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Semi-Classical Approximation in Quantum Mechanics. A survey of old and recent Mathematical results

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Introduction

Non-relativistic quantum mechanics was founded on the correspondence principle of Bohr : "When the Planck constant $\hbar$ can be considered small with respect to the other parameters such as masses and distances, quantum theory approaches classical Newton theory".

Making the Planck constant small in equations of quantum mechanics is a rather singular limit and then many difficult mathematical problems occur. Until the years 1960/70 the mathematical tools used came essentially from perturbation theory (like for example in the book of Kato [92]). In the seventies, Maslov and Hörmander introduced a new efficient tool which is now known as microlocal analysis and which contains in particular an accurate calculus for classes of operators defined by Fourier integrals which is suitable for constructing approximations for quantum propagators.

The goal of this report is to show how some mathematical problems arising in semi-classical approximation have been solved using ideas coming from microlocal analysis, i.e Fourier analysis in the phase space of the classical mechanics.

Let us say that all the Hamiltonians considered here are smooth. In particular Coulomb potentials are not considered. Singular potentials need a separate study (see for example [88]).

In this survey the following topics will be considered.

1. Propagation of quantum and classical observables. How can the classical evolution be recovered from the quantum evolution?

2. Time dependent WKB approximations.

3. Trace formulas and eigenvalue asymptotics.

4. Quantum signature of classical chaos.

5. Scattering states, limiting absorption principle, asymptotics for the spectral shift function (scattering phase).

6. Propagation of coherent states or wave packets.

The parts 1 and 2 introduce the main technical mathematical tools used in the paper. In the other parts we present more advanced results obtained during the last fifteen years on the subject. The title of this survey is quite general. The topics we have selected here reflect only the knowledge, the ability and the taste of the author.

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Main Notations used in the paper

- $X = \mathbb{R}^n$ with its natural Euclidean structure. For $x \in X$, $x = (x_1, \cdots, x_n)$, $|x| = (x_1^2 + \cdots + x_n^2)^{\frac{1}{2}}$ and $\langle x \rangle = (1 + |x|^2)^{1/2}$
- X^* is the dual space of X, $Z = X \times X^*$ is the phase space, the natural duality between X^* and X is denoted by $< x, \xi >$, $x \in X$, $\xi \in X^*$.
- $\mathcal{S}(X)$ is the Schwartz space of smooth, rapidely decreasing complex valued functions on X.
- $\mathcal{S}'(X)$ is the Schwartz space of tempered distributions on X.
- $\mathcal{L}(E, F)$ is the linear space of linear continuous maps from E to F where E, F are topological linear spaces.
- If $E = F$ is a Hilbert space, the norm on E and the operator norm on$\mathcal{L}(E, E)$ are both denoted by $\|\cdot\|$, when it is not confusing.
  If T is a linear operator in E, T^* denotes the adjoint of T.
- For $z \in \mathbb{C}$, $\Re z$ is its real part, $\Im z$ its imaginary part, $|z|$ its modulus, $\bar{z}$ the conjugate of z.
  For $x \in \mathbb{R}$, $x_+ = \max(x, 0)$, $x_- = \max(-x, 0)$.
- If $u(\hbar)$ is a complex valued function of $\hbar \in]0, 1]$, and $\{u_j\}$ a sequence of complex numbers,
  $$u(\hbar) \asymp \sum_{j \geq 0} u_j \hbar^j$$
  will denote an asymptotic expansion in the sense of Poincaré : $\forall N \in \mathbb{N}$, $\exists C_N$ such that
  $$|u(\hbar) - \sum_{j=0}^{j=N} u_j \hbar^n| \leq C_N \hbar^{N+1}, \quad \forall \hbar \in]0, 1].$$
- ∇ is the gradient operator on X, $D_x = i^{-1}\nabla$.
  The following notations are also used:
  $\nabla := \partial_x := \frac{\partial}{\partial x}$, $\partial_x^\alpha = \partial_{x_1}^{\alpha_1} \cdots \partial_{x_n}^{\alpha_n}$, $D_x^\alpha = i^{-|\alpha|}\partial_x^\alpha$ where
  $|\alpha| = \alpha_1 + \cdots + \alpha_n$.
- $\triangle$ is the Laplace operator on X, $\triangle = \sum \frac{\partial^2}{\partial {x_j}^2}$.
- H denotes a generic *classical Hamiltonian* and $\hat{H}$ denotes a *quantization* of H.
- If F is a finite set, $\#F$ is the number of elements in F.

1 Propagation of Observables

1.1 Hamiltonian classical mechanics

Let us begin with a quick review of classical mechanics to introduce our notation. (For more details see Abraham-Marsden [1] or Arnold [9]). Let us start with some well known facts in classical mechanics. Let us denote by $X = \mathbb{R}^n$ the configuration space of a classical mechanical system with n degrees of freedom. The corresponding phase space is $Z = X \times X^*$ which is a symplectic linear space equipped with the symplectic form defined as

$$\sigma(x, \xi; y, \eta) = \langle \xi, y \rangle - \langle \eta, x \rangle, \quad x, y \in X, \ \xi, \eta \in X^*.$$

A classical Hamiltonian is a smooth real function $H \ : X \times X^* \mapsto \mathbb{R}$. The basic example is $H(x, \xi) = \frac{|\xi|^2}{2m} + V(x)$ $(m > 0)$.
The motion of the system is determined by the system of Hamilton's equations

$$\begin{aligned} \frac{dx}{dt} &= \frac{\partial H}{\partial \xi}(x, \xi) \\ \frac{d\xi}{dt} &= -\frac{\partial H}{\partial x}(x, \xi). \end{aligned} \tag{1.1}$$

The equations (1.1) generate a flow Φ_H^t on the phase space Z, defined by $\Phi_H^t(x(0), \xi(0)) = (x(t), \xi(t))$; $\Phi_H^0 = 1\!\!1$. Φ_H^t exists locally by the Cauchy-Lipchitz theorem for O.D.E. But we need more assumptions on H to define Φ_H^t globally on Z. Moreover, Φ_H^t, when it exists, is a symplectic diffeomorphism (canonical transformation) group of transformations on Z, i.e it leaves σ invariant and satisfies $\Phi_H^{t+s} = \Phi_H^t \cdot \Phi_H^s$.
Some elementary examples :
1) $H(x, \xi) = \frac{|\xi|^2}{2m}$, $\Phi_H^t(x, \xi) = (x + t\frac{\xi}{m}, \xi)$, the flow is free motion along straight lines.
2) $H(x, \xi) = \frac{|\xi|^2}{2m} + \frac{|x|^2}{2}$, $\Phi_H^t(x, \xi) = (x(t), \xi(t))$, with,

$$x(t) = x\cos(\frac{t}{\sqrt{m}}) + \frac{\xi}{\sqrt{m}}\sin(\frac{t}{\sqrt{m}}), \tag{1.2}$$

$$\xi(t) = -\sqrt{m}x\sin(\frac{t}{\sqrt{m}}) + \xi\cos(\frac{t}{\sqrt{m}}). \tag{1.3}$$

So we see that Φ_H^t is a periodic motion along ellipses in phase space.
The main general properties satisfied by Φ_H^t are volume conservation and energy conservation. That means that the Lebesgue measure on Z is preserved by Φ_H^t and the level sets $\Sigma_E = H^{-1}(E) = \{z \in Z, \ H(z) = E\}$ are invariant under Φ_H^t. Furthermore, if E is not a critical value for H (i.e $\nabla H(z) \neq 0$ for $z \in \Sigma_E$), we can define the Liouville measure on Σ_E by $dL_E = \frac{d\Sigma_E}{|\nabla H|}$ which is invariant under Φ^t ($d\Sigma_E$ is the natural Euclidean measure on Σ_E).
Let us recall here a proof of this last property which will be used later.
Let f be a smooth, compactly support function on Z such that for $z \in \mathrm{supp}(f)$ we have $\nabla H(z) \neq 0$. Then we have the following formula :

$$\int_Z f(z)dz = \int_{\mathbb{R}} \left(\int_{\Sigma_E} f(z) dL_E(z) \right) dE. \tag{1.4}$$

We can deduce, for each fixed E_0, the following identity

$$\frac{d}{dE}\int_{E_0\le H(z)\le E} f(z)dz = \int_{\Sigma_E} f(z)dL_E(z). \tag{1.5}$$

So the volume invariance of Φ^t_H in Z implies the invariance of the Liouville measure on Σ_E. A particular and interesting case appears when Σ_E is a compact subset of phase space. With this property, the Hamiltonian flow is well defined, at every time $t \in \mathbb{R}$, on Σ_E. Moreover the Liouville measure can be normalized as a probability measure ν_E on Σ_E, $dL_E = \gamma_E d\nu_E$, where $\gamma_E = L_E(\Sigma_E)$.

A *classical observable* A is a complex valued function (or a Schwartz distribution) defined on phase space Z (Examples: coordinates of position x_j, coordinates of momentum ξ_j, kinetic energy, etc...).
The time evolution of a C^1-smooth, time independent observable can be easily computed

$$\frac{d}{dt}A(\Phi^t(z)) = \{H, A\}(\Phi^t(z)), \tag{1.6}$$

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

$$\{H, A\} = \frac{\partial H}{\partial x}\cdot\frac{\partial A}{\partial \xi} - \frac{\partial H}{\partial \xi}\cdot\frac{\partial A}{\partial x}. \tag{1.7}$$

Remark 1.1 *1) (1.6) is equivalent to (1.1).*
2) The Poisson bracket is preserved by Φ^t_H.
3) A is constant along a trajectory of the motion of the Hamiltonian H if and only if the Poisson bracket $\{H, A\}$ vanishes along this trajectory.

1.2 Quantum evolutions

Let us start with the usual Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V\psi, \tag{1.8}$$

where $\Delta = \sum_{1\le j\le n}\frac{\partial^2}{\partial x_j}$, $x = (x_1, \cdots, x_n)$, are coordinates for x and V is a real function (potential energy) defined on the configuration space X.
Under mild conditions on V, the Schödinger equation has a unique solution $\psi(t, x)$ with $\psi(t, .) \in L^2(X)$ where $\psi(0, x) = \psi_0(x)$ is the given initial data. For example, if V is bounded below and $V \in L^2_{loc}(X)$ then $\hat{H}$ is essentially self-adjoint (i.e there exists a unique self adjoint extension of $\hat{H}$ as a unbounded operator in $L^2(X)$ starting from the space of smooth, compact support functions, see [93]). The quantum evolution is driven by the unitary group $U_H(t) = \mathrm{e}^{-\frac{it}{\hbar}\hat{H}}$, defined by the functional calculus [121].
Now let us introduce a quantum observable $\hat{A}$, i.e a self-adjoint operator in $L^2(X)$. The

time evolution is given by $\hat{A}(t) = U_H(-t)\hat{A}U_H(t)$ and satisfies the Heisenberg-von Neumann equation

$$\frac{d\hat{A}(t)}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}], \tag{1.9}$$

where $[\hat{H}, \hat{A}]$ is the commutator $\hat{H}\hat{A} - \hat{A}\hat{H}$. For the moment, we will not be careful about the domain of definition of these operators.
Because we are concerned here with the correspondance between classical mechanics and quantum mechanics, we shall consider quantum observables with a classical analogue, in a suitable sense. So we have to define a correspondence between quantum and classical observables $A \leftrightarrow \hat{A}$ according to the Bohr prescription :
(i) $A \leftrightarrow \hat{A}$ is *linear*
(ii) *position observables* : $x_j \leftrightarrow \hat{x}_j$: multiplication operator by x_j
(iii) *moment observables* : $\xi_j \leftrightarrow \hat{\xi}_j$: differential operator $\frac{\hbar}{i}\frac{\partial}{\partial x_j}$.
Let us remark that if the observables A, B depend only on the position variable (or on the moment variables) then $\hat{A}\cdot\hat{B} = \widehat{A.B}$ but, this is no longer true for a mixed observable. This is related to the non-commutativity for product of the quantum observables and the Heisenberg identity. More explicitly we have $[\hat{x}_j, \hat{\xi}_j] = i\hbar$ so, the quantum observable corresponding to $x_1\xi_1$ is not determined by the rules (i), (ii), (iii).
We do not want to discuss here the quantization problem in its full generality (see for example [55]). One way to choose a reasonable and convenient quantization procedure is the following, which is called the Weyl quantization (see [84]). Let L_ζ be a real linear form on the phase space Z, where $\zeta = (\alpha, \beta)$, $L_\zeta(z) = \langle \zeta, z\rangle$, $\alpha \in X^*$, $\beta \in X$. $\widehat{L_\zeta}$ is a well defined quantum Hamiltonian (i.e a essentially self adjoint operator in $L^2(X)$). Its propagator $W_\zeta(t) = \mathrm{e}^{\frac{-it}{\hbar}\widehat{L_\zeta}}$ can be easily computed; for $\psi \in \mathcal{S}(X)$, we have explicitly

$$W_\zeta(t)\psi(x) = \mathrm{e}^{\frac{i}{\hbar}\alpha(tx+t^2\beta/2)}\psi(x + t\beta). \tag{1.10}$$

So, the Weyl prescription is defined by the conditions (i), (ii), (iii) and
(iv) $\mathrm{e}^{itL_\zeta} \leftrightarrow W_\zeta(t)$.
Let us consider a classical observable $A \in \mathcal{S}(Z)$. The inverse Fourier formula, where $\tilde{A}$ denotes the Fourier transform of A in variable $z \in Z$, gives

$$A(z) = (2\pi)^{-2n} \int_Z \tilde{A}(\zeta)\mathrm{e}^{i\langle\zeta,z\rangle}d\zeta.$$

$\hat{A}$ is clearly uniquely defined by the rules (i) to (iv). More explicitly, for $\psi \in \mathcal{S}(X)$, we have

$$\hat{A}\psi = (2\pi)^{-2n} \int_Z \tilde{A}(\zeta)W_\zeta(1)\psi d\zeta \tag{1.11}$$

and with more computations, we get the usual formula

$$\hat{A}\psi(x) = (2\pi\hbar)^{-n} \int\int A\left(\frac{x+y}{2}, \xi\right) \mathrm{e}^{i\hbar^{-1}\langle x-y,\xi\rangle}\psi(y)dyd\xi. \tag{1.12}$$

Sometimes, we shall use also the notation $\hat{A} = Op_\hbar^w A$ ($\hbar$-Weyl quantization).

Let us introduce now a suitable set of classical observables for which the $\hbar$-Weyl quantization will have nice properties.

