\mu_{\hbar,t}(x)=\mu\big(\frac{x-q_t}{\sqrt{\hbar}}\big)$.

Moreover, For T *large, the estimate is uniform if the condition* $(\star\star)$ *of the theorem 4.1 is fulfilled*

Corollary 4.5 **(Finite Time, Large N)**. — *Let us assume here that* $T<+\infty$.

There exist ε_T, $c>0,\hbar_0>0$, $a>0$ *such that if we choose* $N_\hbar=[\frac{a}{\hbar}]-1$ *we have*

$$\|\hbar^{(N_\hbar+3)/2}R_z^{(N_\hbar+1)}(t)\mathrm{e}^{\varepsilon\mu_{\hbar,t}}\|_{L^2}\leq\exp\left(-\frac{c}{\hbar}\right), \tag{141}$$

for every $t\in I_T$, $\hbar\in]0,\hbar_0]$, $0\leq\varepsilon\leq\varepsilon_T$. *Moreover, we have*

$$\|\psi_z^{(N_\hbar)}(t)-U(t,t_0)\varphi_z\|_{L^2}\leq\exp\left(-\frac{c}{\hbar}\right). \tag{142}$$

Corollary 4.6 **(Large Time, Large N)**. — *Let us assume that* $T=+\infty$ *and there exist* $\gamma\geq 0$, $\delta\geq 0$, $C_1\geq 0$, *such that* $|F_{t,t_0}|\leq\exp(\gamma|t|)$, $|z_t|\leq\exp(\delta|t|)$ *and that the condition* $(\star\star)$ *of the theorem 4.1 is fulfilled. Then for every* $\theta\in]0,1[$ *there exists* $a_\theta>0$ *such that if we choose* $N_{\hbar,\theta}=[\frac{a_\theta}{\hbar^\theta}]-1$ *there exist* $c_\theta>0,\hbar_\theta>0$ *such that*

$$\|\hbar^{(N_{\hbar,\theta}+2)/2}R_z^{(N_{\hbar,\theta}+1)}(t)\mathrm{e}^{\varepsilon\mu_{\hbar,t}}\|_{L^2}\leq\exp\left(-\frac{c_\theta}{\hbar^\theta}\right) \tag{143}$$

for every $|t|\leq\frac{1-\theta}{6\gamma}\log(\hbar^{-1})$, $\forall\hbar\in\hbar\in]0,\hbar_\theta]$. *Moreover we have:*

$$\|\psi^{(N_{\hbar,\theta})}(t)-U(t,t_0)\varphi_z\|_{L^2}\leq\exp\left(-\frac{c_\theta}{\hbar^\theta}\right), \tag{144}$$

under the conditions of (143).

Remark 4.7. — We have consider here standard Gaussian. All the results are true and proved in the same way for Gaussian coherent states defined by g^Γ, for any $\Gamma\in\Sigma_d^+$.

All the results in this subsection can be easily deduced from theorem 4.1. Proposition 4.3 and theorem 4.4 are easily proved using the estimates of subsection 2.2. The proof of the corollaries are consequences of theorem 4.4 and Stirling formula for the Gamma function, which entails: for some positive constant $c > 0$, $C > 0$, we have, for all $u \geq 1$,

$$cu^{u+\frac{1}{2}} \leq \Gamma(u) \leq Cu^{u+\frac{1}{2}}. \tag{145}$$

Let us now begin the proof of theorem 4.1.

Proof. — Let us remark that the integral kernel $\mathrm{e}^{-|X-X'|^2/4}$ defines a bounded linear operator from $L^2(\mathbb{R}^{2d}, \mathrm{e}^{\lambda|X|})dX$ into $L^2(\mathbb{R}^{2d}, \mathrm{e}^{\lambda|X|}dX)$, for every $\lambda \geq 0$. So the proof is almost the same for any $\lambda \geq 0$ and we shall assume for simplicity that $\lambda = 0$.

The first step is to estimate $B_j(t, X)$ by induction on j using the computations of section 2.

For $B_0(t, X) = \mathrm{e}^{-\frac{|X|^2}{4}}$ the necessary estimate was already proved in lemma 2.7. For technical reason it is easier to prove the following more sophisticated induction formula. There exists $C_{\lambda,T} > 0$ such that

$$\begin{aligned}\left\|X^\alpha \partial_X^\beta B_j(t, X)\right\|_{L^2(\mathbb{R}^{2d}, \mathrm{e}^{\lambda|X|}dX)} &\leq \sum_{1\leq m\leq j} C_{\lambda,T}^{2j+4m+|\alpha|+|\beta|} |F|_T^{3j} \\ &\quad (j + 2m + |\alpha| + |\beta|)^{\frac{j+2m+|\alpha|+|\beta|}{2}} \binom{j-1}{m-1} \frac{|t - t_0|^m}{m!}.\end{aligned} \tag{146}$$

In section 2 we have established the induction formula (92),

$$\partial_t B_j(t, X) = \sum_{\substack{k+\ell=j+2 \\ \ell\geq 3}} \int_{\mathbb{R}^{2d}} K_\ell(t, X, X')B_k(t, X')\, dX', \tag{147}$$

where

$$\begin{aligned}K_\ell(t, X, X') = \sum_{|\gamma|=\ell} \frac{1}{\gamma!} \partial_X^\gamma H(t, z_t) \sum_{\beta\leq\gamma} C_\beta^\gamma 2^{-|\beta|} \left(\frac{F_t(X + X')}{2}\right)^{\gamma-\alpha} \cdot \\ \cdot H_\beta \left(\frac{F_t J(X - X')}{2}\right) \mathrm{e}^{-|X-X'|^2/4} \mathrm{e}^{-(i/2)\sigma(X',X)}.\end{aligned} \tag{148}$$

Using the multinomial formula, we have

$$\begin{aligned}K_\ell(t, X, X') = \sum_{|\gamma|=\ell} \frac{1}{\gamma!} \partial_X^\gamma H(t, z_t) \sum_{\substack{\beta\leq\gamma \\ \alpha\leq\gamma-\beta}} \binom{\beta}{\gamma} \binom{\gamma-\beta}{\alpha} \left(\frac{F_t(X - X')}{2}\right)^\alpha \cdot \\ \cdot H_\beta \left(\frac{F_t J(X - X')}{2}\right) \mathrm{e}^{-|X-X'|^2/4} \left(F_t X'\right)^{\gamma-\beta-\alpha} \mathrm{e}^{-(i/2)\sigma(X',X)}.\end{aligned} \tag{149}$$

We shall denote by C_0 a generic constant, depending only on d, and we assume for simplicity that condition $(\star)$ is satisfied. Let us denote: $|\gamma| = \ell$, $|\alpha| = r$, $|\beta| = v$. We have $r + v \leq \ell$ and

$$\binom{\beta}{\gamma}\binom{\gamma-\beta}{\alpha} \leq C_0^\ell \frac{\ell!}{r!v!(\ell-r-v)!}. \tag{150}$$

From the Hermite polynomial estimates (lemma 2.7) we get

$$\left\| \left(\frac{F_t(X-X')}{2}\right)^\alpha H_\beta\left(\frac{F_tJ(X-X')}{2}\right) \mathrm{e}^{-|X-X'|^2/4} \right\|_{L^1(\mathbb{R}^{2d})} \leq C_0^{r+v+1}|F_t|^{r+v}\Gamma\left(\frac{r+v}{2}\right). \tag{151}$$

Let us assume that inequality (146) is proved for $k = 0, \cdots, j-1$. Let us prove it for $k = j$, if $C = C_{\lambda,T}$ is choosen large enough. Because $X^\alpha\partial_X^\beta B_j(t,X)$ has the same analytic expression as $B_j(t,X)$, it is enough to prove (146) for $\alpha = \beta = 0$. Using (149) and induction assumption, we have

$$\begin{aligned} \|\partial_t B_j(t,X)\|_{L^2(\mathbb{R}^{2d})} &\leq |F|_T^{3j} \sum_{\substack{\ell+k=j+2\\ \ell\geq 3}} \sum_{\{1\leq m\leq k\}} \sum_{\{r+v\leq\ell\}} R^\ell C_0^{r+v} C^{2k+4m+\ell-r-v}. \\ &|F|_T^{3j} \frac{\ell!}{r!v!(\ell-r-v)!}\Gamma(\frac{r+v}{2}) \cdot (k+\ell-r-v+2m)^{(k+\ell-r-v+2m)/2}. \end{aligned} \tag{152}$$

To estimate the h.r.s of (152) we use Stirling formula and remark that the function $u \mapsto \frac{(a+u)^{(a+u)/2}}{u^{u/2}}$ is increasing. So we get

$$\begin{aligned} &\sum_{r+v\leq\ell} \frac{\ell!}{r!v!(\ell-r-v)!}\Gamma\left(\frac{r+v}{2}\right)(k+\ell-r-v+2m)^{(k+\ell-r-v+2m)/2} \\ &\leq C_0^\ell \frac{\ell^\ell}{r^{r/2}v^{v/2}(\ell-r-v)^{(\ell-r-v)/2}} \frac{(k+\ell-r-v+2m)^{(k+\ell-r-v+2m)/2}}{\ell-r-v)^{(\ell-r-v)/2}} \\ &\leq C_0^\ell(k+\ell+2m)^{(k+\ell+2m)/2}, \end{aligned} \tag{153}$$

with a constant C_0 large enough.

Now, using the formula $\sum_{m\leq k\leq j-1}\binom{k-1}{m-1} = \binom{j-1}{m}$ and integration in time we get (146) for $\alpha = \beta = 0$, where $C = C_{\lambda,T}$ is choosen large enough, depending only on R and C_0. The proof is easily extended to any α, β, with the same choice of C.

The second step in the proof is to estimate the remainder term $\tilde{R}_z^{(N+1)}$. Let us recall a useful formula already used in section.2.

$$\tilde{R_z}^{(N+1)}(t,X) = \sum_{\substack{j+k=N+2\\ k\geq 3}} \int_{\mathbb{R}^{2d}} B_j(t,X')\langle Op_1^w[R_k(t)\circ F_t]g_{X'}, g_X\rangle\, dX' \tag{154}$$

where

$$R_k(t,X) = \frac{\hbar^{k/2-1}}{k!} \sum_{|\gamma|=k} \int_0^1 \partial_X^\gamma H(t, z_t + \theta\sqrt{\hbar}X)X^\gamma(1-\theta)^{k-1}\, d\theta. \tag{155}$$

We use the same method as in the first step to estimate $B_j(t,X)$. Using (154) and (155) we get:

$$\tilde{R}_z^{(N+1)}(t,X) = \sum_{\substack{j+k=N+2\\ k\geq 3}} \int_{\mathbb{R}^{2d}} B_j(t,X') K_\ell^{(R)}(t,X,X')\, dX', \tag{156}$$

where

$$\begin{aligned} K_\ell^{(R)}(t,X,X') = \sum_{|\gamma|=\ell} \partial_Y^\gamma H\left[\left[t, z_t + \theta\sqrt{\hbar}F_t\left(Y + \frac{X+X'}{2}\right)\right]\right]\cdot \\ \left(F_t\left(Y+\frac{X+X'}{2}\right)\right)^\gamma . \exp\left(-|Y|^2 + i\sigma(Y, X-X') - \frac{i}{2}\sigma(X,X')\right) dY. \end{aligned} \tag{157}$$

As in the first step of the proof, we expand $\left(Y + \frac{X+X'}{2}\right)^\gamma$ by the multinomial formula in monomials $Y^\alpha (X-X')^\beta X'^\delta$. The difference here with the first step is that we need to improve the exponential decrease of $K_\ell^{(R)}(t,X,X')$ in $|X-X'|$. This can be done by the complex deformation of $\mathbb{R}^{2d}$ in Y, $Y \mapsto Y - i\varepsilon\frac{J(X-X')}{\langle X-X'\rangle}$, for $\varepsilon > 0$, small enough. This is possible because $H(t,X)$ is supposed to be analytic. Hence we can finish the proof of (136), using the estimates (135) on the $B_j(t,X)$ and accurate computations on factorials used for their proof in the first step. □

4.2. Gevrey type estimates

***Theorem 4.8* (Gevrey).** — *Let us assume that conditions (A_0) and (A_{Gs}) are satisfied, for some $s > 1$. Then the following uniform estimates hold. For every $\lambda > 0$, there exists $C_\lambda > 0$ such that for all $j \in \mathbb{N}$, $\alpha, \beta \in \mathbb{N}^{2d}$, $N \geq 0$ we have*

$$\begin{aligned} \left\| X^\alpha \partial_X^\beta B_j(t,X)\right\|_{L^2(\mathbb{R}^{2d}, e^{\lambda|X|^{1/s}}dX)} \leq \\ C_{\lambda,T}^{3j+1+|\alpha|+|\beta|} |F|_T^{3j} (1+|t-t_0|)^j j^{(s-2)j} (3j+|\alpha|+|\beta|)^{\frac{3j+|\alpha|+|\beta|}{2}}. \end{aligned} \tag{158}$$

Moreover if there exists $R > 0$ such that for all $\gamma \in \mathbb{N}^{2d}$ we have

$$(s\star) \quad |\partial_X^\gamma H(t,z_t)| \leq R^\gamma \gamma!^s, \quad \forall t \in \mathbb{R}$$

then $\sup_{T>0} C_{\lambda,T} := C_\lambda < +\infty$. Furthermore for every $\lambda < \rho$ there exists C'_λ such that for all $\alpha, \beta \in \mathbb{N}^{2d}$, $N \geq 1$, $\nu\sqrt{\hbar}|F|_T \leq 2(\rho - \lambda)$, we have

$$\begin{aligned} \left\| z^\alpha \partial_X^\beta \tilde{R}_z^{N+1}(t,X)\right\|_{L^2(\mathbb{R}^{2d}, e^{\lambda|X|^{1/s}}dX)} \leq \hbar^{(N+3)/2} (C'_{\lambda,T})^{3N+3+|\alpha|+|\beta|} |F|_T|^{3N+3} \\ (1+|t-t_0|)^{N+1} (N+1)^{(s-2)(N+1)} (3N+3+|\alpha|+|\beta|)^{\frac{3N+3+|\alpha|+|\beta|}{2}}, \end{aligned} \tag{159}$$

and if the condition $(s\star\star)$ is fulfilled, then $\sup_{T>0} C'_{\lambda,T} := C'_\lambda < +\infty$, where

$$(s\star\star) \quad |\partial_X^\gamma H(t, z_t + Y)| \leq R^\gamma \gamma!^s e^{\nu|Y|^{1/s}}, \quad \forall t \in \mathbb{R},\ Y \in \mathbb{R}^{2d}.$$

Theorem 4.9. — *With the notations of subsection (2.1) and under the assumptions of Theorem 4.8, $\psi_z^{(N)}(t,x)$ satisfies the Schrödinger equation*

$$i\hbar\partial_t\psi_z^{(N)}(t,x) = \widehat{H}(t)\psi_z^{(N)}(t,x) + \hbar^{(N+3)/2}R_z^{(N+1)}(t,x), \tag{160}$$

$$\text{where } \psi_z^{(N)}(t,x) = \mathrm{e}^{i\delta_t/\hbar}\mathcal{T}(z_t)\Lambda_\hbar\mathcal{M}[F_{t,t_0}]\left(\sum_{0\le j\le N}\hbar^{j/2}b_j(t)g\right). \tag{161}$$

We have the following estimates. For every $m\in\mathbb{N}$, $r\in[1,+\infty]$, $\lambda>0$ and $\varepsilon\le\min\{1,\frac{\lambda}{|F|_T|}\}$, there exists $C_{r,m,\lambda,\varepsilon}>0$ such that for every $j\ge 0$ and every $t\in I_T$ we have, with $s_\star=2s-1$,

$$\|\mathcal{M}[F_{t,t_0}]b_j(t)g\mathrm{e}^{\varepsilon\mu^{1/s}}\|_{r,m,1}\le (C_{r,m,\lambda,\varepsilon})^{j+1}(1+|F|_T)^{2d}j^{s_\star j/2}|F|_T^{3j}(1+|t-t_0|)^j. \tag{162}$$

The remainder term controled with the following weight estimates:
for every $m\in\mathbb{N}$, $r\in[1,+\infty]$, there exists $m'\ge 0$ such that for every $\varepsilon<\min\{1,\frac{\rho}{|F_{t,t_0}|}\}$, there exist $C>0$ and $\kappa>0$ such that we have

$$\begin{aligned}&\|\hbar^{(N+3)/2}R_z^{(N+1)}(t)\mathrm{e}^{\varepsilon\mu_{\hbar,t}^{1/s}}\|_{r,m,\hbar}\le\\ &\qquad C^{N+1}(N+1)^{s^\star(N+1)/2}\left(\sqrt{\hbar}|F|_T|^3\right)^{N+1}\hbar^{-m'}(1+|t-t_0|)^{N+1}\end{aligned} \tag{163}$$

for all $N\ge 0$, $t\in I_T$ and $\hbar>0$ with the condition $\sqrt{\hbar}|F_{t,t_0}|\le\kappa$.

Proof. — As in the analytic case, the main result is theorem 4.8, theorem 4.9 will follow easily.

Let us first consider Gevrey estimates for the $B_j(t,X)$. They are obtained with a small modification of the analytic case. It is easy to see that the induction formula (146) is still valid if we modify it by a factor $\Gamma((s-1)j)$ in the r.h.s of (146).

To estimate the remainder term we need to use almost-analytic extensions for Gevrey-s functions as it was used in [**26**] (see Appendix A for more details).