Definition 1.2 *$A \in \mathcal{O}(m)$, $m \in \mathbb{R}$, if and only if $Z \xrightarrow{A} \mathbb{C}$ is C^∞ in Z and for every multiindex γ there exists $C > 0$ such that*

$$|\frac{\partial^\gamma}{\partial z^\gamma} A(z)| \leq C\langle z\rangle^m, \ \forall z \in Z.$$

Let us denote $\mathcal{O}(+\infty) = \cup_m \mathcal{O}(m)$. We have obviously $\cap_m \mathcal{O}(m) = \mathcal{S}(Z)$.

For every $A \in \mathcal{O}(m)$ we have the following elementary properties:

1. $\hat{A}$ is a linear continuous mapping on $\mathcal{S}(X)$.
2. $\hat{A}^\star = \widehat{\bar{A}}$ and $\hat{A}$ is a linear continuous mapping on $\mathcal{S}'(X)$.

We have an operational calculus defined by :

The product rule for quantum observables

Let $A, B \in \mathcal{S}(Z)$. We look for a classical observable C such that $\hat{A} \cdot \hat{B} = \hat{C}$. Some computations with the Fourier transform give the following formula

$$C(x,\xi) = \exp(\frac{i\hbar}{2}\sigma(D_x, D_\xi; D_y, D_\eta))a_1(x,\xi)a_2(y,\eta)|_{(x,\xi)=(y,\eta)}, \tag{1.13}$$

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

$$C(x,\xi) = \sum_{j\geq 0} \frac{1}{j!}(\frac{i}{2}\sigma(D_x, D_\xi; D_y, D_\eta))^j a_1(x,\xi)a_2(y,\eta)|_{(x,\xi)=(y,\eta)}\hbar^j. \tag{1.14}$$

We can easily see that in general C 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.

Definition 1.3 *We say that A is a semi-classical observable of weight m if it exists $\hbar_0 > 0$ and a sequence $A_j \in \mathcal{O}(m)$, $j \in \mathbb{N}$, so that A is a map from $]0, \hbar_0]$ into $\mathcal{O}(m)$ satisfying the following asymptotic condition : for every $N \in \mathbb{N}$ and every $\gamma \in \mathbb{N}^{2n}$ there exists $C_N > 0$ such that for all $\hbar \in]0,1[$ we have*

$$\sup_Z \langle z\rangle^{-m} \left| \frac{\partial^\gamma}{\partial z^\gamma}\left(A(\hbar, z) - \sum_{0\leq j\leq N} \hbar^j A_j(z)\right)\right| \leq C_N \hbar^{N+1}, \tag{1.15}$$

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

Now we state the product rule

Theorem 1.4 *For every $A \in \mathcal{O}(m)$ and $B \in \mathcal{O}(p)$, there exists a unique $C \in \mathcal{O}_{sc}(m+p)$ such that $\hat{A} \cdot \hat{B} = \hat{C}$ with $C \asymp \sum_{j \geq 0} \hbar^j C_j$. The C_j are given by*

$$C_j(x,\xi) = \frac{1}{2^j} \sum_{|\alpha+\beta|=j} \frac{(-1)^{|\beta|}}{\alpha!\beta!} (D_x^\beta \partial_\xi^\alpha A).(D_x^\alpha \partial_\xi^\beta B)(x,\xi).$$

Corollary 1.5 *Under the assumption of the theorem, we have the well known correspondence between the commutator for quantum observables and the Poisson bracket for classical observables, $\frac{i}{\hbar}[\hat{A}, \hat{B}] \in \hat{\mathcal{O}}_{sc}(m+p)$ and its principal symbol is the Poisson bracket $\{A, B\}$.*

Let us recall also some other useful properties concerning Weyl quantization. Detailed proofs can be found in [84] and [122].

- if $A \in \mathcal{O}(0)$ then $\hat{A}$ is bounded in $L^2(X)$ (Calderon-Vaillancourt theorem).
- if $A \in L^2(Z)$ then $\hat{A}$ is an Hilbert-Schmidt operator in $L^2(X)$ and its Hilbert-Schmidt norm is
$$\|\hat{A}\|_{HS} = (2\pi\hbar)^{-n/2} \left(\int_Z |A(z)|^2 dz \right)^{1/2}.$$
- if $A \in \mathcal{O}(m)$ with $m < -2n$ then $\hat{A}$ is a trace-class operator. Moreover we have
$$\mathrm{tr}(\hat{A}) = (2\pi\hbar)^{-n} \int_Z A(z) dz. \tag{1.16}$$
- $A, B \in L^2(Z)$ then $\hat{A} \cdot \hat{B}$ is a trace class operator in $L^2(X)$ and
$$\mathrm{tr}(\hat{A} \cdot \hat{B}) = (2\pi\hbar)^{-n} \int_Z A(z)B(z) dz.$$

Now, we come to the main result of this section which gives a proof of the correspondence between quantum and classical dynamics. As we shall see this theorem is a useful tool for semi-classical analysis although its proof is an easy application of Weyl calculus rules recalled above. The microlocal version of the following result is due to Egorov [49]. R. Beals [17] found a nice simple proof.

Theorem 1.6 (the Semiclassical Propagation Theorem) *Let us consider a Hamiltonian $H \in \mathcal{O}_{sc}(2)$ satisfying :*

$$|\partial_z^\gamma H_j(z)| \leq C_\gamma, \text{ for } |\gamma| + j \geq 2; \tag{1.17}$$
$$\hbar^{-2}(H - H_0 - \hbar H_1) \in \mathcal{O}_{sc}(0). \tag{1.18}$$

Let us introduce an observable $A \in \mathcal{O}(m)$, $m \in \mathbb{R}$. Then we have :
(a) For $\hbar$ small enough, $\hat{H}$ is essentially self-adjoint in $L^2(X)$, with core $\mathcal{S}(X)$, hence the

quantum evolution $U_H(t) = \exp(-\frac{it}{\hbar}\hat{H})$ *is well defined for all* $t \in \mathbb{R}$.
(b) For each $t \in \mathbb{R}$, $\hat{A}(t) = U_H(-t)\hat{A}U_H(t) \in \hat{\mathcal{O}}_{sc}(m)$. *Its symbol has an asymptotic expansion,* $A(t) \asymp \sum_{j\geq 0} \hbar^j A_j(t)$, *in* $\mathcal{O}_{sc}(m)$, *which is uniform in* t, *for* t *bounded. Moreover* $A_j(t)$ *can be computed by the following formulas*

$$A_0(t,z) = A(\Phi^t(z)), \tag{1.19}$$

$$A_1(t,z) = \int_0^t \{A(\Phi^\tau), H_1\}\Phi^{t-\tau}(z)d\tau \tag{1.20}$$

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

$$A_j(t,z) = \sum_{\substack{|(\alpha,\beta)|+k=j+1\\ 0\leq \ell\leq j-1}} \Gamma(\alpha,\beta)\int_0^t [(\partial_\xi^\alpha \partial_x^\beta H_k)(\partial_\xi{}^\alpha \partial_x{}^\beta A_\ell)(\Phi^\tau)](\Phi^{t-\tau}(z))d\tau, \tag{1.21}$$

with

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

Sketch of proof
We admit here that $\hat{H}$ is essentially self-adjoint (for a proof see [122]).
Let us remark that, under the assumption of the theorem, the classical flow for H_0 exists globally. Indeed, the Hamiltonian vector field $(\partial_\xi H_0, -\partial_x H_0)$ has a sublinear growing at infinity so, no classical trajectory can blow up in a finite time. Moreover, using usual methods in non linear O.D.E (variation equation) we can prove that $A(\Phi^t) \in \mathcal{O}(m)$ with semi-norm uniformly bounded for t bounded.
Now, from the Heisenberg equation and the classical equations of motion we get

$$\frac{d}{ds} U_H(-s)\widehat{A_0}(t-s)U_H(s) = \tag{1.22}$$
$$U_H(-s)\left\{\frac{i}{\hbar}[\hat{H}, \widehat{A_0}(t-s)] - \{\widehat{H, A_0}\}(\Phi^{t-s})\right\} U_H(s),$$

where $A_0(t) = A(\Phi^t)$. But, from the corollary of the product rule, the principal symbol of $\frac{i}{\hbar}[\hat{H}, \widehat{A_0}(t-s)] - \{\widehat{H, A_0}\}(\Phi^{t-s})$ vanishes. So, at the first stage, using the product rule formula, we get the approximation

$$U_H(-t)\hat{A}U_H(t) - \widehat{A_0}(t) = \tag{1.23}$$
$$\int_0^t U_H(-s)\left(\frac{i}{\hbar}[\hat{H}, \widehat{A_0}(t-s)] - \{\widehat{H, A_0}\}\Phi^{t-s}\right) U_H(s)ds.$$

Now, it is not difficult to obtain, by induction, the full asymptotics in $\hbar$. ∎

Remark 1.7 *If* $H = H_0$ *is a polynomial function of degree* ≤ 2 *on the phase space* Z *then the propagation theorem assumes a simpler form :* $A(t) = A(\Phi^t_H)$ *and the remainder term is null. This comes from the following exact formula, for all* $B \in \mathcal{O}(+\infty)$*:*

$$\frac{i}{\hbar}[\hat{H}, \hat{B}] = \{\widehat{H, B}\}. \tag{1.24}$$

In particular for $H = L_\zeta$ we have

$$W(\zeta)\hat{B}W(-\zeta) = \widehat{B}_\zeta, \text{ where } B_\zeta(z) = B(z-\zeta). \tag{1.25}$$

As a first application of the propagation theorem we show how to recover the classical evolution from the quantum evolution, in the classical limit $\hbar \searrow 0$. Let us introduce the standard Gaussian function $\psi_0(x) = (\pi\hbar)^{-n/4}\exp\left(-\frac{|x|^2}{2\hbar}\right)$, and the Gaussian $\varphi_\zeta = W(-\zeta)\psi_0$, peaked at the point ζ of phase space.

Corollary 1.8 *For every observable $A \in \mathcal{O}(m)$ we have*

$$\lim_{\hbar\searrow 0}\langle \hat{A}U_H(t)\varphi_\zeta, U_H(t)\varphi_\zeta\rangle = A(\Phi_H^t(\zeta)) \tag{1.26}$$

and the limit is uniform in time t on every bounded set.

Proof
Let us introduce the orthogonal projector, Π_{ψ_0}, on ψ_0 and its classical analogue π_{ψ_0} such that $\widehat{\pi_{\psi_0}} = \Pi_{\psi_0}$ (i.e π_{ψ_0} is the Wigner transform of ψ_0). A direct computation gives

$$\pi_{\psi_0}(z) = 2^n\mathrm{e}^{-\frac{|z|^2}{\hbar}}.$$

Now for every $B \in \mathcal{O}(m)$ we have

$$\langle \hat{B}\psi_0, \psi_0\rangle = \mathrm{tr}(\hat{B}\Pi_{\psi_0}) \tag{1.27}$$

$$= (\pi\hbar)^{-n}\int_Z B(z)\exp(-\left(\frac{|z|^2}{\hbar}\right))dz. \tag{1.28}$$

But we have

$$\langle \hat{A}U_H(t)\varphi_\zeta, U_H(t)\varphi_\zeta\rangle = \mathrm{tr}[W(\zeta)U_H(-t)AU_H(t)W(-\zeta)\Pi_{\psi_0}].$$

So by the propagation theorem we easily get

$$\lim_{\hbar\searrow 0}\langle \hat{A}U_H(t)\varphi_\zeta, U_H(t)\varphi_\zeta\rangle = \lim_{\hbar\searrow 0}(\pi\hbar)^{-n}\int_Z A(\Phi^t(z+\zeta))\mathrm{e}^{-\frac{|z|^2}{\hbar}}dz \tag{1.29}$$

$$= A(\Phi^t(\zeta)). \tag{1.30}$$

∎

Remark 1.9 *The last result has a long history beginning with Ehrenfest (1930) and continuing with Hepp (1974), Robert [122], Wang [139]. In particular Wang proved that it can be extended to time-dependent Hamiltonians and unbounded observables.*
Corollary (1.8) still holds for more general Hamiltonians, but the proof requires more refined localization in the phase space (see below).

Now let us give a geometrical interpretation of the above results by introducing the notions of essential support and frequency set. These notions are the analogue for the semi-classical approximation of the wave front sets in optics and micro-local analysis [84].
Let us begin with the following definitions.

Definition 1.10 (A. Voros[138]) *Let us consider a map :* $]0,\hbar_0[\stackrel{A}{\to}\mathcal{S}'(Z)$.

1. *A is said to be negligible (semiclassically negligible) in an open subset $\mathcal{V}$ of Z if for all $B\in C_0^\infty(\mathcal{V})$ we have*
$$\langle A(\hbar),B\rangle = O(\hbar^\infty).$$
2. *The essential support of A, denoted by $ES[A]$, is the closed subset of Z defined by :* $ES[A]$ is the complement of the greatest negligible open set of Z for A.
3. *If $\hat{A}$ is a map from $]0,\hbar_0[$ into $\mathcal{L}(\mathcal{S}(X),\mathcal{S}'(X))$ we call the essential support of $\hat{A}$ the set $ES[A]$ where A is the Weyl symbol of $\hat{A}$ ($A\in\mathcal{S}'(Z)$). We shall use the notation $ES[A]=ES[\hat{A}]$.*

Remark 1.11 *The Weyl quantization can be extented so that to every $A\in\mathcal{S}'(Z)$ we can associate $\hat{A}\in\mathcal{L}(\mathcal{S}(X),\mathcal{S}'(X))$ and the correspondence is bijective. This is the Weyl analogue of the Schwartz kernel theorem (for a proof see[122]). A natural formula , extending the trace duality, is the following. For $u,v\in\mathcal{S}(X)$ let us denote by $\pi_{u,v}$ the Weyl symbol of the rank one operator : $\psi\mapsto\langle\psi,u\rangle v$,*

$$\langle\hat{A}u,v\rangle = (2\pi\hbar)^{-n}\langle A,\pi_{u,v}\rangle, \tag{1.31}$$

$\pi_{u,v}$ is called the Wigner function of (u,v).

A related notion is the following

Definition 1.12 (Guillemin-Sternberg [62]) *Let Ω be an open subset of X and consider a map $]0,\hbar_0]\stackrel{T}{\to}\mathcal{D}'(\Omega)$. The frequency set of T, denoted by $\mathrm{FS}[T]$, is defined as a subset of the phase space Z, by its complement, as follows :*
we say that $z_0=(x_0,\xi_0)\notin\mathrm{FS}[T]$ if there exists a neighborhood $U\times V$ of (x_0,ξ_0) in $X\times X^*$ such that for every $\psi\in C_0^\infty(U)$ and every $\xi\in V$ we have

$$\langle\psi(x)\exp(-i\hbar^{-1}\langle x,\xi\rangle),T_x(\hbar)\rangle = O(\hbar^\infty), \tag{1.32}$$

uniformly in $\xi\in V$. $T_x(\hbar)$ means that the distribution $T(\hbar)$ acts in the x- variable.

$\mathrm{FS}[T]$ is clearly a closed subset of the phase space Z. The proofs of the following results can be found in [122]. Let us consider a $\hbar$ dependent state $\psi(\hbar)$ for $\hbar\in]0,\hbar_0[$, satisfying the condition

(f) there exists $M,\ell\in\mathbb{N}, C>0$ such that $\|(-\hbar^2\Delta+|x|^2)^{-M}\psi(\hbar)\|\le C\hbar^{-\ell}$.

Let us denote by $\overline{\psi(\hbar)}\otimes\psi(\hbar)$ the operator $u\mapsto\langle u,\overline{\psi(\hbar)}\rangle\psi(\hbar)$.

Proposition 1.13 *Under the condition* (f) *we have*

$$\mathrm{ES}[\overline{\psi(\hbar)} \otimes \psi(\hbar)] = \mathrm{FS}[\psi].$$

Moreover the following conditions are equivalent

1. $z_0 = (x_0, \xi_0) \notin \mathrm{FS}[\psi]$.

2. *There exists an open neighborhood* w *of* z_0 *such that*

$$\forall A \in C_0^\infty(\omega), \ \ \langle \hat{A}\psi(\hbar), \overline{\psi(\hbar)}\rangle = O(\hbar^\infty).$$

3. *There exists some* $\hat{A} \in \hat{O}_{sc}(m)$ *such that* $A(z_0) \neq 0$ *(* A_0 *is the principal symbol of* A*) and* $\|\hat{A}\psi(\hbar)\| = O(\hbar^\infty)$.

Example 1.14 1. $\mathrm{FS}[\varphi_\zeta] = \{\zeta\}$.

2. *Let us us consider a WKB state :* $\psi(\hbar) = a(x)\exp(i\hbar^{-1}S(x))$ *where* a *is a smooth complex valued function and* S *is a smooth real valued function. The non stationary phase theorem [121] easily gives*

$$\mathrm{FS}[\psi] \subseteq \{(x,\xi), \ x \in \mathrm{supp}(a), \ \xi = \nabla S(x)\}.$$

Now we come to the following geometrical interpretation of the propagation theorem

Proposition 1.15 *Let us consider the Schrödinger equation*

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi, \qquad \psi(0) = \psi_0, \tag{1.33}$$

where $\|\psi_0\| = 1$ *and* H *satisfies the assumption of the propagation theorem. Then we have :* $\mathrm{FS}[\psi(t)] = \Phi^t_{H_0}(\mathrm{FS}[\psi_0])$, $\forall t \in \mathbb{R}$.

Proof
If $z_0 \notin \Phi^t_{H_0}(\mathrm{FS}[\psi_0])$ then there exists $B_{-t} \in C_0^\infty(Z)$ such that $\hat{B}_{-t}(\Phi^t_{H_0}(z_0)) \neq 0$ and $\|\widehat{B_{-t}L}\psi_0\| = O(\hbar^\infty)$. Now let us consider $\hat{B} = U_H(t)\hat{B}_{-t}U_H(-t)$. Then we have $B_0(z_0) \neq 0$ and $\|\hat{B}\psi(t)\| = O(\hbar^\infty)$ so $z_0 \notin \mathrm{FS}[\psi(t)]$. Using that $\Phi^t_{H_0}$ is a diffeomorphism we get the result. ∎

Remark 1.16 For an extension of the notion of the frequency set, taking into account growth in the momentum variable (like in microlocal analysis), see Colin-Parisse [35].

2 Time Dependent W.K.B Approximations

The starting point of the Wentsel-Kramers-Brillouin approximation for an $\hbar$-dependent quantum state, $\psi(\hbar) \in \mathcal{S}'(X)$, is the following ansatz

$$\psi_\hbar(x) = \int_\Theta e^{i\hbar^{-1}\phi(x,\theta)} A(\hbar, x, \theta) d\theta. \tag{2.1}$$

where $\Theta = \mathbb{R}^N$ is some Euclidean space ("frequency variables set"), ϕ is a real phase, and A a complex amplitude which satisfies $A(\hbar, x, \theta) \asymp \sum_{j\geq 0} \hbar^j A_j(x, \theta)$ in a suitable sense to be defined. In particular $\psi(\hbar)$ can also be the Schwartz kernel of some quantum observable, by replacing the representation space X by $X \times X$.
The main application we have in mind is to the propagator of the time dependent Schrödinger operator $K(\hbar, t, x, y)$ which is the Schwartz kernel of the unitary operator $U_H(t)$ introduced in section 1. So $K(\hbar)$ satisfies

$$i\hbar\frac{\partial}{\partial t} K(\hbar, t, \cdot, y) = \hat{H} K(\hbar, t, \cdot, y), \tag{2.2}$$

$$K(\hbar, 0, x, y) = \delta(x - y). \tag{2.3}$$

The ansatz is to write

$$K(\hbar, t, x, y) = \int_\Theta e^{i\hbar^{-1}\phi(t,x,\theta,y)} A(\hbar, x, \theta, y) d\theta. \tag{2.4}$$

To give a rigorous meaning to (2.1) and (2.4) we review now some facts on classes of Fourier integrals.

2.1 Fourier Integrals

We shall assume that the phase ϕ satisfies the following conditions,

$$\phi \in C^\infty(X \times \Theta, \mathbb{R}), \text{and } \forall\gamma \in \mathbb{N}^{N+n}, \exists C > 0, \text{such that} \quad |\partial^\gamma_{x,\theta}\phi(x, \theta)| \leq C\langle(x, \theta)\rangle^{(2-|\gamma|)_+}, \tag{2.5}$$

$$\exists C > 0 \text{ such that } C^{-1}\langle(x, \theta)\rangle \leq \langle(\nabla_{x,\theta}\phi(x, \theta), x)\rangle \leq C\langle(x, \theta)\rangle \tag{2.6}$$

and that the amplitude A satisfies,

$$A(\hbar) \in C^\infty(X \times \Theta, \mathbb{C}), \text{and } \exists m \in \mathbb{R}, \forall\gamma \in \mathbb{N}^{N+n} \exists C > 0, \text{such that} \quad |\partial^\gamma_{x,\theta} A(\hbar, x, \theta)| \leq C\langle(x, \theta)\rangle^m. \tag{2.7}$$

We shall denote by $T(\phi, A, \hbar)$ the distribution defined by the r.h.s of (2.1), when it has a meaning. So we have, for $\varphi \in \mathcal{S}(X)$,

$$\langle T(\phi, A, \hbar), \varphi\rangle = \int_{\Theta\times X} e^{i\hbar^{-1}\phi(x,\theta)} A(\hbar, x, \theta)\varphi(x) d\theta dx. \tag{2.8}$$

Now we recall the principle of the *non stationary phase method* in order to give a rigorous meaning to the above Fourier integrals. Let us introduce $\chi \in C_0^\infty(\mathbb{R})$, $\chi(u) = 1$ for $u \in [-1, 1]$. To use assumption (2.7) we split the amplitude into two pieces,

$$A(\hbar, \theta, x) = A^{(0)}(\hbar, \theta, x) + A^{(1)}(\hbar, x, \theta), \quad \text{where} \tag{2.9}$$

$$A^{(0)}(\hbar, x, \theta) = \chi\left(\frac{\nabla_{x,\theta}\phi}{\epsilon\langle(x,\theta)\rangle}\right) A(\hbar, \theta, x). \tag{2.10}$$

To (2.9) corresponds the decomposition

$$T(\phi, A, \hbar) = T(\phi, A^{(0)}, \hbar) + T(\phi, A^{(1)}, \hbar).$$

By choosing $\epsilon > 0$ small enough (independently of $\hbar$) we can see that on the support of $A^{(0)}$ we have : $\langle\theta\rangle \leq C\langle x\rangle$. Consequently, $\langle T(\phi, A^{(0)}, \hbar), \varphi\rangle$ is well defined as an absolutely convergent integral. To define $T(\phi, A^{(1)}, \hbar)$ we use an integration by part procedure. On the support of $A^{(1)}$ we have $|\nabla_{x,\theta}\phi| \neq 0$. We introduce the differential operator in $X \times \Theta$

$$\Lambda = \frac{\nabla_{x,\theta}\phi \cdot \nabla_{x,\theta}}{i|\nabla_{x,\theta}\phi(x,\theta)|^2}, \tag{2.11}$$

which satisfies

$$\hbar\Lambda e^{i\hbar^{-1}\phi} = e^{i\hbar^{-1}\phi}. \tag{2.12}$$

By applying a large enough power of Λ, we get an absolutely convergent integral

$$\langle T(\phi, A^{(1)}, \hbar), \varphi\rangle = \hbar^k \int_{X\times\Theta} e^{i\hbar^{-1}\phi(x,\theta)}({}^t\Lambda)^k(A^{(1)}(\hbar, x, \theta)\varphi(x))dxd\theta, \tag{2.13}$$

where ${}^t\Lambda$ is the transpose of Λ. So we define a temperate distribution $T(\phi, A, \hbar)$ by putting

$$\langle T(\phi, A, \hbar), \varphi\rangle = \langle T(\phi, A^{(0)}, \hbar), \varphi\rangle + \langle T(\phi, A^{(1)}, \hbar), \varphi\rangle, \tag{2.14}$$

where the r.h.s is well defined by (2.9). This definition is independent of the procedure as we shall see now. Another logically independent way to define the Fourier integral $\langle T(\phi, A, \hbar), \varphi\rangle$ is to pass through the limit with a cutoff. Let us introduce some $F \in \mathcal{S}(X \times \Theta)$, $F(0) = 1$, and denote $A_\epsilon = F(\epsilon x, \epsilon\theta)A(x, \theta)$. Combining integration by parts and the dominated convergence theorem, we can prove the following proposition (see [74] for detailed estimates).

Proposition 2.1 *For every $\varphi \in \mathcal{S}(X)$,*

$$\lim_{\epsilon\searrow 0}\langle T(\phi, A_\epsilon, \hbar), \varphi\rangle = \langle T(\phi, A, \hbar), \varphi\rangle, \tag{2.15}$$

where $T(\phi, A, \hbar)$ is the tempered Schwartz distribution defined by (2.14).

Let us recall, as an elementary application of this proposition, the Fourier decomposition theorem $\delta(x - y) = (2\pi\hbar)^{-n}\int_X e^{i\hbar^{-1}\langle x-y,\eta\rangle}d\eta$.

We can now define a large class of Fourier integral operators. Let us introduce ϕ and A

defined in $X \times \Theta \times X$ where the above assumptions are satisfied by taking $\Theta \times X$ as a new frequency set. Furthermore we assume that ϕ satisfies

$$\exists C > 0 \text{ such that } C^{-1}\langle(x,\theta,y)\rangle \leq \langle(\nabla_{x,\theta}\phi(x,\theta),x)\rangle \leq C\langle(x,\theta)\rangle, \tag{2.16}$$

$$C^{-1}\langle(x,\theta,y)\rangle \leq \langle(\nabla_{\theta,y}\phi(\theta,y),y)\rangle \leq C\langle(x,\theta,y)\rangle. \tag{2.17}$$

Under assumptions (2.16), using the oscillating integral procedure, we define a continuous linear operator from $\mathcal{S}(X)$ into $\mathcal{S}'(X)$ by

$$\langle \mathcal{I}(\phi,A,\hbar)\varphi_1,\varphi_2\rangle = \int_{X\times\Theta\times X} \mathrm{e}^{i\hbar^{-1}\phi(x,\theta)} A(\hbar,x,\theta)\varphi_1(y)\varphi_2(x)d\theta dy dx. \tag{2.18}$$

The basic properties of this class of Fourier Integral Operators (FIO) are summed up in the following

Proposition 2.2 (see [74]) *1. $\mathcal{I}(\phi,A,\hbar)$ is a continuous linear operator in $\mathcal{S}(X)$ and we have the following properties*

2. *The adjoint operator $\mathcal{I}(\phi,A,\hbar)^*$ is in the same class, $\mathcal{I}(\phi,A,\hbar)^* = \mathcal{I}(\phi^*,A^*,\hbar)$, with $\phi^*(x,\theta,y) = -\phi(y,\theta,x)$, $A^*(x,\theta,y) = \bar{A}(y,\theta,x)$.*

3. *$\mathcal{I}(\phi,A,\hbar)$ is a linear continuous operator in $\mathcal{S}'(\mathcal{X})$.*

4. *The product of two FIO is a FIO. More precisely,*

$$\mathcal{I}(\phi_1,A_1,\hbar)\cdot\mathcal{I}(\phi_2,A_2,\hbar) = \mathcal{I}(\phi,A,\hbar), \tag{2.19}$$

where

$$\Theta = \Theta_1 \times X \times \Theta_2, \tag{2.20}$$

$$A(x,\theta,z) = A_1(x,\theta_1,y)A_2(y,\theta_2,z), \tag{2.21}$$

$$\phi(x,\theta,z) = \phi_1(x,\theta_1,y) + \phi_2(y,\theta_2,z), \tag{2.22}$$

with $\theta = (\theta_1,y,\theta_2)$. In particular $A \in \mathcal{O}_m(X\times\Theta\times X)$ where $m = m_1 + m_2$ and $A_i \in \mathcal{O}_m(X\times\Theta_i\times X)$.