Let us consider the space $\mathcal{G}(R,s,\nu)$ of C^∞ functions f defined on $\mathbb{R}^m$ and satisfying

$$|\partial_X^\gamma f(X)|\le R^{|\gamma|+1}|\gamma|^{s|\gamma|}\mathrm{e}^{\nu|X|^{1/s}},\quad\forall X\in\mathbb{R}^m.$$

Let us define $N_\rho=\left[(R\rho)^{1/(1-s)}\right]$ and for $X,Y\in\mathbb{R}^m$,

$$f_{R,\rho}^{aa}(X+iY)=\sum_{|\gamma|\le N_\rho}\frac{(iY)^\gamma}{\gamma!}\partial_X^\gamma f(X). \tag{164}$$

In the following proposition (proved in an appendix E) we sum up the main properties we need concerning almost-analytic extensions.

Proposition 4.10. — *Let be $f\in\mathcal{G}_s(\rho,R,\nu)$. Then for every $\theta\in]0,1[$ there exists C_θ such that for every $\rho>0$ we have:*

$$|f_{R,\rho}^{aa}(X+iY)|\le RC_\theta\mathrm{e}^{\nu|X|^{1/s}},\ \forall X\in\mathbb{R}^m,|Y|\le\theta\rho, \tag{165}$$

and there exist $b > 0$ and $\rho_0 > 0$ such that for every $X \in \mathbb{R}^m$ and every $\rho \in]0, \rho_0]$ we have, for $|Y| \le \theta\rho$,

$$|(\partial_X + i\partial_Y) f^{aa}_{R,\rho}(X + iY)| \le C_\theta e^{\nu|X|^{1/s}} \exp\left(-\frac{b}{\rho^{\frac{1}{s-1}}}\right). \tag{166}$$

Remark 4.11. — Let us recall the notation $\partial_{\bar Z} = \frac{1}{2}(\partial_X + i\partial_Y)$, where $Z = X + iY$. In the second part of the proposition, we see that if f is analytic, $s = 1$ and $\partial_{\bar Z} f = 0$. If $s > 1$ and if ρ is small then $\partial_{\bar Z} f$ will be small. This is the usefull property of almost analytic extensions.

We can now finish the proof of estimate for remainder in the Gevrey case by revisiting the proof of theorem 4.1. Let us work with an almost analytic extension in X, $H^{aa}_{R,\rho}(t, X + iY)$. The contour deformation will be defined here in the following way, from $\mathbb{R}^{2d}$ to $\mathbb{C}^{2d}$,

$$\mathbb{R}^{2d} \ni Z \longmapsto Z - i\varepsilon \frac{J(X - X')}{\langle X - X' \rangle^r}, \quad \text{for } \varepsilon > 0.$$

and the Cauchy theorem is replaced here by the Stokes theorem,

$$\int_{\partial\mathcal{U}} f(u)\, du = \int_{\mathcal{U}} \frac{df}{d\bar u}\, du \wedge d\bar u$$

where f is C^1 on the smooth domain $\mathcal{U}$ of $\mathbb{R}^2$ identified with $\mathbb{C}$, applied successively in variables Z_j $(Z = (Z_1, \cdots, Z_{2d}))$.

So, choosing $r = 2 - \frac{1}{s}$, using proposition 4.10 with $\rho = \varepsilon \frac{|X - X'|}{\langle X - X' \rangle^r}$ and computing as in the proof of (136), we can finish the proof of (159). □

We can get the following exponential small error estimate for the propagation of coherent states in the Gevrey case:

Corollary 4.12. — *Let us assume here that $T < +\infty$. Then there exist $c > 0, \hbar_0 > 0$, $a > 0$, small enough, such that if we choose $N_\hbar = [\frac{a}{\hbar^{1/s_\star}}] - 1$ we have, for every $t \in I_T$, $\hbar \in]0, \hbar_0]$,*

$$\|\psi_z^{(N_\hbar)}(t) - U(t, t_0)\varphi_z\|_{L^2} \le \exp\left(-\frac{c}{\hbar^{1/s_\star}}\right). \tag{167}$$

4.3. Propagation of frequency sets. — It is well known that microlocal analysis describes in the phase space the singularities of solutions of partial differential equations [**25**] and one its paradigm is that singularities are propagated through the trajectories of the Hamiltonian flow of the symbol of the differential operator.

In semi-classical analysis, the singularities of a state are measured by the size of the state in $\hbar$, localized in the phase space.

Definition 4.13. — Let be $\psi^{(\hbar)} \in L^2(\mathbb{R}^d)$ such that $\sup_{0<\hbar\le h_0} \|\psi^{(\hbar)}\| < +\infty$. For every real number $s \ge 1$, the $\mathcal{G}s$-frequency set of ψ is the closed subset $\mathrm{FS}_{\mathcal{G}s}[\psi]$ of the phase space $\mathcal{Z}$ defined as follows.

$X^0 \notin \mathrm{FS}_{\mathcal{G}^s}[\psi]$ if and only if there exists a neighborhood $\mathcal{V}$ of X^0 and $c > 0$ such that

$$|\langle \psi, \varphi_z \rangle| \leq \mathrm{e}^{-\frac{c}{\hbar^{1/s}}}, \ \forall z \in \mathcal{V}. \tag{168}$$

For $s = 1$, $\mathrm{FS}_{\mathcal{G}^1}[\psi^{(\hbar)}] = \mathrm{FS}_{\omega}[\psi^{(\hbar)}]$ is the analytic frequency set.

Remark 4.14. — If in the above definition, $z^0 = (x^0, \xi^0)$ and if we can choose $\mathcal{V} = V \times \mathbb{R}^d$ then (168) is equivalent to $\int_{V_1} |\psi(x)|^2 dx \leq \mathrm{e}^{-\frac{c_1}{\hbar^{1/s}}}$ where V_1 is a neighborhood of x^0 and $c_1 > 0$ (see [**29**]).

Frequency set has several other names: wave front set, essential support, micro-support. There exist several equivalent definitions. For us the most convenient is to use coherent states.

The goal of this subsection is to give a proof of the following propagation theorem.

Theorem 4.15. — *Let us assume that conditions* (A_0) *and* $(A_{\mathcal{G}^s})$ *are satisfied. Let be* $\psi_\hbar$ *a family of states in* $L^2(\mathbb{R}^d)$ *such that* $\sup_{0<\hbar\leq h_0} \|\psi^{(\hbar)}\| < +\infty$. *Then for every* $s' \geq 2s - 1$, *and every* $t \in \mathbb{R}$, $t_0 \in \mathbb{R}$ *we have:*

$$\mathrm{FS}_{\mathcal{G}^{s'}}[U(t,t_0)\psi^{(\hbar)}] = \Phi^{t,t_0}\left(\mathrm{FS}_{\mathcal{G}^{s'}}[\psi]\right) \tag{169}$$

Proof. — This theorem is more or less a consequence of our analytic estimates for $U(t, t_0)\varphi_z$. We detail the proof for the analytic frequency set and $s' = 1$. The proof for $s > 1$ is almost unchanged. We have

(170)

$$\langle U(t,t_0)\psi, \varphi_z\rangle = \langle \psi, U(t_0,t)\varphi_z\rangle = \langle \psi, \psi_z^{(N_\hbar)}(t_0)\rangle + \big\langle \psi, \big(U(t_0,t)\varphi_z - \psi_z^{(N_\hbar)}(t_0)\big)\big\rangle.$$

From corollary 4.5 we get, with $N_\hbar = [\frac{a}{\hbar}]$,

$$|\langle \psi, U(t_0,t)\varphi_z - \psi_z^{(N(\hbar))}(t_0)\rangle| \leq \|\psi\|_{L^2} \exp\left(-\frac{c}{\hbar}\right), \ c > 0. \tag{171}$$

To conclude we need to estimate $\langle \psi, \psi_z^{(N(\hbar))}(t_0)\rangle$ using the two following lemma, which will be proved later.

Lemma 4.16. — *For every symplectic matrix* S *there exists* $C > 0$ *and* $\varepsilon > 0$ *such that for all* $X \in \mathbb{R}^{2d}$, $|Y| \leq \varepsilon$ *and* $\hbar > 0$, *we have*

$$|\langle \varphi_X, \mathcal{M}_\hbar[S]\varphi_Y\rangle| \leq \exp\left(-\frac{|X|^2}{C\hbar}\right), \tag{172}$$

where $\mathcal{M}_\hbar[S] = \Lambda_\hbar \mathcal{M}[S]\Lambda_\hbar^{-1}$.

Lemma 4.17. — *For every* $\lambda > 0$, $T > 0$, *there exists* $C > 0$ *such that for every* $j \geq 1$, $t \in I_T$, $X \in \mathbb{R}^{2d}$, *we have*

$$|B_j(t,X)| \leq C^j \mathrm{e}^{-\lambda|X|} j^{j/2} \exp\left(-\frac{|X|^2}{Cj}\right). \tag{173}$$

In particular, for every $\delta > 0$, $\lambda > 0$, $a \in]0, e^{-1}[$, there exist $C > 0$ such that for $|X| \geq \delta$, $t \in I_T$ and $j\hbar \leq a$, we have

$$|B_j(t, X)| \leq \exp\left(-\frac{1}{C\hbar} - \lambda|X|\right). \tag{174}$$

Let us introduce the notations $f = \Lambda_\hbar\left(\sum_{0\leq j\leq N_\hbar} \hbar^{j/2} b_j(t)g\right)$ and $\tilde{\psi} = \mathcal{F}_\hbar^{\mathcal{B}}\psi$ (Fourier-Bargman transform). Then we have

$$|\langle\psi, \psi_X^{(N_\hbar)}(t_0)\rangle| \leq \int_{\mathbb{R}^{2d}} |\tilde{\psi}(Y)||\langle\varphi_{Y-z}, \mathcal{M}_\hbar f\rangle|\, dY. \tag{175}$$

Let be the constants $\varepsilon > 0$ small enough and $C > 0$ large enough. For $|Y - z| \leq \varepsilon$ we have $|\tilde{\psi}(Y)| \leq \mathrm{e}^{-\frac{1}{C\hbar}}$. Let us consider now the case $|Y - z| \geq \varepsilon$. We have

$$|\langle\varphi_{Y-z}, \mathcal{M}_\hbar f\rangle| \leq (2\pi\hbar)^{-d} \int_{\mathbb{R}^{2d}} |\langle\varphi_{Y-z}, \mathcal{M}_\hbar\varphi_X\rangle||\tilde{f}(X)|\, dX. \tag{176}$$

Using the two above lemmas we have:
if $|X| \leq \varepsilon$,

$$|\langle\varphi_{Y-z}, \mathcal{M}_\hbar\varphi_X\rangle| \leq \exp\left(-\frac{|Y - z|^2}{C\hbar}\right)$$

and if $|X| \geq \varepsilon$

$$|\tilde{f}(X)| \leq \mathrm{e}^{-\lambda|X| - \frac{1}{C\hbar}}.$$

So, finally we get

$$|\langle\psi, \psi_z^{(N_\hbar)}(t_0)\rangle| \leq \mathrm{e}^{-\frac{1}{C\hbar}}. \qquad \square$$

Let us now prove lemma 4.16.

Proof. — Let be $S = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$. Using theorem 1.4 and Fourier transform formula for Gaussian functions we can see that

$$\langle\varphi_X, \mathcal{M}_\hbar[S]\varphi_Y\rangle = \mathrm{e}^{ib(X,Y)},$$

where b is a quadratic form in (X, Y). So by perturbation, it is enough to prove the inequality for $Y = 0$. To do that we can easily compute $2i(\Gamma + i)^{-1} = \mathbb{1} + W$, where $W = (A-D+i(B+C))(A+D+i(B-C))^{-1}$ and prove that that $W^\star W < \mathbb{1}$. The result follows from the Fourier transform formula for Gaussian functions (see Appendix). $\square$

Let us now prove lemma 4.17.

Proof. — Inequality (173) is a little improvement of the theorem 4.1 (135) but it is crucial for our purpose.

So we revisit the proof of (135). We will prove, by induction, the following pointwise estimate, by revisiting the proof of (135).

$$
(177)\quad \begin{aligned} |X^\alpha B_j(t,X)| \leq \sum_{1\leq m\leq j} & C^{2j+4m+|\alpha|+|\beta|}\binom{j-1}{m-1}\frac{|t-t_0|^m}{m!}\cdot \\ & \cdot\left(\sum_{0\leq \ell\leq j} \mathrm{e}^{-\lambda|X|}g^{(\sigma_\ell)}(X)\right)(j+2m+|\alpha|)^{\frac{j+2m+|\alpha|}{2}}, \end{aligned}
$$

where $g^{(\sigma)}(X)$ is the Gaussian probability density in $\mathbb{R}^{2d}$ with mean 0 and variance σ^2, σ_j is an increasing sequence of positive real numbers such that $\lim_{j\to+\infty}\frac{\sigma_j^2}{j}>0$.

To go from the step $j-1$ to the step j in the induction we use the following well known property for convolution of Gaussian functions: $g^{(2)}\star g^{(\sigma_k)} = g^{(\sigma_{k+1})}$ where $\sigma_{k+1}^2 = 4+\sigma_k^2$. So we have $\sigma_j^2 = 2+4j$, starting with $\sigma_0^2 = 2$. Hence we get (173).

Let us prove (174). We want to estimate $(j\hbar)^{j/2}\mathrm{e}^{-\frac{\delta}{Cj\hbar}}$. To do that we consider the one variable function $\ell(u) = \frac{x\log x}{2\hbar} - \frac{b}{u}$ where b is a small positive constant. For $\hbar$ small enough and $a\in\,]0,\mathrm{e}^{-1}[$ we see that ℓ is increasing on $]0,a]$ and, for some $c>0$, $f(a)\leq -\frac{c}{\hbar}$. So, we get, for $1\leq j\leq \frac{a}{\hbar}$, $(j\hbar)^{j/2}\mathrm{e}^{-\frac{\delta}{Cj\hbar}} \leq \mathrm{e}^{-\frac{c}{\hbar}}$. □

Remark 4.18. — Several proofs are known for the propagation of analytic frequency set. For analytic singularities it is due to Hanges. Another simple proof in the semiclassical frame work is due to Martinez [**29**].

5. Scattering States Asymptotics

5.1. What is scattering theory?— There are many books on this subject. For good references concerning as well classical and quantum mechanics, we shall mention here [**10**], [**36**].

Let us only recall some basic facts and notations concerning classical and quantum scattering. We consider a classical Hamiltonian H for a particle moving in a curve space and in an electro-magnetic field. We shall assume that

$$H(q,p) = \frac{1}{2}g(q)p\cdot p + a(q)\cdot p + V(q),\ q\in\mathbb{R}^d,\ p\in\mathbb{R}^d,$$

$g(q)$ is a smooth definite positive matrice and there exist $c>0, C>0$ such that

$$(178)\qquad c|p|^2 \leq g(q)p\cdot p \leq C|p|^2,\quad \forall (q,p)\in\mathbb{R}^{2d}.$$

$a(q)$ is a smooth linear form on $\mathbb{R}^d$ and $V(q)$ is a smooth scalar potential. In what follows it will be assumed that $H(q,p)$ is a *short range perturbation* of $H^{(0)}(q,p) = \frac{|p|^2}{2}$ in the following sense. There exists $\rho>1$, $c>0$, $C>0$, C_α, for $\alpha\in\mathbb{N}^d$ such that

$$
(179)\quad \begin{aligned} & |\partial_q^\alpha(\mathbb{1}-g(q))| + |\partial_q^\alpha a(q)| + |\partial_q^\alpha V(q)| \leq \\ & \qquad C_\alpha < q >^{-\rho-|\alpha|},\quad \forall q\in\mathbb{R}^d,\ \text{where } \partial_q^\alpha = \frac{\partial^\alpha}{\partial q^\alpha}. \end{aligned}
$$

H and $H^{(0)}$ define two Hamiltonian flows Φ^t, Φ_0^t, on the phase space $\mathbb{R}^{2d}$ for all $t \in \mathbb{R}$. Scattering means here comparaison of the two dynamics Φ^t, Φ_0^t. The free dynamic is explicit: $\Phi_0^t(q^0, p^0) = (q^0 + tp^0, p^0)$. The interacting dynamic is the main object of study. The methods of [**10**] and [**36**] can be used to prove existence of the classical wave operators, defined by

$$\Omega_{\pm}^{c\ell} X = \lim_{t\to\pm\infty} \Phi^{-t}(\Phi_0^t X). \tag{180}$$

This limit exists for every $X \in \mathcal{Z}_0$, where $\mathcal{Z}_0 = \{(q,p) \in \mathbb{R}^{2d},\ p \neq 0\}$, and is uniform on every compact of $\mathcal{Z}_0$. We also have, for all $X \in \mathcal{Z}_0$,

$$\lim_{t\to\pm\infty} \left(\Phi^t \Omega_{\pm}^{c\ell}(X) - \Phi_0^t(X)\right) = 0 \tag{181}$$

Moreover, $\Omega_{\pm}^{c\ell}$ are C^∞-smooth symplectic transformations. They intertwine the free and the interacting dynamics:

$$H \circ \Omega_{\pm}^{c\ell} X = H^{(0)}(X), \quad \forall X \in \mathcal{Z}_0, \qquad \text{and} \quad \Phi^t \circ \Omega_{\pm}^{c\ell} = \Omega_{\pm}^{c\ell} \circ \Phi_0^t \tag{182}$$

The classical scattering matrix $S^{c\ell}$ is defined by $S^{c\ell} = (\Omega_{+}^{c\ell})^{-1}\Omega_{-}^{c\ell}$. This definition make sense because we can prove (see [**36**]) that modulo a closed set $\mathcal{N}_0$ of Lebesgue mesure 0 in $\mathcal{Z}$ ($\mathcal{Z}\backslash\mathcal{Z}_0 \subseteq \mathcal{N}_0$) we have:

$$\Omega_{+}^{c\ell}(\mathcal{Z}_0) = \Omega_{-}^{c\ell}(\mathcal{Z}_0)$$

Moreover $S^{c\ell}$ is smooth in $\mathcal{Z}\backslash\mathcal{N}_0$ and commutes with the free evolution: $S^{c\ell}\Phi_0^t = \Phi_0^t S^{c\ell}$. The scattering operator has the following kinematic interpretation.