Remark 2.3 *For applications it is often necessary to consider more restrictive classes of amplitudes.*

2.2 Semi-Classical Approximation of Quantum Propagators

To be specific let us start with the basic example of quantum Hamiltonians defined by

$$\hat{H}(V) = -\hbar^2\Delta + V, \tag{2.23}$$

where V is an electric potential which is assumed to be smooth and satisfy the following decay estimates,

$$\forall\alpha, \text{multiindex}, \exists C_\alpha \quad \text{such that} \quad \forall x \in \mathbb{R}^n,$$
$$|\partial_x^\alpha V(x)| \leq C_\alpha \langle x\rangle^{(2-|\alpha|)_+}. \tag{2.24}$$

More generally $\hat{H}$ can be choosen as in the propagation theorem. We shall see later that this growth condition can be overcome by using a suitable localization, In particular for application to bound state energies.
From the above considerations, we make the following ansatz for the kernel of the propagator of the Schrödinger Hamiltonian,

$$K(\hbar, t, x, y) = (2\pi\hbar)^{-n} \int_{X^*} e^{i\hbar^{-1}(S(t,x,\eta)-\langle y,\eta\rangle)} (\sum_{j\geq 0} \hbar^j A_j(t, x, \eta))d\eta, \tag{2.25}$$

with the following conditions at time $t = 0$,

$$S(0, x, \eta) = \langle x, \eta\rangle, \tag{2.26}$$
$$A_0(0, x, \eta) = 1, \tag{2.27}$$
$$A_j(0, x, \eta) = 0, \text{ for } j \geq 1. \tag{2.28}$$

Now by writing the equation

$$(i\hbar\frac{\partial}{\partial t} - \hat{H}K(\hbar, \cdot, y)) \equiv 0$$

and formally computing the $\hbar$-expansion, we get the following equations

$$\begin{aligned} \partial_t S(t, x, \eta) + H(x, \partial_x S(t, x, \eta)) &= 0, \\ S(0, x, \eta) &= \langle x, \eta\rangle, \end{aligned} \tag{2.29}$$

which is the Hamilton-Jacobi (or eikonal) equation, and the transport equations

$$\begin{aligned} i\partial_t A_0(t, x, \eta) &= \mathcal{L}(x, \eta, D_x)A_0(t, x, \eta), && (2.30) \\ A_0(0, x, \eta) &= 1, \\ i\partial_t A_j(t, x, \eta) &= \mathcal{L}(x, \eta, D_x)A_j(t, x, \eta) + F_j(A_0, \cdots, A_{j_1}), && (2.31) \\ A_j(0, x, \eta) &= 0, \ (j \geq 1), \end{aligned}$$

where

$$\mathcal{L}(x, \eta, D_x)B = \partial_\xi H \cdot D_x B + (2i)^{-1}[\mathrm{tr}(\partial^2_{\xi,\xi} H(x, \partial_x S) \cdot \partial^2_{x,x} + \partial^2_{x,p} H(x, \partial_x S)]B$$

and F_j is a polynomial expression in a finite number of derivatives of $A_0, \cdots, A_j$ with uniformly bounded coefficients.
Under our assumptions, the derivatives of order ≥ 2 of H are uniformly bounded, hence we can solve the equations (2.29) and (2.30) for $|t|$ small enough. So we have a sequence of approximations $U_{H,N}(t)$ for $U_H(t)$ which satisfy

Theorem 2.4 ([73]) *There exists $T > 0$ small enough such that*

1. *The Hamilton-Jacobi equation (2.29) has a unique solution $S(t,x,\eta)$. Moreover it is the generating function of the flow Φ_H^t i.e, we have*

$$\Phi_H^{-t}(x,\partial_x S(t,x,\eta)) = (\partial_\eta S(t,x,\eta),\eta))$$

and satisfies

$$|\partial_z^\gamma S(t,z)| \le C\langle z\rangle^{(2-|\gamma|)_+}.$$

2. *The transport equations (2.30) have a unique solution $A_j(t,x,\eta)$, solved by induction, defined and C^∞-smooth in $[-T,T]\times Z$, and satifies estimates*

$$|\partial_t^k\partial_z^\gamma A_j(t,z)| \le C,\ \ \forall (t,z)\in[-T,T]\times Z.$$

3. *Let us introduce the Fourier-Integral operator :*

$$U_{H,N}(t)\varphi(x) = (2\pi\hbar)^{-n}\int_Z e^{i\hbar^{-1}(S(t,x,\eta)-\langle y,\eta\rangle)}\Big(\sum_{0\le j\le N}\hbar^j A_j(t,x,\eta)\Big)\varphi(y)dyd\eta. \tag{2.32}$$

Then we have a remainder term estimate in L^2-norm

$$\sup_{|t|\le T}\|U_H(t)-U_{H,N}(t)\| = O(\hbar^N). \tag{2.33}$$

Sketch of proof (see [122] for details)
The Hamilton-Jacobi equation is solved by the usual method (integration along the classical flow). The time T is determined by the presence of caustics. Furthermore we have here to take care about the estimates. The transport equations are solved by induction and direct integration along the classical flow.
The error estimate is a consequence of the above equations which give

$$(i\hbar\partial_t - \hat{H})U_{H,N}(t) = R_N(\hbar,t), \tag{2.34}$$

where $R_N(\hbar,t)$ is a Fourier-Integral operator

$$R_N(\hbar,t)\varphi(x) = (2\pi\hbar)^{-n}\int_Z e^{i\hbar^{-1}(S(t,x,\eta)-\langle y,\eta\rangle)}r_N(\hbar,t,x,\eta)dxd\eta, \tag{2.35}$$

where the amplitude $\hbar^{-N-1}r_N(\hbar,t,\cdot)$ is in $\mathcal{O}(0)$ for $t\in[-T,T]$, $\hbar\in]0;\hbar_0]$. From this we can prove there exists $C>0$ such that

$$\|R_N(\hbar,t)\| \le C\hbar^{N+1}, \forall t\in[-T,T],\ \forall\hbar\in]0;\hbar_0]. \tag{2.36}$$

∎

Now we want to construct approximations for $U_H(t)$ for every time t. This can be done using the group property. Let us fix $T_1\in]0,T/2]$ and consider the time interval $t\in]kT_1,(k+1)T_1[$. Assume first $k\ge 1$. We have

$$U_H(t) = U_H(t-kT_1)\cdot U_H(T_1)^k,$$

which can be approximate by

$$V_{H,N}(t) = U_{H,N}(t - kT_1) \cdot U_{H,N}(T_1)^k.$$

We can get easily, from the Theorem (2.4), that the following estimate is true

$$\sup_{kT_1 \le t \le k+1} \|U_H(t) - V_{H,N}(t)\| = O(\hbar^N). \tag{2.37}$$

It remains to show that $V_{H,N}(t)$ is a Fourier-Integral operator. By applying the product rule for FIO (2.2), we get $V_{H,N}(t) = \mathcal{I}(\phi, B, \hbar)$ with

$$\phi(t, x, \theta, y) = S(t - kT_1, x, \eta_{k+1}) - \langle y_{k+1}, \eta_{k+1}\rangle + \sum_{1 \le j \le k} S(T_1; y_{j+1}, \eta_j) - \langle y_j, \eta_j\rangle,$$

$$y = y_1, \ \theta = (\eta_1, y_2, \eta_2, \cdots, y_{k+1}, \eta_{k+1}) \in (\mathbb{R}^n)^{2k+1},$$

$$B(\hbar, t, x, \theta, y) = A^{(N)}(\hbar, t - kT_1, x, \eta_{k+1} \prod_{j=1}^{j=k} A^{(N)}(\hbar, T_1, y_{j+1}, \eta_j),$$

where

$$A^{(N)}(\hbar, t, x, \eta) = \sum_{0 \le j \le N} \hbar^j A_j(t, x, \eta).$$

We have an analogous formula for $k \le -1$ by taking the FIO

$$V_{H,N}(t) = U_{H,N}(t - kT_1) \cdot U_{H,N}(-T_1)^{-k}.$$

In particular (2.37) still holds.
From this we can easily compute the frequency set of the Schwartz kernel $K(\hbar, t)$ of $U_H(t)$ using the non stationary phase theorem.

Corollary 2.5 *We have the following result*

$$FS[K(\hbar, t)] = \{(x, \xi, y, -\eta) \in Z \times Z, \ \Phi_H^t(x, \xi) = (y, \eta)\}.$$

Remark 2.6 *A lot of methods have been introduced to compute semiclassical approximations for $U_H(t)$. The most popular in physics is the approach by Feynman integrals which, although very intuitive, is hard to prove rigorously. Recently Ben-Arous and Castell proposed a probabilistic approach using an almost analytic extension from the heat kernel [14]. The analytic approach explained here gives a quite complicated Fourier-Integral Operator, when the time t becomes large, because caustics may appear. Hence, to get a better representation we have to use the Hörmander-Maslov theory (see [54, 84]). In section 6 of this survey we shall present another approach, using coherent states, which avoïds the difficulties coming from caustics.*

3 Trace Formulas and Eigenvalue Asymptotics

In this section we will consider the stationary Schrödinger equation and its bound states, i.e

$$(\hat{H} - E)\psi = 0, \quad E \in \mathbb{R}, \quad \psi \in L^2(X), \|\psi\| = 1. \tag{3.1}$$

The most popular example is the harmonic oscillator $\hat{H} = -\hbar^2\Delta + |x|^2$, for which one can compute an explicit orthonormal basis of eigenfunctions in $L^2(X)$ (bound states), ψ_α, with eigenvalues $E_\alpha(\hbar) = (2|\alpha| + 1)\hbar$.

Let us introduce some global assumptions on the Hamiltonians we want to consider here. We start with a quantum Hamiltonian $\hat{H}$ coming from a semiclassical observable H. We assume that $H(\hbar, z)$ has an asymptotic expansion:

$$H(\hbar, z) \asymp \sum_{0\le j<+\infty} \hbar^j H_j(z), \tag{3.2}$$

with the following properties:

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

(As_2) H_0 is bounded below : there exits $c_0 > 0$ and $\gamma_0 \in \mathbb{R}$ such that $c_0 \le H_0(z) + \gamma_0$. 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* :

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

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

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

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

Under these assumptions it is well known that $\hat{H}$ has a unique self-adjoint extension in $L^2(X)$ [93] and the propagator:

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

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

To simplify the notations the subscript H is sometimes omitted and we write U and Φ instead of U_H and Φ_H. Sometimes we also implicitly assume that $H = H_0$.

Examples of Hamiltonians satisfying (As_1) to (As_4)

1.
$$\hat{H} = -\hbar^2(\nabla - i\vec{a}(x))^2 + V(x).$$

The electric potential V and the magnetic potential $\vec{a}$ are smooth on $\mathbb{R}^n$ and satisfy:

$$\begin{aligned} \liminf_{|x|\to+\infty} V(x) &> E, \\ \exists\gamma > 0 \text{ such that } \forall\alpha, \ |\partial_x^\alpha V(x)| &\le c_\alpha(V(x) + \gamma), \\ \exists M > 0 \text{ such that } |V(x)| &\le C(V(y) + \gamma)(1 + |x - y|)^M, \\ |\partial_x^\alpha \vec{a}(x)| &\le c_\alpha(V(x) + \gamma)^{1/2}. \end{aligned} \tag{3.3}$$

2.

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

V is as in example 1 and $\{g_{ij}\}$ is a smooth Riemannian metric on $\mathbb{R}^n$ satisfying:

$$\exists C \text{ a real number } \exists \mu(x)\ (x \in \mathbb{R}^n) \text{ such that}$$
$$\frac{\mu(x)}{C}|\xi|^2 \leq |\sum g_{ij}(x)\xi_i\xi_j| \leq C\mu(x)|\xi|^2,$$
$$\text{with } \frac{1}{C} \leq \mu(x) \leq C(V(x) + \gamma). \tag{3.4}$$

Let us also give an example of a non local Hamiltonian:

3.

$$\hat{H} = \sqrt{m^2 - \hbar^2\Delta} + V(x), \tag{3.5}$$

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

In this section we are interested in this section in bound states. So, let us consider a classical energy interval $I_{c\ell} =]\lambda_-, \lambda_+[,\ \ \lambda_- < \lambda_+$ and assume:
(As_5) *$H_0^{-1}(I_{c\ell})$ is a bounded set of the phase space $\mathbb{R}^{2n}$.*
This implies that for every closed interval $J = [E_-, E_+] \subset I_{c\ell}$, and for $\hbar > 0$ small enough, the spectrum of $\hat{H}$ in J is purely discrete ([73]). In what follows we fix such an interval J.
For some energy level $E \in]E_-, E_+[$, we assume :
(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

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

A useful tool in analyzing the spectrum of $\hat{H}$ is the following functional calculus result proved in [73].

Theorem 3.1 *Let H be a semiclassical Hamiltonian satisfying assumptions (As_1) to (As_4). Let f be a smooth real valued function satisfying $f \in S^r(\mathbb{R})$, $r \in \mathbb{R}$, which means*

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

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

$$H_f(\hbar, z) \asymp \sum_{j \geq 0} \hbar^j H_{f,j}(z). \tag{3.6}$$

In particular we have

$$H_{f,0}(z) = f(H_0(z)), \tag{3.7}$$
$$H_{f,1}(z) = H_1(z) f'(H_0(z)), \tag{3.8}$$
$$\text{and for, } j \geq 2\ \ H_{f,j} = \sum_{1 \leq 1 \leq 2j-1} (-1)^k (k!) d_{j,k}(H) f^{(k)}(H_0), \tag{3.9}$$

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

Remark 3.2 *The starting point of the proof is a careful study of the resolvent* $(\hat{H} - z)^{-1}$ *(corresponding to* $f(\lambda) = (\lambda - z)^{-1}$*). In this case we can construct a parametrix with a good control in* $\hbar$ *and* z *for* $z \in \mathbb{C}\backslash\mathbb{R}$*. For* f *holomorphic in a neighborhood of the real axis we can use the Cauchy integral to define* $f(\hat{H})$*. That works in particular with* $f(\lambda) = (\gamma_0 + \lambda)^s$*. Then using the Mellin transform we can prove the theorem for general smooth* f*. This is the strategy followed in [73]. An alternative and more direct strategy was introduced in [45] using almost analytic extension.*

From this theorem follows the following trace formula

Theorem 3.3 *Let us assume that assumptions* (As_1) *to* (As_5) *are satisfied. Then we have*

1. *For every closed interval* $J := [E_-, E_+] \subset I_{c\ell}$*, and for* $\hbar_0$ *small enough, the spectrum of* $\hat{H}$ *in* J *is purely discrete* $\forall \hbar \in]0, \hbar_0]$*.*
   Let us denote by Π_J *the spectral projector of* $\hat{H}$ *in* J*. Then*

2. Π_J *is finite dimensional and the following estimate holds*

$$\mathrm{tr}(\Pi_J) = O(\hbar^{-n}), \quad \text{as } \hbar \searrow 0.$$

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

$$\mathrm{tr}[g(\hat{H})] \asymp \sum_{j \geq 0} \hbar^{j-n} T_j(g), \tag{3.10}$$

   where T_j *are distributions in* I*. In particular we have*

$$\begin{aligned} T_0(g) &= (2\pi)^{-n} \int_Z g(H_0(z))dz, & (3.11)\\ T_1(g) &= (2\pi)^{-n} \int_Z g'(H_0(z))H_1(z)dz, & (3.12)\\ T_J(g) &= (2\pi)^{-n} \int_Z \sum_{1 \leq 1 \leq 2j-1} (-1)^k (k!) d_{j,k}(H) g^{(k)}(H_0(z))dz & (3.13) \end{aligned}$$

   for $j \geq 2$*.*

Let us denote by $E_j(\hbar)$, $1 \leq j \leq N$, the eigenvalues of $\hat{H}$ in J, each enumerated with its multiplicity. ($N = O(\hbar^{-n})$). Let us introduce now the density of states defined by

$$\rho_J(\hbar) = \sum_{1 \leq j \leq N} \delta(E - E_j(\hbar)), \tag{3.14}$$

or equivalently its $\hbar$-Fourier transform

$$\begin{aligned} S_J(\hbar) &= \sum_{1 \leq j \leq N} \mathrm{e}^{-it\hbar^{-1} E_J(\hbar)} & (3.15)\\ &= \mathrm{tr}[\Pi_J U_H(t)]. & (3.16) \end{aligned}$$

It is convenient to smooth out the spectral projector Π_J and consider instead

$$S_\chi(\hbar) = \mathrm{tr}[\chi(\hat{H})U_H(t)], \quad \text{with } \chi \in C_0^\infty(I). \tag{3.17}$$

The first information we can get now is a result known as the Poisson relation proved by Chazarain [28, 29] and extended to more general Hamiltonians by Helffer-Robert [73, 122].

Theorem 3.4 *The frequency set of the distribution $S_\chi(\hbar)$ satisfies*

$$FS[S_\chi(\hbar)] \subseteq \{(t,\tau), \text{ such that } \tau \in J \text{ and } \exists z \in Z, H_0(z) = -\tau, \Phi^t_{H_0}(z) = z\}. \tag{3.18}$$

Sketch of proof
Let us remark that the results of section 2 do not apply directly to $U_H(t)$ because the conditions on the derivatives are not satisfied globally. But we have introduced an energy localization χ and the essential support of $\chi(\hat{H})$ is a compact set of the phase space Z. So we need here a semiclassical approximation for $U_{H,\chi} := U_H(t)\chi(\hat{H})$. This can be constructed as in section 2 because everything is localized in a compact set of the phase space. Hence we can construct a Fourier integral operator $U_{H,\chi,N}(t)$ for short time such that $U_{H,\chi,N}(0) = \chi(\hat{H})$. Using the group property, we get approximations for arbitrary time t. The phases are the same as in section 2 but they are defined only on bounded set; it is sufficient here because the amplitudes are compactly supported.
Then the theorem is easily proved by computing the critical points of the phase ϕ and using the non stationary phase theorem.

Example 3.5 *Let us consider the one dimensional harmonic oscillator*

$$\hat{H} = -\frac{\hbar^2}{2}\frac{d^2}{dx^2} + \frac{x^2}{2},$$

with eigenvalues $E_j(\hbar) = (j + \frac{1}{2})\hbar$, $j \in \mathbb{N}$. Then we get a Schwartz tempered distribution

$$S(\hbar) = \sum \mathrm{e}^{-i\frac{t}{\hbar}(j+\frac{1}{2})}$$

and using the well known Poisson formula

$$\sum_{k\in\mathbb{Z}} \hat{f}(k)\mathrm{e}^{ikx} = 2\pi \sum_{k\in\mathbb{Z}} f(x + 2k\pi),$$

it is an exercise to prove

$$FS[S] = \{(2k\pi, \tau), \tau > 0\} \cup \mathbb{R} \times \{0\}.$$

Let us remark that the period set of the Hamiltonian $H(z) = \frac{|z|^2}{2}$ is $2\pi\mathbb{Z}$.

The next step in the understanding of the discrete spectrum for general Hamiltonians is to analyze the contributions of the periodic trajectories to the distribution $S_\chi(\hbar)$. The

main result in this field is known as the *Gutzwiller trace formula.* The simplest model is the classical Poisson formula recalled above.
As remarked in particular by Guillemin-Uribe [64] and Helffer [70], the general Gutzwiller trace formula is obtained by applying the stationary phase theorem to $\langle S_\chi(\hbar), \varphi\rangle$ for any $\varphi \in C_0^\infty(\mathbb{R})$, using the W.K.B approximations of the propagator. This is not very difficult if φ is supported in a small interval around 0. But if φ is supported in an arbitrary compact interval the problem is not so easy. As we have seen in section 2, the phase of the Fourier-Integral operator which is a semi-classical approximation of the propagator is quite complicated.
Let us remark also that after a suitable energy localization we can assume that H satisfies the assumptions of Theorem (2.4).
To state the result, we need an assumption on the classical trajectories. Let us introduce

$$\Gamma_E = \{(T, z) \in \mathbb{R} \times \Sigma_E,\ \Phi_H^T(z) = z\};\ \ \Sigma_E = \{z \in Z,\ H(z) = E\},$$

where $E \in]E_-, E_+[$.

Definition 3.6 *The Hamiltonian flow Φ_H^t is said to be clean on Σ_E if the following conditions holds :*

1. *Γ_E is a smooth submanifold of $\Sigma_E \times \mathbb{R}$.*
2. *At each point $(z, T) \in \Gamma_E$, the tangent space is determined by*

$$\mathrm{T}_{(z,T)}\Gamma_E = \{(\zeta, \tau) \in \mathbb{R} \times \mathrm{T}_z,\ \tau\mathcal{H}_H(z) + \nabla_z\Phi_H^t(z)\cdot\zeta = \zeta\},$$

where $\mathcal{H}_H(z) = (\nabla_\xi H(z), -\nabla_x H(z))$ (Hamiltonian vector field).

Remark 3.7 *This notion of cleanness was introduced by Duistermaat-Guillemin [48] and Guillemin-Uribe [64]. The condition 2 comes naturally by differentiation of the equation $\Phi_H^t(z) = z$.*

Theorem 3.8 (Gutzwiller trace formula; [70, 47, 105, 112]) *Let $\hat{H}$ be a semiclassical Hamiltonian satisfying (As_1) to (As_6). Then, there exists $\gamma_k \in \mathcal{D}'(\mathbb{R})$ such that for every $\varphi \in C^\infty(\mathbb{R})$, with Fourier transform $\hat{\varphi} \in C_0^\infty(\mathbb{R})$, we have*

$$\sum_{E_j(\hbar)\in[E_-,E_+]} \varphi\left(\frac{E_j(\hbar) - E}{\hbar}\right) \asymp \sum_{j\geq 0} \tau_j(\hat{\varphi})\hbar^{-n+j+1}. \tag{3.19}$$

The τ_j are distributions in $\mathbb{R}$ with support on the set of periods of the closed trajectories. In (3.19) the distributions τ_j are oscillating in $\hbar$. They have the following structure. Let us denote by $[\Gamma_E]$ the set of connected components of Γ_E, then

$$\tau_j(\hat{\varphi}) = \sum_{Y\in[\Gamma_E],Y\cap Supp(\hat{\varphi})\neq\emptyset} \hbar^{n-1+(1-d_Y)/2}e^{i\sigma_Y}e^{i\frac{S_Y}{\hbar}}a_{j,Y}, \tag{3.20}$$

where $d_Y = \dim(Y)$, S_Y is the action along T-periodic paths, $\sigma_Y = m_Y \frac{\pi}{4}$, $m_Y \in \mathbb{Z}$ is a Maslov index.
In particular for the leading term we have

$$a_{0,Y} = (2\pi)^{-(1+d_Y)/2} \int_Y e^{i\beta} \hat{\varphi} d\nu_Y,$$

where $\beta(z,T) = \int_0^T H_1(\Phi^t(z))dt$, $\hat{\varphi}(z,T) = \hat{\varphi}(T)$ and ν_Y is a natural density on Y. In particular for $Y = \Sigma_E \times \{0\}$, ν_Y is the Liouville measure on Σ_E.

Corollary 3.9 *Let us assume that all the periodic orbit γ on Σ_E are non degenerate i.e. their Poincaré map P_γ does not have the eigenvalue 1. Then the cleanness assumption is fulfilled and we have*

$$\sum_{E_j(\hbar)\in[E_-,E_+]} \varphi\left(\frac{E_j(\hbar)-E}{\hbar}\right) \asymp (2\pi\hbar)^{-n}\left(\hat{\varphi}(0)L_E(\Sigma_E)\hbar + \sum_{j\geq 2} c_{0,j}(\hat{\varphi})\hbar^j\right) +$$
$$\sum_\gamma \left(\frac{e^{i\frac{S_\gamma}{\hbar}+\sigma_\gamma}}{|\det(1-P_\gamma)|^{1/2}}\hat{\varphi}(T_\gamma)\frac{T^*_\gamma}{2\pi}e^{-i\int_\gamma H_1} + e^{i\frac{S_\gamma}{\hbar}+\sigma_\gamma}\left(\sum_{j\geq 1} c_{\gamma,j}(\hat{\varphi})\hbar^j\right)\right), \tag{3.21}$$

where

- T^*_γ *is the primitive period of* γ.
- $\sigma_\gamma = m_\gamma \frac{\pi}{4}$ *with* $m_\gamma \in \mathbb{Z}$, *the Maslov index of* γ.
- S_γ *is the classical action along* γ.
- $c_{0,j}$ *are distributions supported in* $\{0\}$.
- $c_{\gamma,j}$ *are distributions supported in* T_γ.

The first line in (3.21) is the contribution of 0 (biggest contribution) and the second line represents the contributions of the other periods which are in supp(φ).

Remark 3.10 *During the last 25 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 poeple: Colin de Verdière [30, 31], Chazarain [28], Duistermaat-Guillemin [48]. The first proof in the semi-classical setting is given in the paper [64] 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 $\mathbb{R}^n$ was considered by Brummelhuis-Uribe (1991). Complete proofs of the Gutzwiller trace formula were obtained during the period 1991/95 by Dozias [47], Meinrencken [105], Paul-Uribe[110]. Recently, in his thesis [95], Khuat-Duy proved a trace formula for degenerate critical energy levels.*

In the Gutzwiller trace formula there is a big contribution at $T = 0$, given by the first line of (3.21), which gives the well known Weyl formula. Let us denote by $N_J(\hbar)$ the number of bound states of $\hat{H}$ in $J = [E_-, E_+]$. The following results hold.

Theorem 3.11 (Weyl asymptotic formula) *Under the assumptions (As_1) to (As_6), if $E_\pm \in I_{cl}$, are regular values for H_0, then we have:*

$$N_J(\hbar) = (2\pi\hbar)^{-n} Vol_Z\{H_0^{-1}(J)\} + O(\hbar^{1-n}). \tag{3.22}$$

Remark 3.12 *When end points of $I_{c\ell}$ are critical for H_0 but are non degenerate then a Weyl formula holds, with a leading term depending on the geometry of the critical manifold (see Brummelhuis-Paul-Uribe [21]).*

The remainder estimate in (3.22) can be improved, if we add the following condition
(As_7) *The Liouville measure of the closed trajectories on Σ_E is zero*
(that means: $\nu_E\{(x,\xi) \in \Sigma_E,\ \exists t \neq 0,\ \Phi^t(x,\xi) = (x,\xi)\} = 0$).

Theorem 3.13 *Let us assume that the assumptions of theorem (3.11) hold and that (As_7) holds for $E = E_-$ and $E = E_+$.*
Then we have a two term asymptotic expansion :

$$N_J(\hbar) = (2\pi\hbar)^{-n} Vol_Z\{H_0^{-1}(J)\} + c_1\hbar^{1-n} + o(\hbar^{1-n}), \tag{3.23}$$

with

$$c_1 = (2\pi)^{-n}\left(\int_{\Sigma_{E_-}} H_1 dL_{E_-} - \int_{\Sigma_{E_+}} H_1 dL_{E_+}\right).$$

The remainder estimate in (3.22) is the semi-classical analogue of a basic result of Hörmander [83]. It has been proved in [29, 73, 87] under different assumptions. The remainder estimate (3.23) is the semi-classical analogue of a theorem of Duistermaat-Guillemin [48] and was proved in [113, 87]. In [114] the authors extend to this setting a nice result of Safarov [131] giving an oscillating second term in the general case i.e without the condition (As_7).
A simple example of Hamiltonians, in $\mathbb{R}^2$, satisfying the assumption (As_7) is the following

$$\hat{H} = -\hbar^2\Delta + a^2x^2 + b^2y^2,$$

with $a > 0,\ b > 0,\ \frac{a}{b}$ not rational.
The difficult part of the above Weyl formula (3.22) is surely the remainder estimate or the second term for (3.23). Let us remark that in the general case it is not possible to improve the $O(\hbar^{1-n})$ estimate. This is easily seen from the example of the harmonic oscillator where the term

$$\hbar^{n-1}(N_J(\hbar) - c_0\hbar^{-n})$$

is oscillating as $\hbar$ tends to 0.
Let us remark that using the functional calculus stated in Theorem (3.3) it is not difficult to get a less accurate estimate : for every $\delta \in]0, 1/2[$

$$N_J(\hbar) = (2\pi\hbar)^{-n} Vol_Z\{H_0^{-1}(J)\} + O(\hbar^{\delta-n}). \tag{3.24}$$

Until recently the accurate estimate with $\delta = 1$ was proved only by time dependent methods. Dimassi-Sjöstrand [45] succeeded improving the functional calculus and gave a stationary proof of the $O(\hbar^{1-n})$ estimate.
Here we shall explain the time dependent method introduced by Levitan and Hörmander [83]. The first step is to consider the Gutzwiller trace formula with test functions supported in a small time interval $]-T, T[$, $T > 0$. So for $\theta \in C_0^\infty(]-T, T[)$ let us introduce

$$\begin{aligned} G_\theta(\hbar, E) &= \sum \chi(E_j(\hbar))\hat{\theta}\left(\frac{E_j(\hbar) - E}{\hbar}\right) && (3.25)\\ &= \mathrm{tr}[\chi(\hat{H}) \int U_H(t)\theta(t)\mathrm{e}^{\frac{itE}{\hbar}} dt], && (3.26)\end{aligned}$$

where $\chi \in C_0^\infty]E-\epsilon, E+\epsilon[$; $\chi \equiv 1$ on $[E-\epsilon/2, E+\epsilon/2]$. We can use the W.K.B approximation for $U_H(t)$ introduced in section 2. We remark that 0 is the only period of the classical flow in $]-T, T[$, for T small enough, with energy E. Applying the stationary phase theorem [84], we get

Theorem 3.14 *Let us assume that $J_0 = [E_0 - \epsilon, E_0 + \epsilon]$ with $\epsilon > 0$ small enough, $J_0 \subset I_{c\ell}$ and J_0 is non critical for H_0. Then for every $E \in J_0$ and every $N \geq 1$ we have*

$$G_\theta(\hbar, E) = (2\pi\hbar)^{1-n}[\sum_{0 \leq j \leq N} \hbar^j \gamma_j(\theta, E) + O(\hbar^{N+1})]. \tag{3.27}$$

Moreover the estimate is uniform in $E \in J_0$ and the leading term is given by

$$\gamma_0(\theta, E) = \theta(0)\chi(E) \int_{\Sigma_E} dL_E.$$

Furthermore if $\theta(t) \equiv 1$ in a neighborhood of 0 and if $\chi(t) \equiv 1$ in a neighborhood of J_0 then the coefficients γ_j are related to the coefficients computed in the weak form of the trace formula (see Theorem (3.3)), for $E \in J_0$, and

$$\begin{aligned} \gamma_j(\theta, E) &= \sum_{1 \leq k \leq 2j-1} \frac{d^k}{dE^k}\left(\int_{\Sigma_E} d_{jk}(H) dL_E\right), && (3.28)\\ \gamma_1 &= -\frac{d}{dE}\left(\int_{\Sigma_E} H_1 dL_E\right). && (3.29)\end{aligned}$$

The second step in proving the Weyl formula with $O(\hbar^{1-n})$ estimate consists in energy localization and a tauberian argument. Let us first remark that for the weak form of the trace formula it is sufficient to estimate

$$N_\chi(\hbar, E) = \sum_{E_j(\hbar) \leq E} \chi(E_j(\hbar)),$$

where $\chi \in C_0^\infty(]E_+ - \epsilon, E_+ + \epsilon[)$, $\epsilon > 0$ small enough, $\chi \geq 0$. Let us remark that we have

$$(2\pi\hbar)^{-1}G_\theta(\hbar, E) = \frac{d}{dE}(N_\chi(\hbar) * \zeta_\hbar)(E),$$

where $\zeta_\hbar(u) = (2\pi\hbar)^{-1}\hat{\theta}(-u/\hbar)$ hence we have $\int \zeta_\hbar(u)du = \theta(0)$. This explains why a tauberian argument concerning convolutions gives the conclusion of Theorem (3.11) (see [73] for the details).