Let us start with a point X_- in $\mathcal{Z}_0$ and its free evolution $\Phi_0^t X_-$. There exists a unique interacting evolution $\Phi^t(X)$, which is close to $\Phi_0^t(X_-)$ for $t \searrow -\infty$. Moreover there exists a unique point $X_+ \in \mathcal{Z}_0$ such that $\Phi^t(X)$ is close to $\Phi_0^t(X_+)$ for $t \nearrow +\infty$. X, X_+ are given by $X = \Omega_{-}^{c\ell} X_-$ and $X_+ = S^{c\ell} X_-$. Using [**10**], we can get a more precise result. Let I be an open interval of $\mathbb{R}$ and assume that I is *non-trapping* for H, which means that for every X such that $H(X) \in I$, we have $\lim\limits_{t\to\pm\infty} |\Phi^t(X)| = +\infty$. Then we have

Proposition 5.1. — *If I is a non-trapping energy interval for I then $S^{c\ell}$ is defined everywhere in $H^{-1}(I)$ and is a C^∞ smooth symplectic map.*

On the quantum side the scattering operator is defined in a analogue way. The quantum dynamics are now given by the evolution unitary groups: $U(t) = \mathrm{e}^{-\frac{it}{\hbar}\hat{H}}$ and $U_0(t) = \mathrm{e}^{-\frac{it}{\hbar}\widehat{H}^0}$. The free evolution is also explicit

$$U_0(t)\psi(x) = (2\pi\hbar)^{-d} \iint_{\mathbb{R}^{2d}} \mathrm{e}^{\frac{i}{\hbar}\left(-t\frac{\xi^2}{2} + (x-y)\cdot\xi\right)} \psi(y)\, dy\, d\xi \tag{183}$$

Let us remark that the operator $\hat{H}$ is essentially self-adjoint so $U(t)$ is a well defined unitary group in $L^2(\mathbb{R}^d)$.

Assumptions (179) implies that we can define the wave operators $\Omega_\pm$ and the scattering operator $S^{(\hbar)} = (\Omega_+)^\star\Omega_-$ (see [**36**] and [**10**] and the methods explained in these books). Recall that $\Omega_\pm = \lim_{t\to\pm\infty} U(-t)U_0(t)$, the ranges of $\Omega_\pm$ are equal to the absolutely continuous subspace of $\hat{H}$ and we have

$$\Omega_\pm U_0(t) = U(t)\Omega_\pm, \quad S^{(\hbar)}U_0(t) = U_0(t)S^{(\hbar)}, \quad \forall t \in \mathbb{R}. \tag{184}$$

The scattering operator $S = S^{(\hbar)}$ depends on the Planck constant $\hbar$ so the correspondence principle in quantum mechanics binds $\lim_{\hbar\to 0} S^{(\hbar)}$ and the classical scattering operator $S^{c\ell}$. There are many papers on this subject [**51**], [**39**], [**18**], [**21**]. Here we want to check this classical limit by using a coherent states approach, like in [**18**] and [**21**]. Using a different technical approach, we shall extend here their results to more general perturbations of the Laplace operator. It could be possible to consider as well more general free Hamiltonians (like Dirac operator) and long range perturbations.

5.2. quantum scattering and coherent states. — The statement of the main results in this section are direct and natural extensions to the scattering case of the propagation of coherent state proved at finite time in section1, Theorem 0.1.

Theorem 5.2. — *For every $N \geq 1$, every $z_- \in \mathcal{Z}\backslash\mathcal{N}_0$ and every $\Gamma_- \in \Sigma_d^+$ (Siegel space), we have the following semi-classical approximation for the scattering operator $S^{(\hbar)}$ acting on the Gaussian coherent state $\varphi_{z_-}^{\Gamma_-}$,*

$$S^{(\hbar)}\varphi_{z_-}^{\Gamma_-} = \mathrm{e}^{i\delta_+/\hbar}\mathcal{T}(z_+)\Lambda_\hbar\mathcal{M}[G_+]\left(\sum_{0\leq j\leq N}\hbar^{j/2}b_j g^{\Gamma_-}\right) + \mathcal{O}(\hbar^{(N+1)/2}) \tag{185}$$

where we use the following notations:
- $z_+ = S^{c\ell}z_-, \ z_\pm = (q_\pm, p_\pm)$
- $z_t = (q_t, p_t)$ *is the interacting scattering trajectory:* $z_t = \Phi^t(\Omega_-^{c\ell}z_-)$
- $\delta_+ = \int_{-\infty}^{+\infty}(p_t\dot{q}_t - H(z_t))dt - \frac{q_+p_+ - q_-p_-}{2}$
- $G_+ = \frac{\partial z_+}{\partial z_-}$
- b_j *is a polynomial of degree* $\leq 3j$, $b_0 = 1$
- *The error term* $\mathcal{O}(\hbar^{(N+1)/2})$ *is estimated in the* L^2*-norm.*

Proof. — Let us denote $\psi_- = \varphi_{z_-}^{\Gamma_-}$ and $\psi_+ = S^{(\hbar)}\varphi_{z_-}^{\Gamma_-}$. Using the definition of $S^{(\hbar)}$ we have

$$\psi_+ = \lim_{t\to+\infty}\left(\lim_{s\to-\infty} U_0(t)U(t-s)U_0(s)\right)\psi_-. \tag{186}$$

The strategy of the proof consists in applying the propagation theorem 0.1 at fixed time to $U(t-s)$ in (186) and then to see what happens in the limits $s \to -\infty$ and $t \to +\infty$.

Let us denote F_t^0 the Jacobi stability matrix for the free evolution and $F^t(z)$ the Jacobi stability matrix along the trajectory $\Phi^t(z)$. Let us first remark that we have the explicit formula

$$F_t^0 = \begin{pmatrix} \mathbb{1}_d & t\mathbb{1}_d \\ 0 & \mathbb{1}_d \end{pmatrix}. \tag{187}$$

To check the two successive limits in equality (186), uniformly in $\hbar$, we obviously need large time estimates concerning classical scattering trajectories and their stability matrices.

Proposition 5.3. — *Under the assumptions of Theorem (5.2), there exists a unique (scattering) solution of the Hamilton equation $\dot{z}_t = J\nabla H(z_t)$ such that*

$$\dot{z}_t - \partial_t \Phi_0^t z_+ = \mathcal{O}(\langle t\rangle^{-\rho}), \text{ for } t \to +\infty \tag{188}$$

$$\dot{z}_t - \partial_t \Phi_0^t z_- = \mathcal{O}(\langle t\rangle^{-\rho}), \text{ for } t \to -\infty \tag{189}$$

Proposition 5.4. — *Let us denote $G_{t,s} = F_{t-s}(\Phi_0^s z_-)F_s^0$. Then we have*
i) $\lim_{s\to-\infty} G_{t,s} = G_t$ *exists,* $\forall t \geq 0$
ii) $\lim_{t\to+\infty} F_{-t}^0 G_t = G_+$ *exists*
iii) $G_t = \frac{\partial z_t}{\partial z_-}$ *and* $G_+ = \frac{\partial z_+}{\partial z_-}$.

These two propositions and the following one will be proved later. The main step in the proof is to solve the following asymptotic Cauchy problem for the Schrödinger equation with data given at time $t = -\infty$.

$$i\hbar\partial_s \psi_{z_-}^{(N)}(s) = \hat{H}\psi_{z_-}^{(N)}(s) + O(\hbar^{(N+3)/2} f_N(s)) \tag{190}$$

$$\lim_{s\to-\infty} U_0(-s)\psi_{z_-}^{(N)}(s) = \varphi_{z_-}^{\Gamma_-} \tag{191}$$

where $f_N \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$ is independent on $\hbar$. The following proposition is an extension for infinite times of results proved in section 1 for finite time.

Proposition 5.5. — *The problem (190) has a solution which can be computed in the following way.*

$$\psi_{z_-}^{(N)}(t,x) = \mathrm{e}^{i\delta_t(z_t)/\hbar}\mathcal{T}(z_-)\Lambda_\hbar \mathcal{M}[G_t]\left(\sum_{0\leq j\leq N} \hbar^{j/2} b_j(t,z_-) g^{\Gamma_-}\right) \tag{192}$$

the $b_j(t,z_-,x)$ are uniquely defined by the following induction formula for $j \geq 1$, starting with $b_0(t,x) \equiv 1$,

$$\partial_t b_j(t,z_-,x)g(x) = \sum_{k+\ell=j+2,\ \ell\geq 3} Op_1^w[K_\ell^{\#}(t)](b_k(t,\cdot)g)(x) \tag{193}$$

$$\lim_{t\to-\infty} b_j(t,z_-,x) = 0. \tag{194}$$

with

$$K_j^{\#}(t,X) = K_j(t,G_t(X)) = \sum_{|\gamma|=j} \frac{1}{\gamma!}\partial_X^\gamma H(z_t)(G_t X)^\gamma, \quad X \in \mathbb{R}^{2d}.$$

$b_j(t,z_-,x)$ is a polynomial of degree $\le 3j$ in variable $x\in\mathbb{R}^d$ with complex time dependent coefficients depending on the scattering trajectory z_t starting from z_- at time $t=-\infty$.

Moreover we have the remainder uniform estimate

$$i\hbar\partial_t\psi_{z_-}^{(N)}(t)=\hat{H}\psi_{z_-}^{(N)}(t)+\mathcal{O}(\hbar^{(N+3)/2}\langle t\rangle^{-\rho})\tag{195}$$

uniformly in $\hbar\in\,]0,1]$ and $t\ge 0$.

Proof. — Without going into the details, which are similar to the finite time case, we remark that in the induction formula we can use the following estimates to get uniform decreasing in time estimates for $b_j(t,z_-,x)$. First, there exists $c>0$ and $T_0>0$ such that, for $t\ge T_0$ we have $|q_t|\ge ct$. Using the short range assumption and conservation of the classical energy, for $|\gamma|\ge 3$, there exists $C\gamma$ such that

$$|\partial_X^\gamma H(z_t)|\le C_\gamma\langle t\rangle^{\rho-1},\ \forall t\ge 0.\tag{196}$$

Therefore, we can get (195) using (196) and (193). □

Let us now finish the proof of the Theorem.

Using Proposition (5.5) and Duhamel formula we get

$$U(t)\psi_{z_-}^{(N)}(s)=\psi_{z_-}^{(N)}(t+s)+\mathcal{O}(\hbar^{(N+1)/2}),\tag{197}$$

uniformly in $t,s\in\mathbb{R}$.

But we have

(198)
$$\|\psi_{z_-}^{(N)}(t)-U(t-s)U_0(s)\psi_{z_-}\|\le\|\psi_{z_-}^{(N)}(t)-U(t-s)\psi_{z_-}^{(N)}(s)\|+\|U_0(s)\psi_--\psi_{z_-}^{(N)}(s)\|.$$

We know that $\lim_{s\to-\infty}\|U_0(s)\psi_--\psi_{z_-}^{(N)}(s)\|=0$. Going to the limit $s\to-\infty$, we get, uniformly in $t\ge 0$,

$$\|\psi_{z_-}^{(N)}(t)-U(t)\Omega_-\psi_-\|=\mathcal{O}(\hbar^{(N+1)/2}).\tag{199}$$

Then we can compute $U_0(-t)\psi_{z_-}^{(N)}(t)$ in the the limit $t\to+\infty$ and we find out that $S^{(\hbar)}\psi_-=\psi_+^{(N)}+O(\hbar^{(N+1)/2})$ where $\psi_+^{(N)}=\lim_{t\to+\infty}U_0(-t)\psi_{z_-}^{(N)}(t)$. □

Let us now prove Proposition 5.3, following the book [**36**].

Proof. — Let us denote $u(t)=z_t-\Phi_0^t z_-$. We have to solve the integral equation

$$u(t)=\Phi_0^t(z_-)+\int_{-\infty}^t(J\nabla H(u(s)+\Phi_0^s(z_-))\,ds.\tag{200}$$

We can choose $T_1<0$ such that the map K defined by

$$Ku(t)=\int_{-\infty}^t(J\nabla H(u(s)+\Phi_0^s(z_-))\,ds$$

is a contraction in the complete metric space $\mathcal{C}_{T_1}$ of continuous functions u from $]-\infty,T_1]$ into $\mathbb{R}^{2d}$ such that $\sup_{t\le T_1}|u(t)|\le 1$, with the natural distance. So we can apply the fixed point theorem to get the Proposition using standard technics. □

Let us prove Proposition 5.4, using the same setting as in Proposition 5.3.

Proof. — $G_{t,s}$ is solution of the differential equation

$$\partial_t G_{t,s} = J\partial_z^2(\Phi^{t-s}(\Phi_0^s(z_-))G_{t,s}, \quad G_{s,s} = \mathbb{1}_{2d}.$$

So we get the integral equation

$$G_{t,s} - F_t^0 = \int_s^t J\partial_z^2 H(\Phi^{r-s}(\Phi_0^s(z_-))(G_{r,s} - F_r^0)\, dr.$$

As in Proposition 5.3, we get that G_t is well defined and satisfies

$$G_t - F_t^0 = \int_{-\infty}^t J\partial_z^2 H(\Phi^{r-s}(\Phi_0^s(z_-))G_r\, dr. \tag{201}$$

Moreover we can easily see, using C^∞ dependance in the fixed point theorem depending on parameters, that $G_t = \frac{\partial z_t}{\partial z_-}$.

Now we have only to prove that $F_{-t}^0 G_t$ has a limit for $t \to +\infty$. For that, let us compute

$$\partial_t(F_{-t}^0 G_t) = F_{-t}^0 J\left(\partial_z^2 H(z_t) - \partial_z^2 H_0\right) G_t.$$

Then we get $\partial_t(F_{-t}^0 G_t) = O(\langle t\rangle^{-\rho})$ for $t \to +\infty$, so the limit exists. □

Proof. — Let us now prove Proposition 5.5.

We begin by applying the propagation Theorem of coherent states for $U(t-s)\psi_{z_s^0}^{\Gamma_s^0}$, where $z_s^0 = \Phi_0^s(z_-)$ and $\Gamma_s^0 = \mathcal{M}(F_s^0)$. Let us remark that we have $\Gamma_s^0 = \Gamma_-(\mathbb{1}+s\Gamma_-)^{-1}$ but we shall not use here this explicit formula.

From Theorem 0.1, we get for every $N \geq 0$,

$$i\hbar\partial_t\psi_z^{(N)}(t,s,x) = \widehat{H}(t)\psi^{(N)}(t,s,x) + R_z^{(N)}(t,s,x) \tag{202}$$

where

$$\psi_{z_-}^{(N)}(t,s,x) = \mathrm{e}^{i\delta_{t,s}/\hbar}\mathcal{T}(z_t)\Lambda_\hbar\mathcal{M}[F_{t,s}F_s^0]\left(\sum_{0\leq j\leq N}\hbar^{j/2}b_j(t,s)g^{\Gamma_-}\right) \tag{203}$$

and

$$\begin{aligned} R_{z_-}^{(N)}(t,s,x) = {} & \mathrm{e}^{i\delta_{t,s}/\hbar}\hbar^{(N+3)/2} \\ & \cdot\left(\sum_{\substack{j+k=N+2\\ k\geq 3}}\mathcal{T}(z_t)\Lambda_\hbar\mathcal{M}[F_{t,s}F_s^0]Op_1^w\left(R_k(t,s)\circ[F_{t,s}F_s^0]\right)(b_j(t,s)g^{\Gamma_-})\right), \end{aligned} \tag{204}$$

where $F_{t,s} = F_{t-s}(\Phi_0^s z_-)$ (it is the stability matrix at $\Phi^{t-s}(\Phi_0^z(z_-))$). Moreover, the polynomials $b_j(t,s,x)$ are uniquely defined by the following induction formula for $j \geq 1$, starting with $b_0(s,s,x) \equiv 1$,

$$\partial_t b_j(t,s,x)g(x) = \sum_{k+\ell=j+2,\ \ell\geq 3} Op_1^w[K_\ell^\#(t,s)](b_k(t,\cdot)g^{\Gamma_-})(x) \tag{205}$$

$$b_j(s,s,x) = 0. \tag{206}$$

where

$$K_\ell^{\#}(t,s,X) = \sum_{|\gamma|=j} \frac{1}{\gamma!}\partial_X^\gamma H(\Phi^{t-s}(\Phi_0^s z_-))(F_{t-s}F_s^0 X)^\gamma, \quad X \in \mathbb{R}^{2d}.$$

So, using Propositions 5.3, 5.4, we can easily control the limit $s \to -\infty$ in equations (203), (204) and we get the proof of the proposition. □

Remark 5.6. — In Theorem 5.2 the error is estimate in the L^2-norm. The same result also holds in Sobolev norm H^s, for any $s \geq 0$, with the norm: $\|\psi\|_{H^s} = \|(-\hbar^2\triangle + 1)^{s/2}\psi\|_{L^2}$. This is a direct consequence of the commutation of $S^{(\hbar)}$ with the free Hamiltonian $\hat{H}^0 = -\frac{\hbar^2}{2}\triangle$. In particular Theorem 5.2 is true for the L^∞-norm.

The following corollaries are straightforward consequences of the Theorem 5.2 and properties of the metaplectic representation stated in section 1.

Corollary 5.7. — *For every $N \in \mathbb{N}$ we have*

$$S^{(\hbar)}\varphi_{z_-}^{\Gamma_-} = \mathrm{e}^{i\frac{\delta_+}{\hbar}} \sum_{0\leq j\leq N} \hbar^{j/2}\pi_j\left(\frac{x-q_+}{\sqrt{\hbar}}\right)\varphi_{z_+}^{\Gamma_+}(x) + \mathcal{O}(\hbar^\infty), \tag{207}$$

where $z_+ = S^{c\ell}(z_-)$, $\Gamma_+ = \varSigma_{G_+}(\Gamma_-)$, $\pi_j(y)$ are polynomials of degree $\leq 3j$ in $y \in \mathbb{R}^d$. In particular $\pi_0 = 1$.

Corollary 5.8. — *For any observable $L \in \mathcal{O}^m$, $m \in \mathbb{R}$, we have*

$$\langle \hat{L}S^{(\hbar)}\varphi_{z_-}, S^{(\hbar)}\varphi_{z_-}\rangle = L(S^{c\ell}(z_-)) + \mathcal{O}(\sqrt{\hbar}). \tag{208}$$

In particular we recover the classical scattering operator form the quantum scattering operator in the semi-classical limit.

Proof. — Using corollary (5.7) we have

$$\langle \hat{L}S^{(\hbar)}\varphi_{z_-}, S^{(\hbar)}\varphi_{z_-}\rangle = \langle \hat{L}\varphi_{z_+}^{\Gamma_+}, \varphi_{z_+}^{\Gamma_+}\rangle + \mathcal{O}(\sqrt{\hbar})$$

and the result follows from a trivial extension of lemma (1.2). □

Remark 5.9. — A similar result was proved for the time-delay operator in [**48**]. The proof given here is more general and not needs a global non-trapping assumption. It is enough to know that the scattering trajectory z_t exists.

The following corollary is less direct and concerns scattering evolution of Lagrangian states (also called WKB states). Let us consider a Lagrangian state $\mathcal{L}_{a,\vartheta}(x) = a(x)\mathrm{e}^{\frac{i}{\hbar}\vartheta(x)}$, where a is a C^∞ function with bounded support and ϑ is a real C^∞ function on $\mathbb{R}^d$. Let us introduce the two following conditions.

(L_1) $\{(x, \partial_x\vartheta(x)),\ x \in \mathrm{supp}(a)\} \subseteq \mathcal{Z}\backslash\mathcal{N}_0$.

(L_2) $\det[\partial_q q_+(y, \partial_y\vartheta(y))] \neq 0$ for every $y \in \mathrm{supp}(a)$ such that $q_+(y, \partial_y\vartheta(y)) = x$.

The condition (L_2) means that x is not conjugate to some point in $\mathrm{supp}(a)$.

If the condition (L_2) is satisfied, then by the implicit function theorem, there exist M functions $q^{(m)}$, smooth in a neighborhood of x, $m = 1, \cdots, M$, such that $q_+(y, \partial_y\vartheta(y)) = x$ if and only if there exists $0 \leq m \leq M$, such that $y = q^{(m)}$. We have the following result.

Corollary 5.10. — *If the conditions (L_1) and (L_2) are fulfilled then we have*
(209)
$$S^{(\hbar)}(a\mathrm{e}^{\frac{i}{\hbar}\vartheta})(x) = \sum_{1\leq m\leq M} \mathrm{e}^{\frac{i}{\hbar}\alpha_j + i\sigma_j\frac{\pi}{2}} \left(\det(A_+^{(m)} + B_+^{(m)}\partial_y^2\vartheta(q^{(m)})\right)^{-1/2}(1 + \mathcal{O}(\sqrt{\hbar}))$$

where $A_+^{(m)} = A_+(q^{(m)}, \partial_y\vartheta(q^{(m)}))$, $B_+^{(m)} = B_+(q^{(m)}, \partial_y\vartheta(q^{(m)}))$, and $\sigma_j \in \mathbb{Z}$ are Maslov indices.

Morever, we also have a complete asymptotic expansion in power of $\hbar$.

Proof. — Let us start with the Fourier-Bargman inversion formula

$$S^{(\hbar)}[\mathcal{L}_{a,\vartheta}](x) = (2\pi\hbar)^{-d}\int_{\mathcal{Z}} \langle \mathcal{L}_{a,\vartheta}, \varphi_z\rangle S^{\hbar)}\varphi_z(x)\, dz. \tag{210}$$

Using the non-stationary phase theorem [**25**], for every $N \in \mathbb{N}$ there exist $C_N > 0$ and $R_N > 0$ such that we have

$$|\langle \mathcal{L}_{a,\vartheta}, \varphi_z\rangle| \leq C_N\hbar^N\langle z\rangle^{-N} \tag{211}$$

for all $|z| \geq R_N$ and $\hbar \in]0, 1]$. So the integral in (210) is supported in a bounded set, modulo an error $O(\hbar^\infty)$. By plugging Theorem 5.2 in equation (210) we get

$$S^{(\hbar)}\mathcal{L}_{a,\vartheta}(x) = 2^{-d}(\pi\hbar)^{-3d/2}\int_{\mathcal{K}} \mathrm{e}^{\frac{i}{\hbar}\Psi_x(y,z)}a(y)\det(A_+ + iB_+)^{-1/2}\, dy\, dz + \mathcal{O}(\sqrt{\hbar}) \tag{212}$$

where $\mathcal{K}$ is a large enough bounded set in $\mathcal{Z} \times \mathbb{R}^d$. Let us recall that

$$G_+ = \partial_z z_+ = \begin{pmatrix} A_+ & B_+ \\ C_+ & D_+ \end{pmatrix}$$

is the stability matrix for the scattering trajectory coming from $z_- = z$ in the past. Ψ_x is the following phase function

$$\Psi_x(y, z) = S_+ + p\cdot(q - y) + p_+\cdot(x - q_+) + \frac{i}{2}|y - q|^2 + \frac{1}{2}\Gamma_+(x - q_+)\cdot(x - q_+) \tag{213}$$

with the notations: $S_+ = \int_{-\infty}^{+\infty}(\dot{q}_s p_s - H(q_s, p_s))ds$, $\Gamma_+ = C_+ + iD_+)(A_+ + iB_+)^{-1}$, $(q_s, p_s) = \Phi^s(q, p)$, $q_+, p_+, A_+, B_+, C_+, D_+$ depend on the scattering data at time $-\infty$, $z = (q, p)$. We can easily compute the critical set $\mathcal{C}[\Psi_x]$ defined by $\Im\Psi_x(y, z) = 0$, $\partial_y\Psi_x(y, z) = \partial_z\Psi_x(y, z) = 0$. We find $\mathcal{C}[\Psi_x] = \{(y, z),\ y = q,\ q_+ = x, \partial_y\vartheta(y) = p\}$. So we have to solve the equation $q_+(y, \partial_y\vartheta(y)) = x$, which can be done with condition (L_2). So the phase function Ψ_x has M critical points, $(q^{(m)}, q, p)$, $0 \leq m \leq M$. To apply the stationary phase theorem we have to compute the determinant of the

Hessian matrix $\partial^2_{y,q,p}\Psi_x$ on the critical points $(q^{(m)},q,p)$. Denoting $V=(A_++iB_+)^{-1}B_+$, we have

$$\partial^2_{y,q,p}\Psi_x=\begin{pmatrix} i\mathbb{1}+\partial^2_y\vartheta & -i\mathbb{1} & -\mathbb{1}\\ -i\mathbb{1} & 2i\mathbb{1}+V & iV\\ -\mathbb{1} & iV & -V\end{pmatrix}.$$

By elementary linear algebra we find that for $y=q^{(m)}$ and $z=(q,p)$ we have:

$$\det(\partial^2_{y,q,p}\Psi_x)=\det\left[(-2i)(A_++iB_+)^{-1}(A_++B_+\partial^2_y\vartheta\right]. \tag{214}$$

Then we get the asymptotics (209), following carefully the arguments of the determinants, we can check the Maslov indices. □

Remark 5.11. — Corollary 5.10 was first proved by K. Yajima [**51**] in the momentum representation and by S.L. Robinson [**40**] for the position representation. The proof given here is rather different and more general. It can also be extended to matrix Hamiltonian like Dirac equation with a scalar short range perturbation.

Using the analytic and Gevrey estimates established for finite time, it is not very difficult to extend these estimates to the scattering operator as we have done for the C^∞ case. So we can recover in particular a result of [**21**]. Let us suppose that condition (178) is satisfied and add the following Gevrey condition.

(A_{SG_s}) (Gevrey assumption). Let be $s\geq 1$. There exist $R>0$, $\delta>0$, such that for every $\alpha\in\mathbb{N}^d$, we have

$$\begin{aligned}|\partial_q^\alpha(\mathbb{1}-g(q))|+|\partial_q^\alpha a(q)|+|\partial_q^\alpha V(q)| &\leq C^{|\alpha|\alpha+1}<q>^{-\rho-|\alpha|},\\ &\qquad \forall q\in C^d,\ \text{such that } |\Im(q)|\leq\delta.\end{aligned} \tag{215}$$

Denote $B_j(X)=\langle b_jg^{\Gamma_-},g_X\rangle$.

Lemma 5.12. — *Under condition (A_{SG_s}), there exists $C>0$ such that for every $j\geq 1$, $X\in\mathbb{R}^{2d}$, we have*

$$|B_j(X)|\leq C^j\mathrm{e}^{-\lambda|X|}j^{s_\star j/2}\exp\left(-\frac{|X|^2}{Cj}\right). \tag{216}$$

In particular, for every $\delta>0$, $\lambda>0$, $a\in]0,e^{-1}[$, there exist $C>0$ such that for $|X|\geq\delta$ and $1\leq j\leq\frac{a}{\hbar^{1/s_\star}}$, we have

$$\hbar^{j/2}|B_j(X)|\leq\exp\left(-\frac{1}{C\hbar^{1/s_\star}}-\lambda|X|\right). \tag{217}$$

Proof. — We explain briefly the strategy, the details are left to the reader. Let us introduce $B_j(t,s,X)=\langle b_j(t,s)g,g_X\rangle$. We use the method used before for finite time to estimate $B_j(t,t',X)$ and control the estimates for $t'\to-\infty$ and $t\to-\infty$ by the method used in the scattering case for $\mathcal{O}(\hbar^\infty)$ estimates. Using the estimates already proved for the classical scattering and assumption (A_{SG_s}), we can estimate $B_j(t,s,X)$ with good controls in t,t' and j by induction. □

Let us denote $\psi_{z_+}^{(N_\hbar)} = \mathrm{e}^{i\delta_+/\hbar}\mathcal{T}(z_+)\Lambda_\hbar\mathcal{M}[G_+]\big(\sum_{0\leq j\leq N}\hbar^{j/2}b_j g^{\Gamma_-}\big)$. From lemma 5.12 we get

Theorem 5.13. — *condition (A_{SG_s}), for every $z_-\in\mathcal{Z}\backslash\mathcal{N}_0$ and every $\Gamma_-\in\Sigma_d^+$ there exists $a>0$, $c>0$, $h_0>0$ small enough and for every $r\geq 0$ there exists C_r such that for all $0\leq\hbar\leq h_0$ we have:*

$$\left\|S^{\hbar)}\varphi_{z_-}-\psi_{z_+}^{(N_\hbar)}\right\|_{H^r(\mathbb{R}^d)}\leq C_r\exp\left(-\frac{c}{\hbar^{\frac{1}{2s-1}}}\right). \tag{218}$$

With the same argument as in the finite time case we get the following application.

Corollary 5.14. — *Let be $\psi_\hbar$ such that $\sup_{0<\hbar\leq h_0}\|\psi_\hbar\|<+\infty$. Then for every $s'\geq 2s-1$, we have:*

$$\mathrm{FS}_{\mathcal{G}s'}[S^{(\hbar)}\psi_\hbar]\cap\mathcal{Z}\backslash\mathcal{N}_0=S^{c\ell}\left(\mathrm{FS}_{\mathcal{G}s'}[\psi_\hbar]\right)\cap\mathcal{Z}\backslash\mathcal{N}_0. \tag{219}$$

Remark 5.15. — In [**1**] the author proves that the scattering matrix is a Fourier Integral operator. Our results are weaker because in our case the energy is not fixed but our estimates seems more accurate.

6. Bound States Asymptotics

In this section we will consider the stationary Schrödinger equation and its bound states (ψ,E) which satisfies, by definition,

$$(\hat{H}-E)\psi=0,\ \ E\in\mathbb{R},\ \ \psi\in L^2(\mathbb{R}^d),\|\psi\|=1. \tag{220}$$

A well known example is the harmonic oscillator $\hat{H}=-\hbar^2\triangle+|x|^2$, for which one can compute an explicit orthonormal basis of eigenfunctions in $L^2(\mathbb{R}^d)$, ψ_α, with eigenvalues $E_\alpha=(2|\alpha|+1)\hbar$, for $\alpha\in\mathbb{N}^d$ where $|\alpha|=\alpha_1\cdots+\alpha_d$.

Let us introduce some global assumptions on the Hamiltonians under consideration in this section to study the discrete part if the spectrum.

6.1. Assumptions. — We start with a quantum Hamiltonian $\hat{H}$ coming from a semiclassical observable H. We assume that $H(\hbar,z)$ has an asymptotic expansion:

$$H(\hbar,z)\asymp\sum_{0\leq j<+\infty}\hbar^j H_j(z), \tag{221}$$

with the following properties:

(As_1) *$H(\hbar,z)$ is real valued , $H_j\in C^\infty(\mathcal{Z})$.*

(As_2) H_0 is bounded below[(1)]: there exits $c_0>0$ and $\gamma_0\in\mathbb{R}$ such that $c_0\leq H_0(z)+\gamma_0$. Furthermore $H_0(z)+\gamma_0$ is supposed to be a temperate weight, i.e., *there exist $C>0$, $M\in\mathbb{R}$, such that*:

$$H_0(z)+\gamma_0\leq C(H_0(z')+\gamma)(1+|z-z'|)^M\quad\forall z,z'\in Z.$$

(1) Using the semi-classical functional calculus [**23**] it is not a serious restriction.

(As_3) $\forall j \geq 0$, $\forall \gamma$ *multiindex* $\exists c > 0$ *such that*: $|\partial_z^\gamma H_j| \leq c(H_0 + \gamma_0)$.

(As_4) $\exists N_0$ *such that* $\forall N \geq N_0$, $\forall \gamma$ $\exists c(N, \gamma) > 0$ such that $\forall \hbar \in]0, 1]$, $\forall z \in \mathcal{Z}$ we have:

$$\left| \partial_z^\gamma [H(\hbar; z) - \sum_{0 \leq j \leq N} \hbar^j H_j(z)] \right| \leq c(N, \gamma)\hbar^{N+1}, \quad \forall \hbar \in]0, 1].$$

Under these assumptions it is known that $\hat{H}$ has a unique self-adjoint extension in $L^2(\mathbb{R}^d)$ [**37**] and the propagator:

$$U(t) := \mathrm{e}^{-\frac{it}{\hbar}\hat{H}}$$

is well defined as a unitary operator in $L^2(\mathbb{R}^d)$, for every $t \in \mathbb{R}$.

Some examples of Hamiltonians satisfying (As_1) to (As_4)

$$\hat{H} = -\hbar^2(\nabla - i\vec{a}(x))^2 + V(x). \tag{222}$$

The electric potential V and the magnetic potential $\vec{a}$ are smooth on $\mathbb{R}^d$ and satisfy: $\liminf_{|x| \to +\infty} V(x) > V_0$, $|\partial_x^\alpha V(x)| \leq c_\alpha(V(x) + V_0)$, there exists $M > 0$ such that $|V(x)| \leq C(V(y) + \gamma)(1 + |x - y|)^M$ and $|\partial_x^\alpha \vec{a}(x)| \leq c_\alpha(V(x) + V_0)^{1/2}$.

$$\hat{H} = -\hbar^2 \sum \partial_{x_i} g_{ij}(x) \partial_{x_j} + V(x), \tag{223}$$

where V is as in example 1 and $\{g_{ij}\}$ is a smooth Riemannian metric on $\mathbb{R}^d$ satisfying for some $C > 0$, $\mu(x)$ we have

$$\frac{\mu(x)}{C}|\xi|^2 \leq |\sum g_{ij}(x)\xi_i\xi_j| \leq C\mu(x)|\xi|^2$$

with $\frac{1}{C} \leq \mu(x) \leq C(V(x) + \gamma)$.

We can also consider non-local Hamiltonians like the Klein-Gordon Hamiltonian:

$$\hat{H} = \sqrt{m^2 - \hbar^2\Delta} + V(x), \tag{224}$$

with $m > 0$ and $V(x)$ as above.

6.2. Preliminaries semi-classical results on the discrete spectrum. — We want to consider here bound states of $\hat{H}$ in a fixed energy band. So, let us consider a classical energy interval $I_{c\ell} =]E_- - \varepsilon, E_+ + \varepsilon[$, $E_- < E_+$ such that we have:

(As_5) $H_0^{-1}(I_{c\ell})$ *is a bounded set of the phase space* $\mathbb{R}^{2d}$.

This implies that in the closed interval $I = [E_-, E_+]$, for $\hbar > 0$ small enough, the spectrum of $\hat{H}$ in I is purely discrete ([**23**]).