The proof of Theorem (3.13) uses the same tools but it is more difficult because we have to increase the time interval for the θ function and to control the periodic trajectories (see [113, 122] for the details).

It is also interesting to consider the moments of eigenvalues, which are called Riesz means of order $\gamma \geq 0$, and defined as

$$R_\gamma(\hbar, E) = \sum_{E_j(\hbar)\leq E} \chi(E_j)(E - E_j(\hbar))_+^\gamma,$$

where $E \in J$, $\chi \in C_0^\infty(I)$, $\chi \equiv 1$ in J. (if we know that $H_0^{-1}]-\infty, E_0]$ is compact we can take $\chi \equiv 1$ and $E < E_0$).

For $\gamma = 1$, $R_1(\hbar, E)$ is related to the ground state of a system with Z Fermions where $Z = \hbar^{-3}$. Lieb and Thirring [98] consider the usual Schrödinger case $\hat{H} - \hbar^2\Delta + V$ with a potential V satisfying $\liminf_{|x|\to+\infty} V(x) > 0$. A natural problem is the existence of a universal constant $L_{\gamma,n}$ such that for all V we have

$$R_\gamma(\hbar, 0) \leq L_{\gamma,n}\hbar^{-n} \int_X V_-^{\gamma+n/2}(x)dx, \tag{3.30}$$

where $L_{\gamma,n}$ depends only on γ, $\gamma > max(0, 1 - n/2)$ and n. It is known that $L_{\gamma,n}$ exists for $n = 1, \gamma > 1/2$; $n = 2, \gamma > 0$; $n = 3, \gamma = 0$. We shall see below that for suitable V and $E < 0$ we have

$$\begin{aligned}
\lim_{\hbar\searrow 0} \hbar^n R_\gamma(\hbar, 0) &= (2\pi)^{-n} \int_Z (E - V - |p|^2)_+^\gamma dxdp \\
&= L_{\gamma,n}^{Cl} \int_X (E - V)_+^{\gamma+n/2} dx.
\end{aligned} \tag{3.31}$$

We have clearly $L_{\gamma,n} \geq L_{\gamma,n}^{Cl}$. Moreover

$$\gamma \mapsto \frac{L_{\gamma,n}}{L_{\gamma,n}^{Cl}}$$

is non-increasing. It was proved by Aizenmann-Lieb-Thirring ([3, 98]) that the smallest γ for which $L_{\gamma,n} = L_{\gamma,n}^{Cl}$ is $\gamma_c = 3/2$. The following result is proved in [76]

Theorem 3.15 *1. Let us consider the same assumptions as in Theorem (3.11). Then we have*

$$R_\gamma(\hbar, E) = \hbar^{-n}\left(\sum_{j=0}^{j=N+[\gamma]_+} \hbar^j C_{j,\gamma}(E) + O(\hbar^{1+\gamma+N})\right), \tag{3.32}$$

where we have $C_{j,\gamma}(E) = \lambda_+^\gamma * C_{j,0}(E)$ *and* $[\gamma]_+ = \gamma$ *if* $\gamma \in \mathbb{N}$, $[\gamma]_+ = [\gamma] + 1$ *if* $\gamma \in [0, +\infty[\backslash\mathbb{N}$, $[\gamma]$ *is the largest integer smaller than* γ.

2. *Let us consider the same assumptions as in Theorem (3.13). Then in the asymptotic expansion (3.32) we can replace the estimate big O by a small o, in particular that means that if $\gamma \in \mathbb{N}$ we get one term more in the asymptotics.*

The above results concern the 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 $E \in [E_-, E_+]$ the Hamiltonian flow $\Phi^t_{H_0}$ is periodic on Σ_E with a period T_E. Furthermore we assume that Σ_E is connected and the subprincipal symbol H_1 is null.*
Let us first recall a result in classical mechanics (Guillemin-Sternberg, [62]) :

Proposition 3.16 *Let γ be a closed path of energy E and period T_E. Then the action integral $J(E) = \int_\gamma pdq$ defines a function of E only, C^∞ in E and such that $J'(E) = T_E$. In particular for one degree of freedom systems we have*

$$J(E) = \int_{H_0(z)\leq E} dz.$$

Now we can extend J to an increasing function on $\mathbb{R}$, linear outside a neighborhood of J. Let us introduce the modified Hamiltonian $\hat{K} = (2\pi)^{-1}J(\hat{H})$. Using results stated in section 1, we can see that $\hat{K}$ has all the properties of $\hat{H}$ and furthermore its Hamiltonian flow is 2π-periodic in $\Sigma_F = K_0^{-1}(F)$ for $F \in [F_-, F_+]$ where $F_\pm = J(E_\pm)$. So in what follows we replace $\hat{H}$ by $\hat{K}$, its "energy renormalization".
Let us denote by a the average of the action of a periodic path on $\Sigma_F^{K_0}$ and by $\mu \in \mathbb{Z}$ its Maslov index. ($a = \frac{1}{2\pi}\int_\gamma pdx - 2\pi F$). Under the above assumptions the following results are proved in [77] using ideas introduced before by Colin de Verdière [31] and Weinstein [143].

Theorem 3.17 ([143, 31, 29, 77]) *There exists $C_0 > 0$ and $\hbar_1 > 0$ such that*

$$\text{spect}(\hat{K}) \cap [F_-, F_+] \subseteq \cup_{k\in\mathbb{Z}} I_k(\hbar), \tag{3.33}$$

with

$$I_k(\hbar) = [-a + (k - \frac{\mu}{4})\hbar - C_0\hbar^2, -a + (k - \frac{\mu}{4})\hbar + C_0\hbar^2]$$

for $\hbar \in]0, \hbar_1]$.

Let us remark that this theorem gives the Bohr-Sommerfeld quantization conditions for the energy spectrum, more explicitly,

$$F_k(\hbar) := J(E_k(\hbar)) = (k - \frac{\mu}{4})\hbar - a + O(\hbar^2).$$

Under a stronger assumption on the flow it is possible to give a more accurate result.
(As_9) $\Phi^t_{K_0}$ *has no fixed point in $\Sigma_F^{K_0}$ $\forall F \in [F_- - \epsilon, F_+ + \epsilon]$ and $\forall t \in]0, 2\pi[$.*
Let us denote by $d_k(\hbar)$ the number of eigenvalues of $\hat{K}$ in $I_k(\hbar)$.

Theorem 3.18 ([31, 29, 77]) *Under the above assumptions, for $\hbar$ small enough and $-a+(k-\frac{\mu}{4})\hbar \in [F_-, F_+]$, we have :*

$$d_k(\hbar) \asymp \sum_{j\geq 1} \Gamma_j(-a+(k-\frac{\mu}{4})\hbar)\hbar^{j-n}, \tag{3.34}$$

with $\Gamma_j \in C^\infty([F_-, F_+])$. In particular

$$\Gamma_1(F) = (2\pi)^{-n} \int_{\Sigma_F} dL_F.$$

In the particular case $n = 1$ 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 3.19 ([77]) *Let us assume $n = 1$ and $a = 0$. Then there exists a sequence $f_k \in C^\infty([F_-, F_+])$, for $k \geq 2$, such that*

$$F_\ell(\hbar) + \sum_{k\geq 2} h^k f_k(F_\ell(\hbar)) = (\ell + \frac{1}{2})\hbar + O(\hbar^\infty) \tag{3.35}$$

for $\ell \in \mathbb{Z}$ such that $(\ell+\frac{1}{2})\hbar \in [F_-, F_+]$.
In particular there exists $g_k \in C^\infty([F_-, F_+])$ such that

$$F_\ell(\hbar) = (\ell + \frac{1}{2})\hbar + \sum_{k\geq 2} h^k g_k((\ell + \frac{1}{2})\hbar) + O(\hbar^\infty), \tag{3.36}$$

where $\ell \in Z$ such that $(\ell+\frac{1}{2})\hbar \in [F_-, F_+]$.

When $H_0^{-1}(J)$ is not connected but such that the M connected components are mutually symmetric, under linear symplectic maps, then the above results still hold [77].
Let us consider for example the particular case of the double well problem in one degree of freedom for simplicity. Let us consider a C^∞ smooth potential $V(x)$ such that

$$V(-x) = V(x),\ V \geq 0,\ \liminf_{|x|\to+\infty} V(x) > 0,$$
$$\{V(x) = 0\} \Leftrightarrow \{x = \pm x_0\},\ V''(x_0) := \omega^2 > 0.$$

The spectrum of $\hat{H}$ in $]0, \sigma[$ is a sequence of simple eigenvalues, $\{E_j(\hbar)\}_{j\in\mathbb{N}}$, where $\sigma = \liminf_{|x|\to+\infty} V(x)$. The eigenvalue $E_j(\hbar)$ is associated with an eigenfunction of the same parity as j. Let us introduce the notation $E_{2j}(\hbar) = E_j^e(\hbar)$ and $E_{2j+1}(\hbar) = E_j^o(\hbar)$. The above construction (see [77]) shows that $E_j^o(\hbar)$ and $E_j^e(\hbar)$ have the same asymptotics in $\hbar$ i.e. we have

$$E_j^o(\hbar) - E_j^e(\hbar) = O(\hbar^\infty),$$

under the condition $E_j^o(\hbar) \in [C\hbar, \sigma]$, for $C > 0$ large enough.
The same property is also true in the interval $[0, C\hbar]$ but it is proved by an other method. Furthermore the splitting between two consecutive eigenvalues has the following expansion

Theorem 3.20

$$e^{S_0/\hbar}[E_j^o(\hbar) - E_j^e(\hbar)] \asymp \hbar^{1/2-j} \sum_{k\in\mathbb{N}} \alpha_k^j \hbar^k, \tag{3.37}$$

where $S_0 = \int_{-x_0}^{x_0} \sqrt{V(x)}dx$. *The* α_k^j *are numerical classical coefficients. In particular*

$$\alpha_0^j = \frac{\sqrt{2V(0)}}{j!} 2^{j+1} \omega^{\frac{1}{2}+j} \pi^{-\frac{1}{2}}$$
$$(\lim_{\varepsilon\to 0} \varepsilon^{2j} \exp\{-2\int_{-x_0+\varepsilon}^{0} \frac{(\sqrt{2V(x)})' - (2j+1)\omega}{2\sqrt{2V(x)}} dx\}). \tag{3.38}$$

Several people contributed to this result: E. Harrel[68], Helffer-Sjöstrand [75], B.Simon[135] Recently V. Sordoni proved that the above formula agrees with a formula computed heuristically by Coleman using the method of instantons, path integrals, and generalized determinants [136, 128].

After this discussion of results connected with periodical paths we consider in more detail the signature of the existence of a *non periodical path* on the energy spectrum. The following result is a quantum mechanical analogue of a simple and beautiful result due to Helton [81] for elliptic operators on compact manifolds.

Theorem 3.21 **([38])** *Under the assumptions* (As_1) *to* (As_6) *for* H, *assume furthermore that there exists on* Σ_E *a non periodical trajectory for the flow* $\Phi_{H_0}^t$. *Then for every* $c > 0$, $\delta > 0$ *and every* $\hbar_0 > 0$ *the set:*

$$\mathcal{T}_{E,\delta} := \{\omega_{jk}(\hbar),\ E_j(\hbar), E_k(\hbar) \in [E - c\hbar^{1-\delta}, E + c\hbar^{1-\delta}],\ 0 < \hbar \leq \hbar_0\}$$

is dense in $\mathbb{R}$, *where* $\omega_{jk}(\hbar) = \frac{E_j(\hbar)-E_k(\hbar)}{\hbar}$.