For some energy level $E \in]E_-, E_+[$, let us introduce the assumption:

(As_6) E *is a regular value of* H_0. *That means*: $H_0(x, \xi) = E \Rightarrow \nabla_{(x,\xi)} H_0(x, \xi) \neq 0$).

So, the Liouville measure $d\nu_E$ is well defined on the energy shell

$$\Sigma_E^{H_0} := \{z \in Z,\ H_0(z) = E\}$$

and is given by the formula:

$$d\nu_E(z) = \frac{d\Sigma_E(z)}{|\nabla H_0(z)|},$$

where $d\Sigma_E$ is the canonical Riemannian measure on the hypersurface Σ_E.

A useful tool to start with the study of the spectrum of $\widehat{H}$ is the following functional calculus result proved in [**23**].

Theorem 6.1. — *Let H be a semiclassical Hamiltonian satisfying assumptions (As_1) to (As_4). Let f be a smooth real valued function such that, for some $r \in \mathbb{R}$, we have*

$$\forall k \in \mathbb{N},\ \exists C_k,\ |f^{(k)}(t)| \leq C_k \langle t\rangle^{r-k}, \quad \forall t \in \mathbb{R}.$$

Then $f(\hat{H})$ is a semiclassical observable with a semiclassical symbol $H_f(\hbar, z)$ given by

$$H_f(\hbar, z) \asymp \sum_{j\geq 0} \hbar^j H_{f,j}(z). \tag{225}$$

In particular we have

$$H_{f,0}(z) = f(H_0(z)), \tag{226}$$

$$H_{f,1}(z) = H_1(z) f'(H_0(z)), \tag{227}$$

$$\textit{and for } j \geq 2, \ \ H_{f,j} \ = \sum_{1\leq 1\leq 2j-1} d_{j,k}(H) f^{(k)}(H_0), \tag{228}$$

where $d_{j,k}(H)$ are universal polynomials in $\partial_z^\gamma H_\ell(z)$ with $|\gamma| + \ell \leq j$.

From this theorem we can get the following consequences on the spectrum of $\hat{H}$ (see [**23**]).

Theorem 6.2. — *Let us assume that assumptions (As_1) to (As_5) are satisfied. Then we have:*

(i) For every closed interval $I := [E_-, E_+] \subset I_{c\ell}$, and for $\hbar_0$ small enough, the spectrum of $\hat{H}$ in I is purely discrete $\forall \hbar \in]0, \hbar_0]$.

Let us denote by Π_I the spectral projector of $\hat{H}$ in I. Then:

(ii) Π_I is finite dimensional and the following estimate holds

$$\mathrm{tr}(\Pi_I) = O(\hbar^{-d}), \ \ \textit{as } \hbar \searrow 0.$$

(iii) For all $g \in C_0^\infty(I_{c\ell})$, $g(\hat{H})$ is a trace class operator and we have

$$\mathrm{tr}[g(\hat{H})] \asymp \sum_{j\geq 0} \hbar^{j-d} \tau_j(g), \tag{229}$$

where τ_j are distributions supported in $H_0^{-1}(I_{c\ell})$. In particular we have

$$T_0(g) = (2\pi)^{-d} \int_{\mathcal{Z}} g(H_0(z))\, dz, \tag{230}$$

$$T_1(g) = (2\pi)^{-d} \int_{\mathcal{Z}} g'(H_0(z)) H_1(z)\, dz \tag{231}$$

Let us denote by E_j, $1 \le j \le N$, the eigenvalues of $\hat{H}$ in I, each is enumerated with its multiplicity ($N = \mathcal{O}(\hbar^{-d})$). So, there exists an orthonormal system of bound states, $\psi_j \in L^2(\mathbb{R}^d)$, such that $\widehat{H}\psi_j = E_j\psi_j$, $1 \le j \le N$.

Let us introduce now the density of states defined as a sum of delta functions by

$$\rho_I(E) = \sum_{1 \le j \le N} \delta(E - E_j), \tag{232}$$

or equivalently its $\hbar$-Fourier transform

$$S_I(t) = \sum_{1 \le j \le N} \mathrm{e}^{-it\hbar^{-1}E_j} \tag{233}$$

$$= \mathrm{tr}\,[\Pi_I U(t)]. \tag{234}$$

For technical reason, It is more convenient to smooth out the spectral projector Π_I and to consider the smooth spectral density:

$$G_\rho(E) = \sum_{1 \le j \le N} \rho\left(\frac{E - E_j}{\hbar}\right)\chi(E_j) \tag{235}$$

where ρ is in the Schwartz space $\mathcal{S}(\mathbb{R})$ such that its Fourier transform has a compact support and χ is smooth, with support in $I_{c\ell}$. Applying the inverse Fourier transform to ρ we get

$$G_\rho(E) = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{tr}[U(t)\chi(\hat{H})]\mathrm{e}^{itE/\hbar}\tilde{\rho}(t)\,dt, \tag{236}$$

where $\tilde{\rho}$ is the Fourier transform of ρ.

In the next results we shall analyze the contribution of the periodic trajectories to the smooth spectral density $G_\rho(E)$ using formula (236).

6.3. Trace Formulas. — The main result in this field is known as the *Gutzwiller trace formula* (other names: generalized Poisson formula, Selberg trace formula). The Gutzwiller trace formula is usually obtained by applying the stationary phase theorem to r.h.s of formula (236) using W.K.B approximations of the propagator. Here we shall explain another method, using a coherent states analysis. This was done for the first time with mathematical details in [**7**] but has appeared before in the physicist litterature [**50**].

We shall study the more general weighted spectral density

$$G_{\rho,L}(E,\hbar) = \sum_{j \ge 0} \rho\left(\frac{E_j - E}{\hbar}\right) L_{jj}(\hbar) \tag{237}$$

where the Fourier transform $\tilde{\rho}$ of ρ has a compact support and $L_{jj} = \langle \psi_j, \widehat{L}\psi_j\rangle$, L being a smooth observable of weight 1.

The ideal ρ should be the Dirac delta function, which need too much informations in time for the propagator. So we will try to control the size of the support of $\tilde{\rho}$. To do that we take $\rho_T(t) = T\rho_1(tT)$ with $T \ge 1$, where ρ_1 is non-negative, even, smooth real function, $\int_{\mathbb{R}} \rho_1(t)dt = 1$, $\mathrm{supp}\{\tilde{\rho}_1\} \subset [-1, 1]$, $\tilde{\rho}_1(t) = 1$ for $|t| \le 1/2$.

Let us assume that we have some control of the classical flow $\Phi^t := \Phi^t_{H_0}$ (defined $\forall t \in \mathbb{R}$ in $H_0^{-1}(I)$).

(As_7) *There exists an increasing function* s from $]0, \infty[$ in $[1, +\infty[$ *satisfying* $s(T) \geq T$ *and such that the following estimates are satisfied:*

$$\sup_{H_0(z)\in I,\, |t|\leq T} \left|\partial_z^\gamma \Phi^t(z)\right| \leq C_\gamma s(T)^{|\gamma|} \tag{238}$$

where C_γ *depends only on* $\gamma \in \mathbb{N}^{2d}$.

By applying the propagation theorem for coherent states we can write $G_{\rho_T,L}(E)$ as a Fourier integral with an explicit complex phase. The classical dynamics enter the game in a second step, to analyze the critical points of the phase. Let us describe these steps (see [**7**] for the details of the computations).

(i) modulo a negligible error, we can replace $\hat{L}$ by $\hat{L}_\chi = \chi(\hat{H})\hat{L}\chi(\hat{H})$ where χ is smooth with support in a small neighborhood of E like $]E - \delta_\hbar, E + \delta_\hbar[$ such that $\lim_{\hbar\to 0} \delta_\hbar = 0$.

(ii) using inverse Fourier formula we have the following time dependent representation:

$$G_{\rho_T,L}(E) = \frac{1}{2\pi}\int_{\mathbb{R}} \tilde{\rho}_1\left(\frac{t}{T}\right) \mathrm{tr}\left(\hat{L}_\chi \mathrm{e}^{\frac{it}{\hbar}(E-\hat{H})}\right) dt \tag{239}$$

(iii) if B is a symbol then we have $\hat{B}\psi_z = B(z)\psi_z + \cdots$ where the $\cdots$ are correction terms in half power of $\hbar$ which depend on the Taylor expansion of B at z (Lemma 1.3)

(iv) putting all things together, after some computations, we get for every $N \geq 1$:

$$\boxed{G_{\rho_1,A}(E,\hbar) = (2\pi\hbar)^{-d}\int_{\mathbb{R}_t\times\mathbb{R}^{2d}_z} \tilde{\rho}_1\left(\frac{t}{T}\right) a^{(N)}(t,z,\hbar)\mathrm{e}^{\frac{i}{\hbar}\Psi_E(t,z)}\, dt\, dz + \mathcal{R}_{N,T,\hbar}}. \tag{240}$$

The phase Ψ_E is given by

$$\begin{aligned} \Psi_E(t,z) = t(E - H_0(z)) + &\frac{1}{2}\int_0^t \sigma(z_s - z, \dot{z}_s)ds + \\ &\frac{i}{4}(\mathbb{I}_d - W_t)(\breve{z} - \breve{z}_t)\cdot\overline{(\breve{z} - \breve{z}_t)}, \end{aligned} \tag{241}$$

with $\breve{z} = q + ip$ if $z = (q,p)$ and $W_t = Z_t Y_t^{-1}$ where $Y_t = C_t - B_t + i(A_t + D_t)$, $Z_t = A_t - D_t + i(B_t + C_t)$.

The amplitude $a^{(N)}$ has the following property

$$a^{(N)}(t,z,\hbar) = \sum_{0\leq j\leq N} a_j(t,z)\hbar^j, \tag{242}$$

where each $a_j(t,z)$ is smooth, with support in variable z included in the neighborhood $\Omega = H_0^{-1}[E - \varepsilon, E + \varepsilon]$ ($\varepsilon > 0$) of Σ_E, and estimated for $|t| \leq T$ as follows

$$|a_j(t,z)| \leq C_j s(T)^{6j}(1+T)^{2j}. \tag{243}$$

In particular for $j = 0$ we have

$$a_0(t,z) = \pi^{-d/2}\left[\det(Y_t)\right]^{-1/2}\exp\left(-i\int_0^t H_1(z_s)\,ds\right). \tag{244}$$

The remainder term satisfies

$$\mathcal{R}_{N,T,\hbar} \le C_N s(T)^{6N+\epsilon_d}(1+T)^{2N+1}\hbar^{N+1}. \tag{245}$$

Form the above computations we can easily see that the main contributions in $G_{\rho_T,L}(E)$, for $\hbar$ small, come from the periods of the classical flow, as it is expected. Let us first remark that we have

$$2\mathrm{Im}\Psi_E(t,z) \ge \langle \Im\Gamma_t(\Gamma_t+i)^{-1}(\breve{z}-\breve{z}_t), \Gamma_t+i)^{-1}(\breve{z}-\breve{z}_t)\rangle.$$

Here $\langle,\rangle$ is the Hermitean product on $\mathbb{C}$. Because of positivity of $\Im\Gamma_t$ we get the following lower bound: there exists $c_0 > 0$ such that for every T and $|t| \le T$ we have

$$\Im\Psi_E(t,z) + |\partial_t\Psi_E(t,z)|^2 \ge c_0\left(|H_0(z)-E|^2 + s(T)^{-4}|z-z_t|^2\right). \tag{246}$$

Let us denote $\Pi(E) = \{t \in \mathbb{R},\ \exists z \in H_0^{-1}(E),\ \Phi^t(z) = z\}$. The non-stationary phase theorem applied to (240) and (246) gives the following

***Proposition 6.3* (Poisson relation)**. — *If* $\mathrm{supp}(\tilde{\rho}_T) \cap \Pi(E) = \varnothing$ *then* $G_{\rho_T,L}(E) = \mathcal{O}(\hbar^\infty)$.

The stationary phase theorem with complex phase applied to (240) ([**25**], vol. 1 and Appendix), gives easily the contribution of the 0-period.

Theorem 6.4. — *If* T_0 *is choosen small enough, such that*
$T_0 < \sup\{t > 0,\ \forall z \in \Sigma_E,\ \Phi^t(z) \ne z\}$, *then we have the following asymptotic expansion:*

$$G_{\rho_{T_0},L}(E) \asymp (2\pi\hbar)^{-d}\sum_{j\ge 0}\alpha_{L,j}(E)\hbar^{j+1} \tag{247}$$

where the coefficient $\alpha_{A,j}$ *do not depend on* ρ. *In particular*

$$\alpha_{L,0}(E) = \int_{\Sigma_E} L(z)\,d\nu_E(z), \quad \alpha_{L,1}(E) = \int_{\Sigma_E} H_1(z)L(z)\,d\nu_E(z). \tag{248}$$

Proof. — Using that $\Im\Gamma_t$ is positive, we get that $\Im\Psi_E(t,z) \ge 0$ and from (246) we get that if $\Im\Psi_E(t,z) = 0$ and $\partial_t\Psi_E(t,z) = 0$ then $H_0(z) = E$ and $z_t = z_0$. But $|t|$ is small enough and $\nabla H_0(z) \ne 0$ if $H_0(z) = E$. So we find that $t = 0$. Moreover these conditions also give $\partial_z\Psi_E(0,z) = 0$. Finally the critical set of the phase Ψ_E is defined by the following equation in $\mathbb{R}\times\mathbb{R}^{2d}$

$$\mathcal{C}_E = \{(0,z), H_0(z) = E\}$$

which is a submanifold of codimension 2. Next we can compute the second derivative $\partial^{(2)}_{t,z}\Psi_E$ on the normal space to $\mathcal{C}_E$. The following computation, left to the reader, gives

$$\partial^{(2)}_{t,z}\Psi_E(0,z) = \begin{pmatrix} -\frac{1}{2}|\nabla_z H_0(z)|^2 & i\nabla_z H_0(z)^T \\ i\nabla_z H_0(z) & 0 \end{pmatrix}. \tag{249}$$

Then we see that $\partial^{(2)}_{t,z}\Psi_E$ on the normal space to $\mathcal{C}_E$ is non-degenerate. So we can apply the stationary phase theorem. The leading term comes from the computation $\det[\partial^{(2}_{0,z}\Psi_E] = |\nabla_z H_0(z)|^2$. □

By using a Tauberian argument [**37**], a Weyl formula with an error term ($\mathcal{O}\hbar^{1-d}$) can be obtained from (247). Let us denote $N_I(\hbar) = \mathrm{tr}(\Pi_I)$ (it is the number of states with energy in I). The Weyl formula says

Theorem 6.5. — *If $I = [a,b]$ such that a, b are regular for H_0, then we have*

$$N_I(\hbar) = (2\pi\hbar)^{-d}\int_{[H_0(X)\in I]} dX + \mathcal{O}(\hbar^{1-d}) \tag{250}$$

for $\hbar$ small.

Remark 6.6. — The leading term in the Weyl formula is determined by the volume occupied by the energy in the phase space. Since a proof by H. Weyl (1911) of his formula for the Laplace operator in a bounded domain, a lot of paper have generalized this result in several directions: different geometries and remainder estimates. Between 1968 and 1985 optimal results have been obtained for the remainder term, including the difficult case of boundary value problems. Let us give here some names: Hörmander, Ivrii, Melrose, Chazarain, Helffer-Robert.

The contributions of periodic trajectories can also be computed if we had some specific assumptions on the classical dynamics. The result is called Gutzwiller trace formula. In [**7**] a coherent states analysis was used to give a proof of the Gutzwiller trace formula. Other proofs were known before (see the remark below). Let us recall now the statement. The main assumption is the following. Let $\mathcal{P}_{E,T}$ be the set of all periodic orbits on Σ_E with periods T_γ, $0 < |T_\gamma| \leq T$ (including repetitions and change of orientation). T^*_γ is the primitive period of γ. Assume that all γ in $\mathcal{P}_{E,T}$ are non-degenerate, i.e., 1 is not an eigenvalue for the corresponding "Poincaré map", P_γ (in the Appendix we shall give more explanations concerning the Poincaré map). It is the same to say that 1 is an eigenvalue of F_{T_γ} with algebraic multiplicity 2. In particular, this implies that $\mathcal{P}_{E,T}$ is a finite union of closed path with periods T_{γ_j}, $-T \leq T_{\gamma_1} < \cdots < T_{\gamma_n} \leq T$.

***Theorem 6.7* (Trace Gutzwiller Formula)**. — *Under the above assumptions, for every smooth test function ρ such that* $\mathrm{supp}\{\tilde\rho\} \subset\,]-T, T[$ *, the following asymptotic expansion holds true, modulo $O(\hbar^\infty)$,*

$$\begin{aligned} G_{\rho,L}(E) &\asymp (2\pi\hbar)^{-d}\tilde\rho(0)\sum_{j\geq 0} c_{L,j}(\tilde\rho)\hbar^{j+1} + \\ &+ \sum_{\gamma\in\mathcal{P}_{E,T}} (2\pi)^{d/2-1}\exp\left(i\left(\frac{S_\gamma}{\hbar}+\frac{\sigma_\gamma\pi}{2}\right)\right)|\det(\mathbb{I}-P_\gamma)|^{-1/2}.\left(\sum_{j\geq 0} d^\gamma_{A,j}(\tilde\rho)\hbar^j\right) \end{aligned} \tag{251}$$

where σ_γ is the Maslov index of γ ($\sigma_\gamma \in \mathbb{Z}$), $S_\gamma = \oint_\gamma p\,dq$ is the classical action along γ, $c_{L,j}(\tilde\rho)$ are distributions in $\tilde\rho$ supported in $\{0\}$, in particular

$$c_{L,0}(\tilde\rho) = \tilde\rho(0)\alpha_{L,0}(E),\ \ c_{L,1}(\tilde\rho) = \tilde\rho(0)\alpha_{L,1}(E).$$

$d^\gamma_j(\widetilde\rho)$ are distributions in $\widetilde\rho$ with support $\{T_\gamma\}$. In particular

$$d^\gamma_0(\tilde\rho) = \tilde\rho(T_\gamma)\exp\left(-i\int_0^{T^*_\gamma} H_1(z_u)du\right)\int_0^{T^*_\gamma} L(z_s)\,ds. \tag{252}$$

Proof. — The reader can see in [**7**] the detailed computations concerning the determinant coming from the critical set of the phase Ψ_E in formula (240). □

Remark 6.8. — During the last 35 years the Gutzwiller trace formula was a very active subject of research. The history started with the non-rigorous works of Balian-Bloch and Gutzwiller. Then for elliptic operators on compact manifolds some spectral trace formulas extending the classical Poisson formula, were proved by several people: Colin de Verdière [**44, 45**], Chazarain [**6**], Duistermaat-Guillemin [**13**]. The first proof in the semi-classical setting is given in the paper [**17**] by Guillemin-Uribe (1989) who have considered the particular case of the square root of the Schrödinger operator on a compact manifold. But their work already contains most of the geometrical ingredients used for the general case. The case of the Schrödinger operator on $\mathbb{R}^d$ was considered by Brummelhuis-Uribe (1991). Complete proofs of the Gutzwiller trace formula were obtained during the period 1991/95 by Dozias [**12**], Meinrencken [**30**], Paul-Uribe [**31**]. All these works use the Fourier integral operator theory. More recently (2002), Sjöstrand and Zworski [**42**] found a different proof with a microlocal analysis of the resolvant $(\hat H - \lambda)^{-1}$ close to a periodical trajectory by computing a quantum monodromy.

For larger time we can use the time dependent estimates given above to improve the remainder estimate in the Weyl asymptotic formula. For that, let us introduce some control on the measure of the set of periodic path. We call this property condition (NPC).

Let be $J_E =]E-\delta, E+\delta[$ a small neighborhood of energy E and $s_E(T)$ an increasing function like in (238) for the open set $\Omega_E = H_0^{-1}(J_E)$. We assume for simplicity here that s_E is either an exponential ($s_E(T) = \exp(\Lambda T^b)$, $\Lambda > 0, b > 0$) or a polynomial ($s_E(T) = (1+T)^a$, $a \geq 1$).

The condition is the following:

(NPC) $\forall T_0 > 0$, there exist positive constants $c_1, c_2, \kappa_1, \kappa_2$ such that for all $\lambda \in J_E$ we have

$$\nu_\lambda \left\{ z \in \Sigma_\lambda,\ \exists t,\ T_0 \leq |t| \leq T,\ |\Phi^t(z) - z| \leq c_1 s(T)^{-\kappa_1} \right\} \leq c_2 s(T)^{-\kappa_2}. \tag{253}$$

The following result, which can be proved with using stationary phase arguments, estimates the contribution of the "almost periodic points". We do not give here the details.

Proposition 6.9. — *For all $0 < T_0 < T$, Let us denote $\rho_{T_0 T}(t) = (1-\rho_{T_0})(t)\rho_T(t)$, where $0 < T_0 < T$. Then we have*

$$G_{\rho_{T_0 T}, L}(E) \leq C_3 s(T)^{-\kappa_3} \hbar^{1-d} + C_4 s(T)^{\kappa_4} \hbar^{2-d} \tag{254}$$

for some positive constants $C_3, C_4, \kappa_3, \kappa_4$.

Let us now introduce the integrated spectral density

$$\sigma_{L,I}(\hbar) = \sum_{E_j \in I} L_{jj} \tag{255}$$

where $I = [E', E]$ is such that for some $\lambda' < E' < E < \lambda$, $H_0^{-1}[\lambda', \lambda]$ is a bounded closed set in $\mathcal{Z}$ and E', E are regular for H_0. We have the following two terms Weyl asymptotics with a remainder estimate.

Theorem 6.10. — *Assume that there exist open intervals I_E and $I_{E'}$ satisfying the condition (NPC). Then we have*

$$\begin{aligned} \sigma_{L,I}(\hbar) &= (2\pi\hbar)^{-d} \int_{H_0^{-1}(I)} L(z)dz - (2\pi)^{-d}\hbar^{1-d} \\ &\left(\int_{\Sigma_E} L(z)H_1(z)\, d\nu(z) - \int_{\Sigma_{E'}} L(z)H_1(z)\, d\nu(z) \right) + O\left(\hbar^{1-d}\eta(\hbar)\right) \end{aligned} \tag{256}$$

where $\eta(\hbar) = |\log(\hbar|^{-1/b}$ if $s_E(T) = \exp(\Lambda T^b)$ and $\eta(\hbar) = \hbar^\varepsilon$, for some $\varepsilon > 0$, if $s_E(T) = (1+T)^a$. Furthermore if $I_{E,\delta_1,\delta_2}(\hbar) = [E + \delta_1\hbar, E + \delta_2\hbar]$ with $\delta_1 < \delta_2$ then we have

$$\sum_{E+\delta_1\hbar \leq E_j \leq E+\delta_2\hbar} L_{jj}(\hbar) = (2\pi\hbar)^{1-d}(\delta_2 - \delta_1) \int_{\Sigma_E} L(z)\, d\nu_E + \mathcal{O}\left(\hbar^{1-d}\eta(\hbar)\right). \tag{257}$$

The first part of the theorem is proved in [**34**], at least for $\lim_{\hbar\to 0}\eta(\hbar) = 0$. The improvement concerning the size of η follows ideas coming from [**47**]. A proof can be obtained using (240).

A simple example of Hamiltonians, in $\mathbb{R}^2$, satisfying the (NPC) assumption is the following harmonic oscillator:

$$\hat{H} = -\hbar^2\triangle + a^2x^2 + b^2y^2,$$

with $a > 0,\ b > 0,\ \frac{a}{b}$ not rational.

6.4. Bohr-Sommerfeld quantization rules. — The above results concern the statistics of density of states. Under stronger assumptions it is possible to get asymptotics for invidual eigenvalues. Let us assume that conditions (As_1) to (As_5) hold and introduce the following periodicity condition:

(As_8) *For every* $E \in [E_-, E_+]$*,* Σ_E *is connected and the Hamiltonian flow* $\Phi^t_{H_0}$ *is periodic on* Σ_E *with a period* T_E*.*

(As_9) *For every periodic trajectory* γ *with period* T_E *on* Σ_E*,* $\int_\gamma H_1$ *depends only on* E *(and not on* γ*) .*

Let us first recall a result in classical mechanics (Guillemin-Sternberg, [**16**]):

Proposition 6.11. — *Let us assume that conditions* (As_6)*,* (As_8)*,* (As_9) *are satisfied. Let* γ *be a closed path of energy* E *and period* T_E*. Then the action integral* $\mathcal{J}(E) = \int_\gamma p\,dq$ *defines a function of* E*,* C^∞ *in* $]E_-, E_+[$ *and such that* $\mathcal{J}'(E) = T_E$*. In particular for one degree of freedom systems we have*

$$\mathcal{J}(E) = \int_{H_0(z)\le E} dz.$$

Now we can extend $\mathcal{J}$ to an increasing function on $\mathbb{R}$, linear outside a neighborhood of I. Let us introduce the rescaled Hamiltonian $\hat{K} = (2\pi)^{-1}\mathcal{J}(\hat{H})$. Using properties concerning the functional calculus, we can see that $\hat{K}$ has all the properties of $\hat{H}$ and furthermore its Hamiltonian flow has a constant period 2π in $\Sigma^{K_0}_\lambda = K_0^{-1}(\lambda)$ for $\lambda \in [\lambda_-, \lambda_+]$ where $\lambda_\pm = \frac{1}{2\pi}\mathcal{J}(E_\pm)$. So in what follows we replace $\hat{H}$ by $\hat{K}$, its “energy renormalization”. Indeed, the mapping $\frac{1}{2\pi}\mathcal{J}$ is a bijective correspondence between the spectrum of $\hat{H}$ in $[E_-, E_+]$ and the spectrum of $\hat{K}$ in $[\lambda_-, \lambda_+]$, including mutiplicities, such that $\lambda_j = \frac{1}{2\pi}\mathcal{J}(E_j)$.

Let us denote by a the average of the action of a periodic path on ${\Sigma_\lambda}^{K_0}$ and by $\mu \in \mathbb{Z}$ its Maslov index. ($a = \frac{1}{2\pi}\int_\gamma p\,dx - 2\pi F$). Under the above assumptions the following results were proved in [**23**], using ideas introduced before by Colin de Verdière [**44**] and Weinstein [**49**].

***Theorem 6.12* ([23, 44, 49])**. — *There exists* $C_0 > 0$ *and* $\hbar_1 > 0$ *such that*

$$\operatorname{spect}(\hat{K})\bigcap[\lambda_-, \lambda_+] \subseteq \bigcup_{k\in\mathbb{Z}} I_k(\hbar), \tag{258}$$

with

$$I_k(\hbar) = \Big[-a + \Big(k - \frac{\mu}{4}\Big)\hbar - C_0\hbar^2, -a + (k - \frac{\mu}{4})\hbar + C_0\hbar^2\Big]$$

for $\hbar \in]0, \hbar_1]$.

Let us remark that this theorem gives the usual Bohr-Sommerfeld quantization conditions for the energy spectrum, more explicitly,

$$\lambda_k = \frac{1}{2\pi}\mathcal{J}(E_k) = \Big(k - \frac{\mu}{4}\Big)\hbar - a + O(\hbar^2).$$

Under a stronger assumption on the flow, it is possible to give a more accurate result.

(As_{10}) $\Phi^t_{K_0}$ *has no fixed point in* $\Sigma_F^{K_0}$*,* $\forall\lambda \in [\lambda_- - \epsilon, \lambda_+ + \epsilon]$ *and* $\forall t \in]0, 2\pi[$.

Let us denote by $d_k(\hbar)$ the number of eigenvalues of $\hat{K}$ in the interval $I_k(\hbar)$.

***Theorem 6.13* ([6, 24, 44]).** — *Under the above assumptions, for* $\hbar$ *small enough and* $-a + (k - \frac{\mu}{4})\hbar \in [\lambda_-, \lambda_+]$*, we have:*

$$d_k(\hbar) \asymp \sum_{j\geq 1} \Gamma_j\Big(-a + \Big(k - \frac{\mu}{4}\Big)\hbar\Big)\hbar^{j-d}, \tag{259}$$

with $\Gamma_j \in C^\infty([\lambda_-, \lambda_+])$*. In particular*

$$\Gamma_1(\lambda) = (2\pi)^{-d}\int_{\Sigma_\lambda} d\nu_\lambda.$$

In the particular case $d = 1$ we have $\mu = 2$ and $a = -\min(H_0)$ hence $d_k(\hbar) = 1$. Furthermore the Bohr-Sommerfeld conditions take the following more accurate form

***Theorem 6.14* ([23]).** — *Let us assume* $d = 1$ *and* $a = 0$*. Then there exists a sequence* $f_k \in C^\infty([F_-, F_+])$*, for* $k \geq 2$*, such that*

$$\lambda_\ell + \sum_{k\geq 2} h^k f_k(\lambda_\ell) = \Big(\ell + \frac{1}{2}\Big)\hbar + \mathcal{O}(\hbar^\infty) \tag{260}$$

for $\ell \in \mathbb{Z}$ *such that* $(\ell + \frac{1}{2})\hbar \in [\lambda_-, \lambda_+]$.

In particular there exists $g_k \in C^\infty([\lambda_-, \lambda_+])$ *such that*

$$\lambda_\ell = \Big(\ell + \frac{1}{2}\Big)\hbar + \sum_{k\geq 2} h^k g_k\Big(\Big(\ell + \frac{1}{2}\Big)\hbar\Big) + \mathcal{O}(\hbar^\infty), \tag{261}$$

where $\ell \in Z$ *such that* $(\ell + \frac{1}{2})\hbar \in [F_-, F_+]$.

We can deduce from the above theorem and Taylor formula the Bohr-Sommerfeld quantization rules for the eigenvalues E_n

***Corollary 6.15*.** — *there exists* $\lambda \mapsto b(\lambda, \hbar)$ *and* C^∞ *functions* b_j *defined on* $[\lambda^-, \lambda^+]$ *such that* $b(\lambda, \hbar) = \sum_{j\in\mathbb{N}} b_j(\lambda)\hbar^j + \mathcal{O}(\hbar^\infty)$ *and the spectrum* E_n *of* $\hat{H}$ *is given by*

$$E_n = b\Big(\Big(n + \frac{1}{2}\Big)\hbar, \hbar\Big) + \mathcal{O}(\hbar^\infty), \tag{262}$$

for n *such that* $(n + \frac{1}{2})\hbar \in [\lambda^-, \lambda^+]$*. In particular we have* $b_0(\lambda) = \mathcal{J}^{-1}(2\pi\lambda)$ *and* $\boxed{b_1 = 0}$.

When $H_0^{-1}(I)$ is not connected but such that the M connected components are mutually symmetric, under linear symplectic maps, then the above results still hold [**23**].

Remark 6.16. — For $d = 1$, the methods usually used to prove existence of a complete asymptotic expansion for the eigenvalues of $\hat{H}$ are not suitable to compute the coefficients $b_j(\lambda)$ for $j \geq 2$. This was done recently in [**5**] and [**46**] using the coefficients d_{jk} appearing in the functional calculus (Theorem 6.1).

6.5. A proof of the quantization rules and quasi-modes. — We shall give here a direct proof for the Bohr-Sommerfeld quantization rules by using coherent states, following the Ph.D thesis of J.-M. Bily [**2**]. A similar approach, with more restrictive assumptions, was considered before in [**32**] and [**22**].

The starting point is the following remark. Let be $r > 0$ and suppose that there exists C_r such that for every $\hbar \in]0, 1]$, there exist $E \in \mathbb{R}$ and $\psi \in L^2(\mathbb{R}^d)$, such that

$$\|(\hat{H} - E)\psi\| \leq C_r\hbar^r, \quad \text{and} \quad \liminf_{\hbar\to 0} \|\psi\| := c > 0. \tag{263}$$

If these conditions are satisfied, we shall say that $\hat{H}$ has a quasi-mode of energy E with an error $\mathcal{O}(\hbar^r)$. With quasi-modes we can find some points in the spectrum of $\hat{H}$. More precisely, if $\delta > \frac{C_r}{c}$, the interval $[E - \delta\hbar^r, E + \delta\hbar^r]$ meets the spectrum of $\hat{H}$. This is easily proved by contradiction, using that $\hat{H}$ is self-adjoint. So if the spectrum of $\hat{H}$ is discrete in a neighborhood of E, then we know that $\hat{H}$ has at least one eigenvalue in $[E - \delta\hbar^r, E + \delta\hbar^r]$.

Let us assume that the Hamiltonian $\hat{H}$ satisfied conditions (As_1) to (As_6), $(As_8), (As_9)$.

Using Theorem 6.1 and Proposition 6.11, we can assume that the Hamiltonian flow $\Phi_t^{H_0}$ has a constant period 2π in $H_0^{-1}]E_- - \varepsilon, E_+ + \varepsilon[$, for some $\varepsilon > 0$.

Following an old idea in quantum mechanics (A. Einstein), let us try to construct a quasimode for $\hat{H}$ with energies $E^{(\hbar)}$ close to $E \in [E_-, E_+]$, related with a 2π periodic trajectory $\gamma_E \subset \Sigma_E^{H_0}$, by the Ansatz

$$\psi_{\gamma_E} = \int_0^{2\pi} \mathrm{e}^{\frac{itE^{(\hbar)}}{\hbar}} U(t)\varphi_z \, dt \tag{264}$$

where $z \in \gamma_E$. Let us introduce the real numbers

$$\sigma(\hbar) = \frac{1}{2\pi\hbar} \int_0^{2\pi} [\dot{q}(t)p(t) - H_0(q(t), p(t))] \, dt + \frac{\mu}{4} + b$$

where $t \mapsto (q(t), p(t))$ is a 2π-periodic trajectory γ_E in ${H_0}^{-1}(E)$, $E \in [E_-, E_+]$, μ is the Maslov index of γ and $b = \int_\gamma H_1$. In order that the Ansatz (264) provides a good quasimode, we must check that its mass is not too small.