Proof : Let us reproduce here the proof given in [38]. Let $f \in C_0^\infty(\mathbb{R})$ be such that $f = 0$ on $\mathcal{T}_{E,\delta}$. We have to show that $f \equiv 0$ on $\mathbb{R}$. Let us introduce $\chi \in C_0^\infty(]-c, c[)$ with $\chi(0) = 1$. Following Helton[81] we consider the operator:

$$\hat{A}_{E,f}(\hbar) = \int \hat{f}(t) U(-t,\hbar) \hat{A}_E(\hbar) U(t,\hbar) dt, \tag{3.39}$$

with $A_E(\hbar) = \chi(\frac{\hat{H}-E}{\hbar^{1-\delta}}) \hat{A} \chi(\frac{\hat{H}-E}{\hbar^{1-\delta}})$, $A \in C_0^\infty(\mathbb{R}^{2n})$. By inverse Fourier transform, we also have:

$$\hat{A}_{E,f}(\hbar) = 2\pi \sum_{j,k} f(\omega_{jk}(\hbar)) \chi\left(\frac{E_j(\hbar) - E}{\hbar^{1-\delta}}\right) \chi\left(\frac{E_k(\hbar) - E}{\hbar^{1-\delta}}\right) \Pi_k \hat{A} \Pi_j, \tag{3.40}$$

where Π_k is the projection on the state φ_k.
From (3.39), (3.40) we have:

$$\int \hat{f}(t) U(-t,\hbar) \hat{A}_E(\hbar) U(t,\hbar) dt = 0,\ \forall A \in \mathcal{O}(0). \tag{3.41}$$

From (3.41) we would like to prove that $f \equiv 0$ by going to the classical limit $\hbar \searrow 0$. To do that we first use the semi-classical propagation theorem (section 1) and functional calculus with parameters for pseudodifferential operators ([44]). We test (3.41) by computing the trace of the product with any operator $\hat{B}$, $B \in \mathcal{O}(0)$. We get easily, $\forall B \in \mathcal{O}(0)$,

$$\lim_{\hbar \searrow 0}(2\pi\hbar)^n . Tr\left(\hat{A}_{E,f}(\hbar).\hat{B}\right) = \int\int \hat{f}(t)A\left(\Phi^t_{H_0}(z)\right)\right) B(z)dzdt = 0. \tag{3.42}$$

So we get

$$\int \hat{f}(t)A\left(\Phi^t(z)\right)\right) dt = 0, \ \forall z \in \Sigma_E. \tag{3.43}$$

Now, choose $z_0 \in \Sigma_E$ such that $t \to \Phi^t(z_0)$ is not periodic, we should like to deduce from (3.43) that $\hat{f} \equiv 0$. Using the same arguments as in [74] (p.866-867) we can easily get the following

Lemma 3.22 *For $T > 0$ we can find $\rho_T > 0$ such that the mapping $\Phi : (t, z) \overset{F}{\mapsto} (t, \Phi^t(z))$ is a diffeomorphism from $]-T, T[\times D_{\rho_T}(z_0)$ onto an open neighborhood $\mathcal{N}_T$ of the curve: $\{\Phi^t(z_0), \ -T < t < T\}$; where $D_{\rho_T}(z_0)$ is the euclidean ball with center z_0 and radius ρ_T in the orthogonal plane to the curve at time 0.*
Furthermore, for every g in $C_0^\infty(]-T, T[)$ we can construct some $A \in C_0^\infty(\mathbb{R}^{2n})$ such that: $g(t) = A(\Phi^t(z_0)) + h(t)$, $\forall t \in \mathbb{R}$ with:
(i) $Supp(h) \cap]-T, T[= \emptyset$,
(ii) $\sup_{\mathbb{R}} |h| \leq \sup_{\mathbb{R}} |g|$.

A sketchy proof : Starting with the diffeomorphism F, let us choose $u \in C_0^\infty(D_{\rho_T}(z_0))$, $u(z_0) = 1$, $0 \leq u \leq 1$. We define $B(t, z) := g(t)u(z)$ for $(t, z) \in D_{\rho_T}(z_0)$ and $A(z) := B(F^{-1}(z))$ for $z \in \mathcal{N}_T$. We have clearly $A(\Phi^t(z_0)) = g(t)$ if $|t| \leq T$. For $|t| \geq T$ and $\Phi^t(z_0) \in \mathcal{N}_T$ we have $\Phi^t(z_0) = \Phi^t_1(z)$ with $|t_1| \leq T$, $z \in D_{\rho_T}(z_0)$ so $h(t) = -g(t_1)u(z)$ and we get the announced properties for h. ∎

So, with the above notation, using the above lemma and (3.43) we get:

$$\int \hat{f}(t)g(t)dt = \int \hat{f}(t)h(t)dt \leq \sup_{\mathbb{R}} |g| \int_{|t| \geq T} |\hat{f}(t)|dt,$$

taking T large, we have clearly $\hat{f} \equiv 0$ hence $f \equiv 0$. ∎

Remark 3.23 *Using results obtained by S.Dozias in her thesis [47] we can see that the theorem (6.1) admits a partial converse: if $H_1 = 0$ and if the set $\mathcal{T}_{E,\delta}$ defined in Theorem (6.1) is dense in $\mathbb{R}$ with $\delta < \frac{1}{2}$ then the global flow Φ^t is not periodic on Σ_E. Indeed if the global flow Φ^t is periodic on Σ_E, Dozias proves that there exists $\gamma_0, \gamma_1, C \in \mathbb{R}$; $\varepsilon > 0$ such that:*

$$\text{spectrum}[\hat{H}] \cap [E - c\hbar^{1-\delta}, E + c\hbar^{1-\delta}] \subseteq \bigcup_{k \in \mathbb{Z}} [\gamma_0 + \gamma_1 k\hbar - C\hbar^{1+\varepsilon}, \gamma_0 + \gamma_1 k\hbar + C\hbar^{1+\varepsilon}]. \tag{3.44}$$

Clearly (3.44) entails that $\mathcal{T}_{E,\delta}$ is not dense in $\mathbb{R}$. So the two conditions:
(i) $\mathcal{T}_{E,\delta}$ is dense in $\mathbb{R}$,
(ii) there exists a non periodical path on Σ_E,
are "almost equivalent".

4 Quantum Signature of Classical Chaos

From a mathematical point of view the starting point of the story is a theorem announced and partially proved by Schnirelman in 1974 concerning the equirepartition of eigenfunctions for the Laplace-Beltrami operator, $\triangle_M$, on a constant negative curvature compact manifold M. This theorem was proven rigorously in 1984 by Zelditch [146] whose proof was simplified by Colin de Verdière [33]. Let us recall here the statement. Let ψ_k be an orthonormal basis of eigenfunctions of $\triangle_M$,

$$\triangle_M \psi_k + E_k \psi_k = 0,$$

where $\{E_k\}$ is the increasing sequence of eigenvalues of $-\triangle_M$ with their multiplicities. Then we have the following equirepartition theorem

Theorem 4.1 *There is a subsequence $\{E_{k_j}\}$ of density one, i.e*

$$\lim_{E\nearrow+\infty} \frac{\#\{k, E_k \leq E\}}{\#\{j, E_{k_j} \leq E\}} = 1,$$

such that for every smooth open set $\Omega \subseteq M$ we have

$$\lim_{j\nearrow+\infty} \int_\Omega |\psi_{k_j}|^2 dV_M(x) = \frac{Vol(\Omega)}{Vol(M)}, \tag{4.1}$$

where $dV_M(x)$ is the Riemanniann volume form on M.

In 1987, Helffer-Martinez-Robert [72] have proven a semiclassical version of the Schnirelmann theorem that we want to explain now.
Let us introduce a first chaotic assumption :
(As_{10}) *The dynamical system* $\left(\Sigma_E, d\nu_E, \Phi^t_{H_0}\right)$ *is* ergodic *which means: for every continuous function A on Σ_E, we have, for almost all $z \in \Sigma_E$:*

$$\lim_{T\nearrow+\infty} \frac{1}{T}\int_0^T A(\Phi^t_{H_0}(z))dt = \int_{\Sigma_E} A d\nu_E.$$

Let us recall that ν_E is the Liouville probability measure on Σ_E.
It is not obvious how to construct Hamiltonians H on $Z = \mathbb{R}^{2n}$, for $n \geq 2$, with an ergodic flow on energy shell Σ_E. If $n = 1$ and if Σ_E is connected then the assumption (As_{10}) is fulfilled. For $n = 2$, examples where constructed by Knauf [96] (see also [46]).
Let us remark for future use that , if $n \geq 2$, condition (As_{10}) entails (As_7).
Let us consider now $\hbar$-dependent energy intervals: $I(\hbar) = [E-\delta(\hbar), E+\delta(\hbar)]$, with $\lim_{\hbar\to 0}\delta(\hbar) =$

0, $\delta(\hbar) \geq \epsilon_2 \hbar$, for some $\epsilon_2 > 0$. Let us denote: $\Lambda(\hbar) = \{j,\ E_j(\hbar) \in I(\hbar)\}$ and $N_{I(\hbar)} = \#\Lambda(\hbar)$. Let us introduce the orthonormal system of bound states ψ_k, $\hat{H}\psi_k = E_k(\hbar)\psi_k$, where $E_k(\hbar) \in J$ and the matrix elements $a_{j,k} = \langle \hat{A}\psi_j, \psi_k\rangle$ for $A \in \mathcal{O}(0)$.
In [113] (see also [72]) the following result was implicitly proved.

Theorem 4.2 *Let us consider $A \in \mathcal{O}(0)$ and assume (As_1) to (As_7). Then there exists $c_0 > 0$ such that for every $\epsilon > 0$ there exists C_ϵ and $\eta_\epsilon > 0$ such that for every interval $I \subseteq]E - \eta_\epsilon, E + \eta_\epsilon[$ and every $\hbar \in]0, \hbar_0[$ we have*

$$\left|\mathrm{tr}(\hat{A}\Pi_I - (2\pi\hbar)^{-n} \int_{H_0^{-1}(I)} A(z)dz\right| \leq \epsilon c_0 \hbar^{1-n} + C_\epsilon \hbar^{2-n}, \tag{4.2}$$

where Π_I denotes the spectral projector of $\hat{H}$ on I.

From this theorem we get easily the following result (see also [20]), concerning the semi-classical limit of $N_{I(\hbar)} = \mathrm{tr}\Pi_{I(\hbar)}$ when the size of $I(\hbar)$ is proportional to $\hbar$.

Corollary 4.3 *For $c > 0$ let us denote $I_c(\hbar) = [E - c\hbar, E + c\hbar]$. Then we have*

$$\lim_{\hbar \searrow 0} \hbar^{n-1} N_{I_c(\hbar)}(\hbar) = \frac{2c}{(2\pi)^n} dL_E(\Sigma_E).$$

More generally, for every $A \in \mathcal{O}(0)$, we have

$$\lim_{\hbar \searrow 0} \hbar^{n-1} \mathrm{tr}\left(\hat{A}\Pi_{I_c(\hbar)}\right) = \frac{2c}{(2\pi)^n} \int_{\Sigma_E} A dL_E.$$

Corollary 4.4 *Under the same assumptions as above, we have:*

$$\lim_{\hbar \searrow 0} \frac{\sum_{j \in \Lambda(\hbar)} a_{jj}}{\#\Lambda(\hbar)} = \int_{\Sigma_E} A d\nu_E. \tag{4.3}$$

Remark 4.5 *The corollary (4.4) is still valid under assumptions (As_1) to (As_6) with $\delta(\hbar) \geq C\hbar^\alpha$ for some $C > 0$ and $\alpha < 1$. With this order of width for the energy level window it is not necessary to assume (As_7).*

The first result on quantum signature of classical chaos is the following :

Theorem 4.6 (Ergodic Semi-Classical Theorem) *([72]) Under the assumptions (As_1) to (As_6), $n \geq 2$, and (As_{10}), for every $\hbar > 0$, there exists $M(\hbar) \subseteq \Lambda(\hbar)$, depending only on the Hamiltonian $\hat{H}$, such that :*

$$\lim_{\hbar \searrow 0} \left(\frac{\#M(\hbar)}{\#\Lambda(\hbar)}\right) = 1, \text{ and } \lim_{[\hbar \searrow 0,\, j \in M(\hbar)]} a_{jj}(\hbar) = \int_{\Sigma_E} A d\nu_E, \ \forall A \in \mathcal{O}(0). \tag{4.4}$$

Remark 4.7 *The following question is still open : can we take $M(\hbar) = \Lambda(\hbar)$ in the conclusion of the above lemma, if $n \geq 2$?(it is true for $n = 1$).*

An idea of the proof of the ergodic semi-classical theorem

We have clearly

$$\langle \hat{A}\psi_j, \psi_j\rangle = \frac{1}{T}\int_0^T \langle U_H(-t)\hat{A}U_H(t)\psi_j, \psi_j\rangle dt. \tag{4.5}$$

From the propagation theorem (section 1) we have

$$a_{jj} = \frac{1}{T}\int_0^T \langle \hat{A}(\Phi_H^t)\psi_j, \psi_j\rangle dt + O_T(\hbar).$$

Imagine for a moment that we can invert the limits $\hbar$ tends to 0 and T tends to ∞, we get easily $a_{jj} \overset{\hbar\to 0}{\to} \int_{\Sigma_E} A d\nu_E$. The exact proof is trickier.
Let us replace the Weyl quantization by a positive quantization, the anti-Wick quantization, which is defined in the following way, for $A \in \mathcal{O}(0)$,

$$op_\hbar^{aw}(A)\varphi = (2\pi\hbar)^{-n}\int\int_{\mathbb{R}^{2n}} A(\zeta)\langle\varphi, \varphi_\zeta\rangle\varphi_\zeta d\zeta,$$

where φ_ζ is the Gaussian coherent state centered at ζ defined in section 1.
We have the three following useful properties (see [72]) :
(Aw1) $A \geq 0 \Rightarrow op_\hbar^{aw}(A) \geq 0$.
(Aw2) $op_\hbar^{aw}(A)$ admits an $\hbar$-Weyl symbol $A_w(\hbar)$ given by:

$$A_w(\hbar, x, \xi) = (\pi\hbar)^{-n}\int\int_{\mathbb{R}^{2n}} A(y, \eta)\exp(-\frac{1}{\hbar}[(x-y)^2 + (\xi-\eta)^2])dyd\eta.$$

(Aw3) For every $A \in \mathcal{O}(0)$, $\|op_\hbar^{aw}(A) - op_\hbar^{w}(A)\| = O(\hbar)$ as $\hbar \searrow 0$ where $op_\hbar^w(A) = \hat{A}$.
Thus we can define Radon measures (Husimi measures) on the phase space Z,

$$\int A d\mu_j = \langle op_\hbar^{aw}(A)\psi_j, \psi_j\rangle, \quad A \in \mathcal{S}(Z). \tag{4.6}$$

The distribution $d\mu_j$ is indeed a Radon measure because a positive distribution is a Radon measure according to a well known theorem of L. Schwartz. Let us introduce now the averaged measure

$$dm = \frac{\sum_{j\in\Lambda(\hbar)} d\mu_j}{\#\Lambda(\hbar)}.$$

From the corollary (4.4) and $(Aw3)$ we have, in the sense of weak convergence for Radon measures,

$$\lim_{\hbar\searrow 0} dm = d\nu_E. \tag{4.7}$$

Now using ergodicity the important step, not detailed here (see [72]) is to prove the following proposition

Proposition 4.8 *Under the assumptions* (As_1) *to* (As_6), $n \geq 2$, *and* (As_{10}), *for all* $\epsilon > 0$, *for all* $A \in \mathcal{O}(0)$, *we have*

$$\lim_{\hbar \searrow 0} \left(\frac{\#\{j \in \Lambda(\hbar),\ |\int A d\mu_j - \int A d\nu_E| < \epsilon\}}{\#\Lambda(\hbar)} \right) = 1.$$

From this proposition the semi-classical ergodic theorem follows easily.

Now we want to introduce in the semi-classical context some ideas initiated in the high energy case by S.Zelditch [147]. The point is to estimate the non diagonal matrix elements a_{jk}. We follow here the presentation given in [37]. We begin with a crude estimate which nevertheless explains further restrictions on energy localization.