Proposition 6.17. — *Assume that 2π is the primitive period of γ_E. Then there exists a real number $m_E > 0$ such that*

$$\|\psi_{\gamma_E}\| = m_E\hbar^{1/4} + \mathcal{O}(\hbar^{1/2}). \tag{265}$$

Proof. — Using the propagation of coherent states and the formula giving the action of metaplectic transformations on Gaussians, up to an error term $\mathcal{O}(\sqrt{\hbar})$, we have

$$\begin{aligned}\|\psi_{\gamma_E}\|^2 = (\pi\hbar)^{-d/2}\int_0^{2\pi}\int_0^{2\pi}\int_{\mathbb{R}^d} \mathrm{e}^{\frac{i}{\hbar}\Phi(t,s,x)}\,(\det(A_t+iB_t))^{-1/2}\cdot \\ \cdot\left(\overline{\det(A_s+iB_s)}\right)^{-1/2}\,dt\,ds\,dx,\end{aligned} \tag{266}$$

where the phase Φ is

$$\begin{aligned}\Phi(t,s,x) = (t-s)E + (\delta_t-\delta_s) + \frac{1}{2}(q_s\cdot p_s - q_t\cdot p_t) + \\ x\cdot(p_t-p_s) + \frac{1}{2}\left(\Gamma_t(x-q_t)\cdot(x-q_t) - \overline{\Gamma_s}(x-q_s)\cdot(x-q_s)\right)).\end{aligned} \tag{267}$$

Let us show that we can compute an asymptotics for $\|\psi_{\gamma_E}\|^2$ with the stationary phase Theorem. Using that $\Im(\Gamma_t)$ is positive non-degenerate, we find that

$$\Im(\Phi(t,s,x)) \geq 0, \quad \text{and } \{\Im(\Phi(t,s,x)) = 0\} \Longleftrightarrow \{x = q_t = q_s\} \tag{268}$$

On the set $\{x = q_t = q_s\}$ we have $\partial_x\Phi(t,s,x) = p_t - p_s$. So if $\{x = q_t = q_s\}$ then we have $t = s$ (2π is the primitive period of γ_E) and we get easily that $\partial_s\Phi(t,s,x) = 0$. In the variables (s,x) we have found that $\Phi(t,s,x)$ has one critical point: $(s,x) = (t,q_t)$. Let us compute the hessian matrix $\partial^{(2)}_{s,x}\Phi$ at (t,t,q_t).

$$\partial^{(2)}_{s,x}\Phi(t,t,q_t) = \begin{pmatrix} -(\overline{\Gamma_t}\dot{q}_t - \dot{p}_t)\cdot\dot{q}_t & [\overline{\Gamma_t}(\dot{q}_t-\dot{p}_t)]^T \\ \overline{\Gamma_t}(\dot{q}_t-\dot{p}_t) & 2i\Im\Gamma_t\end{pmatrix}. \tag{269}$$

To compute the determinant, we use the idendity, for $r\in\mathbb{C}$, $u\in\mathbb{C}^d$, $R\in GL(\mathbb{C}^d)$

$$\begin{pmatrix} r & u^T \\ u & R\end{pmatrix}\begin{pmatrix} 1 & 0 \\ -R^{-1}u, \mathbb{1} & \end{pmatrix} = \begin{pmatrix} r - u^T\cdot R^{-1}u & u^T \\ 0 & R\end{pmatrix}. \tag{270}$$

Then we get

$$2\det[-i\partial^2_{s,x}\Phi(t,t,q_t)] = \Gamma_t\dot{q}_t\cdot\dot{q}_t + (\Im(\Gamma_t))^{-1}(\Re\Gamma_t\dot{q}_t - \dot{p}_t)\cdot(\Re\Gamma_t\dot{q}_t-\dot{p}_t)\det[2\Im(\Gamma_t]. \tag{271}$$

But E is not critical, so $(\dot{q}_t,\dot{p}_t) \neq (0,0)$ and we find that $\det[-i\partial^2_{s,x}\Phi(t,t,q_t)] \neq 0$. The stationary phase Theorem (see Appendix), gives

$$\|\psi_{\gamma_E}\|^2 = m_E^2\sqrt{\hbar} + \mathcal{O}(\hbar) \tag{272}$$

with

$$m_E^2 = 2^{(d+1)/2}\sqrt{\pi}\int_0^{2\pi} |\det(A_t+iB_t)|^{-1/2}|\det[-i\partial^2_{s,x}\Phi(t,t,q_t)]|^{-1/2}\,dt. \tag{273}$$

□

We now give one formulation of the Bohr-Sommerfeld quantization rule.

Theorem 6.18. — *Let us assume that the Hamiltonian $\hat{H}$ satisfied conditions (As_1) to (As_6), (As_8), (As_9), with period 2π and that 2π is a primitive period for a periodic trajectory $\gamma_E \subseteq \Sigma_E$.*

Then $\hbar^{-1/4}\psi_{\gamma_E}$ is a quasi-mode for $\hat{H}$, with an error term $\mathcal{O}(\hbar^{7/4})$, if E ***satisfies the quantization condition****:*

$$E = \Big(\frac{\mu}{4} + b + k\Big)\hbar + \frac{1}{2\pi}\int_{\gamma_E} p\,dq. \tag{274}$$

Moreover, the number $a := \frac{1}{2\pi}\int_{\gamma_E} p\,dq - E$ is constant on $[E_-, E_+]$. and choosen $C > 0$ large enough, the intervals

$$I(k,\hbar) = \Big[\Big(\frac{\mu}{4} + b + k\Big)\hbar + \lambda - C\hbar^{7/4}, \Big(\frac{\mu}{4} + b + k\Big)\hbar + \lambda + C\hbar^{7/4}\Big]$$

satisfy: if $I(k,\hbar) \cap [E_-, E_+] \neq \varnothing$ then $\hat{H}$ has an eigenvalue in $I(k,\hbar)$.

Proof. — We use, once more, the propagation of coherent states. Using periodicity of the flow, we have, if $H_0(z) = E$,

$$U(2\pi)\varphi_z = \mathrm{e}^{2i\pi\sigma(\hbar)}\varphi_z + \mathcal{O}(\hbar). \tag{275}$$

Here we have to remark that the term in $\sqrt{\hbar}$ has disappeared. This needs a calculation. We shall see later why the half power of $\hbar$ are absent here.

By integration by parts, we get

$$\begin{aligned} \hat{H}\psi_{\gamma_E} &= i\hbar\int_0^{2\pi} \mathrm{e}^{\frac{itE}{\hbar}}\partial_t U(t)\varphi_z\,dt \\ &= i\hbar\Big(\mathrm{e}^{\frac{2i\pi E}{\hbar}}U(2\pi)\varphi_z - \varphi_z\Big) + E\psi_{\gamma_E} \\ &= E\psi_{\gamma_E} + \mathcal{O}(\hbar^2) \end{aligned} \tag{276}$$

So, we get finally a quasi-mode with an error $\mathcal{O}(\hbar^{7/4})$, using (265). □

Now we want to improve the accuracy of the eigenvalues. Let be a smooth cut-off χ supported in $]E_- - \varepsilon, E_+ + \varepsilon[$, $\chi = 1$ in $[E_-, E_+]$. Let us introduce the real numbers

$$\sigma(\hbar) = \frac{1}{2\pi\hbar}\int_0^{2\pi} [\dot{q}(t)p(t) - H_0(q(t), p(t))]\,dt + \frac{\mu}{4} + b$$

where $t \mapsto (q(t), p(t))$ is a 2π-periodic trajectory γ in ${H_0}^{-1}(E)$, $E \in [E_-, E_+]$, μ is the Maslov index of γ and $b = \int_\gamma H_1$. Let us remark that under our assumptions, $\sigma(\hbar)$ is independant of γ_E and $E \in [E_-, E_+]$.

Theorem 6.19. — *With the above notations and assumptions, the operator $\mathrm{e}^{-2i\pi\sigma(\hbar)}U(2\pi)\chi(\hat{H})$ is a semi-classical observable. More precisely, there exists a semi-classical observable L of order 0, $L = \sum_{j\geq 0}\hbar^j L_j$, such that*

$$\mathrm{e}^{-2i\pi\sigma(\hbar)}U(2\pi)\chi(\hat{H}) = \hat{L}. \tag{277}$$

Moreover we have $L_0(z) = \chi(H_0(z))$ *and for* $j \geq 1$ *the support of* L_j *is in* $H_0^{-1}]E_- - \varepsilon, E_+ + \varepsilon[$.

Proof. — We shall use the propagation Theorem for coherent states with formula (24) to compute the semi-classical Weyl symbol of $\mathrm{e}^{-2i\pi\sigma(\hbar)}U(2\pi)\chi(\hat{H})$. So, we start from the formula

$$L(x,\xi) = (2\pi\hbar)^{-d}\int_{\mathcal{Z}\times\mathbb{R}^d} \mathrm{e}^{-\frac{i}{\hbar}u\xi}U(2\pi)\chi(\hat{H})\varphi_z((x+\frac{u}{2})\overline{\varphi_z(x-\frac{u}{2})}\,dz\,du. \tag{278}$$

This formula is a consequence of results seen in section 1 connecting Weyl symbols, integral kernels and coherent states. Using the propagation Theorem for coherent state and the localization lemmas 1.2 and 1.3, we get

$$\begin{aligned} U(2\pi)\chi(\hat{H})\varphi_z = \mathrm{e}^{2i\pi\sigma(\hbar)}\mathcal{T}(z)\Lambda_\hbar\left(P_{z,0}+\sqrt{\hbar}P_{z,1}+\cdots+\hbar^{N/2}P_{z,N})g\right)\cdot \\ \cdot\,\theta(H(z)) + \hbar^{(N+1)/2}R_{z,N}, \end{aligned} \tag{279}$$

where $P_{z,j}$ is a polynomial of degree $\leq 3j$ and with the same parity as j; $\|R_{z,N}\| = O(1)$; θ is a smooth function, with support in $]E_- - \varepsilon, E_+ + \varepsilon[$, $\theta = 1$ on support of χ. So modulo a negligible error term we have

$$\begin{aligned} L(x,\xi) = 2^{-d}(\pi\hbar)^{-3d/2}\int_{\mathcal{Z}\times\mathbb{R}^d}\theta(H_0(z))\mathrm{e}^{\frac{i}{\hbar}\Phi_{x,\xi}(z,u)}\cdot \\ \cdot\left(\sum_{0\leq j\leq N}\hbar^{j/2}P_{z,j}\left(\frac{x-q-\frac{u}{2}}{\sqrt{\hbar}}\right)\right)dz\,du, \end{aligned} \tag{280}$$

where $z = (q,p) \in \mathbb{R}^d \times \mathbb{R}^d$ and the quadratic phase $\Phi_{x,\xi}$ is defined by

$$\Phi_{x,\xi}(z,u) = u\cdot(p-\xi) + i\left(|x-q|^2 + \frac{|u|^2}{4}\right).$$

Let us translate the variable z by (x,ξ). So in the variable $z' = z - (x,\xi)$ we have

$$\Phi_{x,\xi}(z',u) = \frac{1}{2}\mathcal{A}(z',u)\cdot(z',u),$$

where the matrix $\mathcal{A}$ is defined by

$$\mathcal{A} = \begin{pmatrix} 2i\mathbb{1}_d & 0 & 0 \\ 0 & 0 & \mathbb{1}_d \\ 0 & \mathbb{1}_d & \frac{i}{2}\mathbb{1}_d \end{pmatrix}. \tag{281}$$

So clearly, $\mathcal{A}$ is invertible and $\Im(\mathcal{A})$ is non-negative. To apply the stationary Theorem (see Appendix), we need to compute $\det_+^{-1/2}(i\mathcal{A})$. This follows by computing a Gaussian integral

$$\det{}_+^{-1/2}(i\mathcal{A}) = \pi^{-3d/2}\int_{\mathbb{R}^{3d}}\mathrm{e}^{i\mathcal{A}v\cdot v}\,dv.$$

Using the shape of the matrix $\mathcal{A}$ we get $\det_+^{-1/2}(i\mathcal{A}) = 2^{-d/2}$.

So we get an asymptotic expansion for $L(x,\xi)$ in power of $\sqrt{\hbar}$. But, by computing a little bit more, we found that each half power of $\hbar$ disappears and the Theorem is proved. □

We can use the previous result to improve Theorem 6.18.

Corollary 6.20. — *Suppose that the assumptions of Theorem 6.18 are satisfied. Then there exists smooth function of E, $c_2(E)$, such that $\hbar^{-1/4}\psi_{\gamma_E}$ is a quasi-mode for $\hat{H}$, with an error $\mathcal{O}(\hbar^{9/4})$, if E satisfies the following quantization condition:*

$$E = (\frac{\mu}{4} + b + k)\hbar + \frac{1}{2\pi}\int_{\gamma_E} p\, dq + c_2(E)\hbar^2. \tag{282}$$

Choosen $C > 0$ large enough, the intervals

$$I'(k,\hbar) = [a(k,\hbar) + c_2(a(k,\hbar))\hbar^2 - C\hbar^{9/4}, (a(k,\hbar) + c_2(a(k,\hbar))\hbar^2 + C\hbar^{9/4}]$$

satisfy: if $I'(k,\hbar)\cap[E_-,E_+] \neq \varnothing$ then $\hat{H}$ has an eigenvalue in $I'(k,\hbar)$, where $a(k,\hbar) = (\frac{\mu}{4} + b + k)\hbar + a$.

Remark 6.21. — If $\hat{H}$ satisfied (A_s1) to (As_6), (As_8), (As_9) with a period depending on E and if $\Phi_t^{H_0}$ has no fixed points in Ω for $|t| < T_E$, then we can apply the previous result to $\mathcal{J}(\hat{H})$ to get quasi-modes and approximated eigenvalues for $\hat{H}$.

Now we shall show that in the energy band $[E_-,E_+]$, all the eigenvalues are close to $a(k,\hbar) + c_2(a(k,\hbar))\hbar^2$ modulo $\mathcal{O}(\hbar^{9/4})$ (clustering phenomenum) and moreover we can estimate the number of states in each cluster $I'(k,\hbar)$ for $\hbar$ small enough.

Suppose that $\hat{H}$ satisfies conditions As_1 to As_9 (except (As_7)), with a constant period 2π (remember that after using the action function $\mathcal{J}$ to rescale the periods, this is not a restriction). From Theorem (6.19) we know that, with a suitable cut-off χ, we have

$$\mathrm{e}^{-2i\pi\sigma(\hbar)}U(2\pi)\chi(\hat{H}) = \chi(\hat{H})(\mathbb{1} + \hbar\hat{W}), \tag{283}$$

where W is a semi-classical observable of order 0. But $\hat{W}$ commutes with $\hat{H}$ and, for $\hbar$ small enough, $\log(\mathbb{1} + \hbar\hat{W})$ is well defined. So there exists a semi-classical observable $\hat{V}$ commuting with $\hat{H}$, such that

$$\mathrm{e}^{-\frac{2i\pi}{\hbar}(\hat{H}-\hbar\sigma(\hbar)-\hbar^2\hat{V})}\chi(\hat{H}) = \chi(\hat{H}). \tag{284}$$

Let us consider the compact operators: $\hat{K}^{(1)} = \hat{H}\chi(\hat{H})$ $\hat{K}^{(2)} = (\hat{H} - \hbar\sigma(\hbar) - \hbar^2\hat{V})\chi(\hat{H})$. $\hat{K}^{(1)}$ and $\hat{K}^{(2)}$ commutes, so they have an othonormal basis of joint eigenfunctions. Then using that $\mathrm{Spec}(\hat{K}^{(1)})\cap[E_-,E_+] = \mathbb{Z}\hbar\cap[E_-,E_+]$, we get easily the following statement (see [**23**]) for more details).

Theorem 6.22. — *Under the same conditions as in Theorem 6.19, there exists $C > 0$ such that*

$$\mathrm{Spec}(\hat{H}) \cap [E_-,E_+] \subseteq \bigcup_{k\in\mathbb{Z}} I(k,\hbar). \tag{285}$$

Moreover, if for every $E \in [E_-, E_+]$ there exists a periodic trajectory with primitive period 2π, and if $I(k,\hbar) \subseteq [E_-, E_+]$ then $\mathrm{Spec}(\hat{H}) \cap I(k,\hbar) \neq \varnothing$.

If we assume that the condition (As_{10}) is satisfied, then we can compute the number of states of $\hat{H}$ in $I(k,\hbar)$ for $\hbar$ small. Let us denote

$$d_k(\hbar) = \sum_{\lambda \in \mathrm{Spec}(\hat{H}) \cap I(k,\hbar)} \chi(\lambda).$$

We remark that $d_k(\hbar)$ is a Fourier coefficient, by the following computation

$$\mathrm{tr}\left(\mathrm{e}^{-\frac{it}{\hbar}\hat{H}_\sharp}\chi(\hat{H})\right) = \sum_{k\in\mathbb{Z}} d_k(\hbar)\mathrm{e}^{-itk},$$

where $\hat{H}_\sharp = \hat{H} - \hbar\sigma(\hbar) - \hbar^2\hat{V}$. So we have

$$d_k(\hbar) = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{itk}\mathrm{tr}\left(\mathrm{e}^{-\frac{it}{\hbar}\hat{H}_\sharp}\chi(\hat{H})\right) dt. \tag{286}$$

Choose $\zeta \in C_0^\infty]-3\pi/2, 3\pi/2[$, such that $\sum_{j\in\mathbb{Z}} \zeta(t - 2\pi j) = 1$, we get

$$d_k(\hbar) = \frac{1}{2\pi}\int_{\mathbb{R}} \zeta(t)\mathrm{e}^{itk}\mathrm{tr}\left(\mathrm{e}^{-\frac{it}{\hbar}\hat{H}_\sharp}\chi(\hat{H})\right) dt. \tag{287}$$

We remark now that the integral in (287) is of the same type as the Fourier integrals we meet in the proof of Theorem 6.4. So using the same method, we get the following result

Theorem 6.23. — *Under the assumptions explained above, we have*

$$d_k(\hbar) = \sum_{j\geq 1} f_j((k + \frac{\mu}{4} + b)\hbar + \lambda))\hbar^{j-d} \tag{288}$$

where f_j are smooth functions with support in $]E_- - \varepsilon, E_+ + \varepsilon[$. In particular we have

$$f_1(\tau) = \chi(\tau)\int_{H_0^{-1}(\tau)} \frac{d\Sigma_\tau}{|\nabla_z H_0|} \tag{289}$$

where $d\Sigma_\tau$ is the Riemannian measure on $\Sigma_\tau = H_0^{-1}(\tau)$.

Remark 6.24. — In particular if $d = 1$, we have $f_1(\tau) = \chi(\tau) = 1$ if $\tau \in [E_-, E_+]$. As it is expected, we find exactly one state in each cluster.

A natural question is to compare quasi-modes and exact eigenfunctions. In the 1-D case this can easily done, at least for connected energy levels.

Let us recall the notation $\hat{K}^{(1)} = \hat{H}\chi(\hat{H})$ and suppose that $\hat{H}$ satisfies the conditions of Theorem 6.19. In each intervall $I(k,\hbar)$ we have constructed a quasi-mode which we denote $\psi_k^\sharp$, with energy $\lambda_k^\sharp \in I'(k,\hbar)$. We have the following result.

Proposition 6.25. — *There exists $C>0$ such that for every $(k,\hbar)$ satisfying $I(k,\hbar)\cap[E_-,E_+]\neq\varnothing$, we have*

$$\|(\psi_k^\sharp - \Pi_{I'(k,\hbar)}\psi_k^\sharp\| \leq C\hbar^{5/4}, \tag{290}$$

where Π_I is the spectral projector for $\hat{H}$ on I.

In particular, if $d=1$, the quasi-mode $\psi_k^\sharp$ is close to a genuine eigenfunction. More precisely,

$$\psi_k = \frac{\Pi_{I'(k,\hbar)}\psi_k^\sharp}{\|\Pi_{I'(k,\hbar)}\psi_k^\sharp\|} \tag{291}$$

is an eigenfunction with the eigenvalue λ_k and satisfies

$$\|\psi_k^\sharp - \psi_k\| \leq C\hbar^{5/4}. \tag{292}$$

Proof. — Let us write down

$$\|(\hat{K}^{(1)} - \lambda_k^\sharp)\psi_k^\sharp\|^2 = \sum_j |\lambda_j\chi(\lambda_j) - \lambda_k^\sharp|^2 |\langle\psi_k^\sharp, \psi_j\rangle|^2. \tag{293}$$

But we have choosen $\chi = 1$ on $I'(k,\hbar)$, so using the clustering property for the eigenvalues λ_j and summing on $\lambda_j \notin I'(k,\hbar)$ we get inequality (290).

If $d=1$ we have seen that $\hat{H}$ has only one eigenvalue in $I'(k,\hbar)$, so we get (292) and (291). □

Remark 6.26. — For $d=1$ we can get, by the same method, approximations of eigenvalues and eigenfunctions with an error $\mathcal{O}(\hbar^\infty)$. This has been proved by a different method in [**24**].

Appendix A
Siegel representation

We give here some basic properties of the Siegel representation $S\mapsto \varSigma_S$ of the symplectic group $\mathrm{Sp}(d)$ into the Siegel space Σ_d^+.

Let us prove here the important property stated in Lemma 1.6: If $\Gamma\in\Sigma_d^+$ then $\varSigma_S\Gamma\in\Sigma_d^+$.

Proof. — Let us denote $E := A + B\Gamma, \quad F := C + D\Gamma$. S is symplectic, so we have $S^TJS = J$. Using

$$\begin{pmatrix} E \\ F\end{pmatrix} = S\begin{pmatrix} I \\ \Gamma\end{pmatrix}$$

we get

$$(E^T, F^T)J\begin{pmatrix} E \\ F\end{pmatrix} = \big((I,\Gamma)\big)\, J\begin{pmatrix} I \\ Z\end{pmatrix} = 0,$$

which gives $E^TF = F^TE$ In the same way, we have

$$\begin{aligned}(294)\qquad \frac{1}{2i}(E^T,F^T)J\begin{pmatrix}\bar{E}\\ \bar{F}\end{pmatrix} &= \frac{1}{2i}(I,\Gamma)S^TJS\begin{pmatrix}I\\ \bar{\Gamma}\end{pmatrix}\\ &= \frac{1}{2i}(I,\Gamma)J\begin{pmatrix}I\\ \bar{\Gamma}\end{pmatrix} = \frac{1}{2i}(\bar{\Gamma}-\Gamma) = -\Im\Gamma.\end{aligned}$$

We get the following equation

$$(295)\qquad F^T\bar{E} - E^T\bar{F} = 2i\Im\Gamma.$$

If $x \in \mathbb{C}^n,\ Ex = 0$, we have

$$\bar{E}\bar{x} = x^TE^T = 0$$

hence

$$x^T\Im\Gamma\bar{x} = 0$$

then $x = 0$. Because $\Im\Gamma$ is non-degenerate we get that E and F are injective. So, we can define,

$$(296)\qquad \Sigma(S)\Gamma = (C + D\Gamma)(A + B\Gamma)^{-1}.$$

Let us prove that $\Sigma(S) \in \Sigma_d^+$. We have:

$$\Sigma(S)\Gamma = FE^{-1} \ \Rightarrow (\Sigma(S)\Gamma)^T = (E^{-1})^TF^T = (E^{-1})^TE^TFE^{-1} = FE^{-1} = \Sigma(S)\Gamma.$$

Then $\Sigma(S)\Gamma$ is symmetric. We have also:

$$E^T\frac{FE^{-1} - \bar{F}\bar{E}^{-1}}{2i}\bar{E} = \frac{F^T\bar{E} - E^T\bar{F}}{2i} = \Im\Gamma$$

and this proves that $\Im(\Sigma(S)\Gamma))$ is positive and non-degenerate. □

Appendix B

Proof of Theorem 3.5

The first step is to prove that there exists a unique self-adjoint formal projections $\Pi^+(t)$, smooth in t, such that $\Pi_0^+(t,X) = \pi_+(t,X)$ and

$$(297)\qquad (i\hbar\partial_t - H(t)) \circledast \Pi^+(t) = (i\hbar\partial_t - H(t)) \circledast \Pi^+(t).$$

This equation is equivalent to the following

$$(298)\qquad i\hbar\partial_t\Pi^+(t) = [H(t),\Pi^+(t)]_\circledast.$$

Let us denote $\Pi(t) = \Pi^+(t)$. (The case (-) could be solved in the same way) and $\Pi(t) = \sum_{j\geq 0}\hbar^j\Pi_j(t)$. We shall prove existence of the $\Pi_n(t)$ by induction on n, starting with $\Pi_0(t,X) = \pi_+(t,X)$. Let us denote $\Pi^{(n)}(t) = \sum_{0\leq j\leq n}\hbar^j\Pi_j(t)$. Let us prove by industion on n that we can find $\Pi_{n+1}(t)$ such that

$$(299)\qquad \Pi^{(n+1)}(t) \circledast \Pi^{(n+1)}(t) = \Pi^{(n+1)}(t) + 0(\hbar^{n+2})$$

$$(300)\qquad i\hbar\partial_t\Pi^{(n+1)}(t) = [H(t),\Pi^{(n+1)}(t)]_\circledast + 0(\hbar^{n+2}).$$

Let us denote by $R_n(t,X)$ the coefficient of $\hbar^{n+1}$ in $\Pi^{(n+1)}(t) \circledast \Pi^{(n+1)}(t)$ and by $iS_n(t,X)$ the coefficient of $\hbar^{n+1}$ in $i\hbar\partial_t\Pi^{(n+1)}(t) - [H(t), \Pi^{(n+1)}(t)]_\circledast$. Then the system of equations (299) is equivalent to the following

$$\Pi_{n+1}(t) - (\pi_+(t)\Pi_{n+1}(t) + \Pi_{n+1}(t)\pi_+(t)) = R_n(t) \tag{301}$$

$$[H_0(t), \Pi_{n+1}(t)] = iS_n(t). \tag{302}$$

The matrices $R_n(t)$ and $S_n(t)$ are Hermitean. We also have the following properties, proved by using the induction assumptions and some algebraic computations $\pi_+R_n(t)\pi_- = \pi_-R_n(t)\pi_+ = 0$ and $\pi_+S_n(t)\pi_+ = \pi_-R_n(t)\pi_- = 0$.

We can now solve the equations for $\Pi_{n+1}(t)$ and get the following solution

$$\begin{aligned}\Pi_{n+1}(t) = \pi_-(t)R_n(t)\pi_-(t) - \pi_+(t)R_n(t)\pi_+(t) + \\ \frac{i}{\lambda_+(t) - \lambda_-(t)}\left(\pi_+(t)S_n(t)\pi_-(t) - \pi_-(t)S_n(t)\pi_+(t)\right).\end{aligned} \tag{303}$$

The same proof gives also uniqueness of the $\Pi_n(t)$ for all $n \geq 1$.

Let now prove the second part of the Theorem.

We have to find $H^\pm(t) \in \mathcal{O}_{sc}$, with principal term $\lambda_\pm(t)\mathbb{1}_m$, such that

$$\Pi^\pm(t) \circledast (H(t) - H^\pm(t)) = 0. \tag{304}$$

It is enough to consider + case. The method is the same as in the first part. Let us denote $H^+(t) = \sum_{j\geq 0}\hbar^j H_j^+(t)$, where $H_0^+(t) = \lambda_+(t)\mathbb{1}_m$, and $H^{+,(n)}(t) = \sum_{j\leq n}\hbar^j H_j^+(t)$. We shall prove existence of H_n^+ by induction on n, satisfying

$$\Pi^+(t) \circledast (H(t) - H^{+,(n)}(t)) = O(\hbar^{n+1}). \tag{305}$$

So we get for $H_{n+1}^+(t)$ the following equation

$$\pi_+(t)H_{n+1}^+(t) = W_n(t) \tag{306}$$

where $W_n(t)$ is the coefficient of $\hbar^{n+1}$ in $\Pi^+(t) \circledast (H(t) - H^{+,(n)}(t))$.

Let us remark now that we have $\pi_-(t)W_n(t) = 0$ and $\pi_+W_n(t)\pi_+$ is Hermitean. Then we can solve equation (306) with

$$H_{n+1}^+(t) = \pi_+W_n(t)\pi_+(\pi_+W_n(t)\pi_-\pi_-W_n(t)^*\pi_+.$$

Let us now compute the subprincipal term $H_1^+(t)$.

It is not difficult to find the equation satisfied by $H_1^+(t)$:

$$\begin{aligned}\pi_+(t)H_1^+(t) = \pi_+(t)H_1(t)\pi_+ + \frac{1}{2i}(\lambda_+(t) - \lambda_-(t))\pi_+(t)\{\pi_+(t), \pi_+(t)\} + \\ \frac{1}{i}\pi_+(t)\{\lambda_+(t), \pi_+(t)\} - i\pi_+(t)\partial_t\pi_+(t).\end{aligned} \tag{307}$$

So, we get $\pi_+(t)H_1^+(t)\pi_+(t)$ and $\pi_+(t)H_1^+(t)\pi_-(t)$ and using that $H_1^+(t)$ has to be Hermitean, we get a formula for $H_1^+(t)$ (which is not unique, the part $\pi_-(t)H_1^+(t)\pi_-(t)$ may be any smooth Hermitean matrix. $\square$

Appendix C
About the Poincaré map

Let γ be a closed orbit in σ_E with period T_γ, and let us denote by $F_{\gamma,z}$ the matrix $F_\gamma(z) = F_{T_\gamma}(z)$. F_γ is usually called the "monodromy matrix" of the closed orbit γ. Of course, $F_\gamma(z)$ does depend on on the initial point $z \in \gamma$, but its eigenvalues do not, since the monodromy matrix with a different initial point on γ is conjugate to $F_\gamma(z)$. F_γ has 1 as eigenvalue of algebraic multiplicity at least equal to 2. Let us recall the following definition

Definition C.1. — We say that γ is a non-degenerate orbit if the eigenvalue 1 of F_γ has algebraic multiplicity 2.

Let σ denote the usual symplectic form on $\mathbb{R}^{2d}$

$$\sigma(z, z') = p \cdot q' - p' \cdot q \quad z = (q, p);\ z' = (q', p'). \tag{308}$$

We denote by $\{v_1, v_1'\}$ the eigenspace of F_γ belonging to the eigenvalue 1, and by V its orthogonal complement in the sense of the symplectic form σ

$$V = \left\{z \in \mathbb{R}^{2n}\ :\ \sigma(z, v_1) = \sigma(z, v_1') = 0\right\} \quad . \tag{309}$$

Then, the restriction P_γ of F_γ to V is called the (linearized) "Poincaré map" for γ.

Appendix D
Stationary phase theorems

For details see [**25**]. Let us first consider the simpler case with a quadratic phase. Let be $\mathcal{A}$ a complex symmetric matrix, $m \times m$. We assume that $\Im\mathcal{A}$ is non-negative and $\mathcal{A}$ is non-degenerate. Then we have the Fourier transfor formula for the Gaussian $\mathrm{e}^{i\mathcal{A}x\cdot x/2}$

$$\int_{\mathbb{R}^m} \mathrm{e}^{i\mathcal{A}x\cdot x/2}\mathrm{e}^{-ix\cdot\xi}\, d\xi = (2\pi)^{m/2}\mathrm{det}(-i\mathcal{A})^{1/2}\mathrm{e}^{(i\mathcal{A})^{-1}\xi\cdot\xi/2}.$$

Let be Ω an open set of $\mathbb{R}^m$, a, f smooth functions on Ω, where the support of a is compact. Let us define

$$I(\omega) = \int_{\mathbb{R}^n} a(x)\mathrm{e}^{i\omega f(x)}\, dx$$

***Theorem D.1* (non-degenerate critical point)**. — *Let us assume that $\Im f \geq 0$ in Ω and that for $x \in \Omega$ $\Im f(x) = \partial_x f(x) = 0$, if and only $x = 0$ and that the Hesian matrix $\partial_x^{(2)} f(0) := \mathcal{A}$ is non-degenerated. Then or $\omega \to +\infty$, we have the following asymptotic expansion, modulo $O(\omega^{-\infty})$,*

$$I(\omega) = \left(\frac{2\pi}{\omega}\right)^{d/2} \mathrm{det}_+^{-1/2}(-\mathcal{A}) \left(\sum_{j\geq 0} (\frac{2i}{\omega})^{-j} j!^{-1}(\langle\mathcal{A}^{-1}D_x, D_x\rangle^j f\right)(0) \tag{310}$$

where $\mathrm{det}_+^{-1/2}$ *is defined by continuity of* argdet *on the Siegel space* Σ_n^+.

The following result is a consequence of the previous one (see [**7**] for a proof).

***Theorem D.2* (Non-degenerate critica manifold)**. — *Let $\Omega \subset \mathbb{R}^d$ be an open set, and let $a, f \in C^\infty(\Omega)$ with $\Im f \geq 0$ in Ω and* $\operatorname{supp} a \subset \Omega$. *We define*

$$M = \{x \in \Omega, \Im f(x) = 0, f'(x) = 0\},$$

and assume that M is a smooth, compact and connected submanifold of $\mathbb{R}^d$ of dimension k such that for all $x \in M$ the Hessian, $\partial_x^{(2)} f$, of f is non-degenerate on the normal space N_x to M at x.

Under the conditions above, the integral $J(\omega) = \int_{R^d} e^{i\omega f(x)} a(x)dx$ has the following asymptotic expansion as $\omega \to +\infty$, modulo $O(\omega^{-\infty})$,

$$J(\omega) \equiv \left(\frac{2\pi}{\omega}\right)^{\frac{d-k}{2}} \sum_{j\geq 0} c_j \omega^{-j}.$$

The coefficient c_0 is given by

$$c_0 = e^{i\omega f(m_0)} \int_M \left[\det\left(\frac{f''(m)|N_m}{i}\right)\right]_*^{-1/2} a(m) dV_M(m),$$

where $dV_M(m)$ is the canonical Euclidean volume in M, $m_0 \in M$ is arbitrary, and $[\det P]_*^{-1/2}$ denotes the product of the reciprocals of square roots of the eigenvalues of P chosen with positive real parts. Note that, since $\Im f \geq 0$, the eigenvalues of $\frac{f''(m)|N_m}{i}$ lie in the closed right half plane.

Appendix E
Almost analytic extensions

Let us prove proposition 4.10.

Proof. — For $|Y| \leq \theta\rho$ we have

$$\mathrm{e}^{-\nu|X|^{1/s}} |f_{R,\rho}^{aa}(X+iY)| \leq \sum_{|\gamma|\leq N_\rho} |\gamma|^{|\gamma|(s-1)} R^{|\gamma|+1} (\theta\rho)^{|\gamma|}.$$

Using definition of N_ρ, we see that the generic term in the sum is estimate above by $R\theta^{|\gamma|}$, which has a finite sum because $\theta \in]0,1[$.

To estimate $\partial_{\bar{Z}} f_{R,\rho}^{aa}(X+iY)$, it is enough to assume $m=1$. A direct computation gives

$$\partial_{\bar{Z}} f_{R,\rho}^{aa}(X+iY) = \frac{(iY)^N}{N!} \partial_X^N f(X).$$

So we have, for $|Y| \leq \theta\rho$,

$$\mathrm{e}^{-\nu|X|^{1/s}} \left|\partial_{\bar{Z}} f_{R,\rho}^{aa}(X+iY)\right| \leq CR(\theta\rho R)^{N_\rho} N_\rho^{(s-1)N_\rho} \leq CR\mathrm{e}^{N_\rho \log\theta}.$$

Therefore, using definition of N_ρ and $\theta \in]0,1[$, we get estimate (166). □

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D. Robert, Laboratoire Jean Leray, CNRS-UMR 6629, Université de Nantes, 2 rue de la Houssinière,, F-44322 NANTES Cedex 03, France • *E-mail :* `Didier.Robert@univ-nantes.fr`