Proposition 4.9 ([37]) *Under the assumptions* (As_1) *to* (As_5), *for every* $A \in \mathcal{O}(0)$ *there exists* $c_0 > 0$ *such that we have:*

$$|a_{jk}(\hbar)| \leq c_0 \frac{\hbar}{|E_k(\hbar) - E_j(\hbar)|} \quad \forall E_j,\ E_k \in J_{c\ell},\ E_j(\hbar) \neq E_k(\hbar). \tag{4.8}$$

Proof : Let χ be a smooth cutoff, $\chi = 1$ on $J_{c\ell}$ and compactly supported in $\mathbb{R}$. We have clearly:

$$\langle [\hat{A}, \chi(\hat{H})\hat{H}]\varphi_j, \varphi_k \rangle = (E_j(\hbar) - E_k(\hbar))\langle \hat{A}\varphi_j, \varphi_k \rangle.$$

But from the $\hbar$-Weyl calculus (see section.1) we have the well known commutator estimate:

$$\|[\hat{A}, \chi(\hat{H})\hat{H}]\| = O(\hbar) \text{ as } \hbar \searrow 0.$$

The proposition follows. ∎

Remark 4.10 *(i) The proof of the proposition (4.9) can be iterated to get for every* N *the estimate:* $a_{jk}(\hbar) = O\left(\frac{\hbar}{|E_j - E_k|}\right)^N$.
(ii) The proposition shows that it is sufficient to study a_{jk} *for level spacings of order* $\hbar$ *(only this case is considered in the physics literature).*

Let us formulate a second crude result coming easily from Theorem (4.6):

Proposition 4.11 *Let us assume* (As_1) *to* (As_7) *and* $n \geq 2$. *Then for every* $\hbar > 0$ *there exists* $\square(\hbar) \subseteq \Lambda(\hbar) \times \Lambda(\hbar)$ *such that*

$$\lim_{\hbar \searrow 0} \frac{\#\square(\hbar)}{\#\Lambda(\hbar)^2} = 1, \quad \text{and} \quad \lim_{[\hbar \searrow 0,\ (j,k) \in \square(\hbar)]} a_{jk} = 0. \tag{4.9}$$

Proof : Using Parseval equality for orthonormal systems in Hilbert spaces we get:

$$\begin{aligned}\sum_{(j,k)\in\Lambda(\hbar)^2} |a_{jk}|^2 &= \sum_{j\in\Lambda(\hbar)} \langle \Pi_{I(\hbar)}\hat{A}\varphi_j, \hat{A}\varphi_j\rangle \\ &\leq \sum_{j\in\Lambda(\hbar)} \langle \hat{A}^2\varphi_j, \varphi_j\rangle. \end{aligned} \tag{4.10}$$

But we know that $\lim_{\hbar\searrow 0} \#\Lambda(\hbar) = +\infty$ (see [113]) So, using corollary (4.4) we get:

$$\lim_{\hbar\searrow 0} \frac{1}{\#\Lambda(\hbar)^2} \sum_{(j,k)\in\Lambda(\hbar)^2} |a_{jk}|^2 = 0$$

and we get the proposition using the following abstract lemma whose proof is implicit in [72] (part.3-p.319) ∎

Lemma 4.12 *Let us consider a mapping :*

$$]0, +\infty[\ni \hbar \mapsto \Omega(\hbar) \in \mathcal{F}(\mathbb{N}),$$

where $\mathcal{F}(\mathbb{N})$ is the set of all finite subsets of integers. Let us consider a serie of complex numbers (depending on $\hbar$): $\{(a_j(\hbar)\}_{j\in\mathbb{N}}$ such that :

$$\lim_{\hbar\searrow 0} \frac{1}{\#\Omega(\hbar)} \sum_{j\in\Omega(\hbar)} |a_j(\hbar)| = 0,$$

then there exists $\tilde{\Omega}(\hbar) \subseteq \Omega(\hbar)$ such that :

$$\lim_{\hbar\searrow 0} \frac{\#\tilde{\Omega}(\hbar)}{\#\Omega(\hbar)} = 1 \text{ and } \lim_{[\hbar\searrow 0,\, j\in\tilde{\Omega}(\hbar)]} a_j(\hbar) = 0.$$

A connection between classical chaos and the behaviour of non diagonal matrix elements was established by Zelditch [146] for the Laplace-Beltrami operator on a compact negative curvature manifolds. In [37] these results are extended to the semi-classical setting. Let us formulate now the results concerning the non diagonal matrix elements and classical chaos.

Theorem 4.13 (Ergodic case[37]) *We assume that the assumptions (As_1) to (As_6) and (As_{10}) are fufilled.*
Let us consider an observable $\hat{A} = op_\hbar^w(A)$ with $A \in \mathcal{O}(m)$. Then we have :
(i) For every $\varepsilon > 0$ there exists $T_\varepsilon > 0$ and $\hbar_\varepsilon > 0$ such that:

$$\forall j \in M(\hbar),\ \forall k \in \Lambda(\hbar),\ 0 < \hbar \leq \hbar_\varepsilon;\ j \neq k; |E_j(\hbar) - E_k(\hbar)| \leq \frac{\pi\hbar}{2T_\varepsilon} \Rightarrow |a_{jk}| \leq \varepsilon. \tag{4.11}$$

(ii) For every family of matrix elements $\{a_{jk}\}_{(j,k)\in\Omega(\hbar)}$ satisfying :
(α) $\Omega(\hbar) \subseteq \Lambda(\hbar)^2$ and $(j,k) \in \Omega(\hbar) \Rightarrow j \neq k$,

(β) $\lim_{[\hbar\searrow 0,\ (j,k)\in\Omega(\hbar)]}\left(\frac{E_j(\hbar)-E_k(\hbar)}{\hbar}\right)=0,$

(γ) $\liminf_{\hbar\searrow 0}\left(\frac{\#\Omega(\hbar)}{\#\Lambda(\hbar)}\right)>0,$

there exists $\tilde{\Omega}(\hbar)\subseteq\Omega(\hbar)$ *such that :*

$$\lim_{\hbar\searrow 0}\frac{\#\tilde{\Omega}(\hbar)}{\#\Omega(\hbar)}=1 \text{ and } \lim_{\hbar\searrow 0} a_{jk}=0, \quad \text{uniformly for } (j,k)\in\tilde{\Omega}(\hbar). \tag{4.12}$$

The above statement means : for all $\epsilon>0$, *there exists* $\hbar_\epsilon>0$, *such that for every* $0<\hbar<\hbar_\epsilon$ *and for every* $(j,k)\in\tilde{\Omega}(\hbar)$ *we have* $|a_{jk}|\leq\epsilon$.
Furthermore, the set $M(\hbar)$ *is the same as in Theorem (2-1) and the set* $\tilde{\Omega}(\hbar)$ *of (ii) can also be chosen independently of the observable* $A(\hbar)$.

Remark 4.14 *(1)There exists a lot of non diagonal families satisfying the assumptions of Theorem (3.5) (ii).*
(2) Let us consider the harmonic oscillator in one degree of freedom. For $E>0$ *it is not difficult to construct* $A(\hbar)$ *such that* $\langle A(\hbar)\varphi_j,\varphi_{j+1}\rangle\to 1$ *and* $(2j+1)\hbar\to E$ *as* $\hbar\searrow 0$ *(take* $a(x,\xi)=x$ for $|x|\leq\sqrt{E+1}$ *). We can compare this fact with (21).*

To give further results we introduce a stronger assumption :
(As_{11}) *The dynamical system* $(\Sigma_E, d\nu_E, \Phi^t)$ *is mixing, that means:*

$$\lim_{t\nearrow+\infty}\left(\int_{\Sigma_E}A(\Phi^t(z))A(z)d\nu_E(z)\right)=\left(\int_{\Sigma_E}A(z)d\nu_E(z)\right)^2.$$

Let us also introduce the weak-mixing property :
(As^*_{11}) *The dynamical system* $(\Sigma_E, d\nu_E, \Phi^t)$ *is weak-mixing, that means:*

$$\lim_{T\nearrow+\infty}\frac{1}{2T}\int_{-T}^{T}\left(\int_{\Sigma_E}A(\Phi^t(z))A(z)d\nu_E(z)\right)dt=\left(\int_{\Sigma_E}A(z)d\nu_E(z)\right)^2.$$

Theorem 4.15 (Mixing case, [37]) *Let us assume* (As_1) *to* (As_6) *and* (As_{11}). *Let* $\hat{A}$ *be an observable as in Theorem (4.13).*
(i) There exists $M(\hbar)\subseteq\Lambda(\hbar)$ *(*$M(\hbar)$ *is the same as above) such that:*

$$\lim_{\hbar\searrow 0}\frac{\#M(\hbar)}{\#\Lambda(\hbar)}=1, \quad \lim_{[\hbar\searrow 0\ j\in M(\hbar),\ k\in\Lambda(\hbar),\ j\neq k]} a_{jk}=0, \quad \forall A\in\mathcal{O}(m).$$

(ii) For every family of matrix elements $\{a_{jk}\}_{(j,k)\in\Omega(\hbar)}$ *such that:*
(α) $\Omega(\hbar)\subseteq\Lambda(\hbar)^2$ *and* $(j,k)\in\Omega(\hbar)\Rightarrow j\neq k$,
(β) $\exists\tau\in\mathbb{R}$ *such that* $\lim_{[\hbar\searrow 0,\ (j,k)\in\Omega(\hbar)]}\left(\frac{E_j(\hbar)-E_k(\hbar)}{\hbar}\right)=\tau,$

(γ) $\liminf_{\hbar\searrow 0}\left(\frac{\#\Omega(\hbar)}{\#\Lambda(\hbar)}\right) > 0$,
there exists $\tilde{\Omega}(\hbar) \subset \Omega(\hbar)$ *such that:*

$$\lim_{\hbar\searrow 0}\frac{\#\tilde{\Omega}(\hbar)}{\#\Omega(\hbar)} = 1 \text{ and } \lim_{\hbar\searrow 0} a_{jk} = 0, \quad \text{uniformly for } (j,k) \in \tilde{\Omega}(\hbar). \tag{4.13}$$

The set $\tilde{\Omega}(\hbar)$ *of (ii) can also be chosen independently of the observable* $\hat{A}$.

Let us remark that the observable $\hat{A}$ need not be bounded. This can be applied, for example, to the position or momentum observables (conductivity).
Now we shall discuss some other aspects of Zelditch's work in the semi-classical setting.
Let us consider first the mapping $A \mapsto A(\Phi^t) = V_t(A)$ as a unitary group in $L^2(\Sigma_E)$ (Koopman operator). By Stone's theorem we have

$$\langle A(\Phi^t), A\rangle = \int_{\mathbb{R}} e^{it\tau} d\mu_A(\tau), \tag{4.14}$$

where μ_A is a Radon measure on $\mathbb{R}$ (spectral measure).
On the quantum side let us introduce the Radon measure m_A defined as

$$\int_{\mathbb{R}} f dm_A = \frac{1}{\#\Lambda(\hbar)} \sum_{E_k\in I(\hbar);E_j\in J} f\left(\frac{E_k - E_j}{\hbar}\right)|a_{j,k}|^2. \tag{4.15}$$

Then we have

Proposition 4.16 *Let us assume* (As_1) *to* (As_7). *Then for every* $f \in C(\mathbb{R})$ *we have*

$$\lim_{\hbar\searrow 0}\int_{\mathbb{R}} f dm_A = \int_{\mathbb{R}} f d\mu_A.$$

Idea of Proof: Let us recall the notations $\hat{A}(t) = U(-t)\hat{A}U(t)$, $\omega_{jk} = \frac{E_j - E_k}{\hbar}$. Using the Parseval identity, we get

$$\mathrm{tr}(\Pi_{I(\hbar)}\hat{A}(t)^\star\hat{A}) = \sum_{E_k\in I(\hbar),\ E_j\in J} e^{it\omega_{jk}}|a_{jk}|^2 + O(\hbar^\infty). \tag{4.16}$$

It is enough to consider $f \in \mathcal{S}(\mathbb{R})$. Hence using the inverse Fourier transform and the Lebesgue convergence theorem we get the result as in [148]. ∎

Now we want to discuss a definition given by Sunada [137] and Zelditch [148] concerning quantum ergodicity and quantum mixing (in a semi-classical sense).
Let us recall the following spectral characterizations (see [8]).

- The classical flow Φ^t is ergodic in Σ_E if and only if 1 is a simple eigenvalue of V_t.

- The classical flow Φ^t is weak mixing in Σ_E if and only if the constant functions are the only eigenfunction of V_t in $L^2(\Sigma_E)$.

Let us denote by $\mathcal{S}_0(E)$ the set of observables A such that $A \in \mathcal{S}(Z)$ and $\int_{\Sigma_E} A d\nu_E = 0$. Let us introduce

$$F_T(\tau)A = \frac{1}{2T}\int_{-T}^{T} \mathrm{e}^{-it\tau} V_t(A)dt.$$

We have the following consequence of Wiener theorem

$$s - \lim_{T\to\infty} F_T(\tau) = P_\tau, \tag{4.17}$$

where P_τ is the orthogonal projector onto the eigenfunctions of V_t with eigenvalue $\mathrm{e}^{-it\tau}$. On the quantum side the following limit exists too

$$\bar{A}_T(\tau) := \frac{1}{2T}\int_{-T}^{T} \mathrm{e}^{-it\tau}\hat{A}(t)dt, \text{ then } w - \lim_{T\to\infty} \bar{A}_T(\tau) = \bar{A}(\tau). \tag{4.18}$$

Following Sunada and Zelditch,

Definition 4.17 *1. The quantum evolution $U(t)$ is semi-classically-quantum-ergodic at the energy level E if the following condition holds, for all $A \in \mathcal{S}_0(E)$,*

$$\frac{1}{\#\Lambda(\hbar)} \|\Pi_{I(\hbar)}\bar{A}(0)\Pi_{I(\hbar)}\|^2_{HS} = o(1). \tag{4.19}$$

2. The quantum evolution $U(t)$ is semi-classically-quantum-weak-mixing at the energy level E if the following condition holds for all $A \in \mathcal{S}_0(E)$, for all $\tau \in \mathbb{R}$,

$$\frac{1}{\#\Lambda(\hbar)} \|\Pi_{I(\hbar)}\bar{A}(\tau)\Pi_{I(\hbar)}\|^2_{HS} = o(1). \tag{4.20}$$

Let us remark that we have, by an easy computation,

$$\left\|\Pi_{I(\hbar)}\bar{A}(\tau)\Pi_{I(\hbar)}\right\|^2_{HS} = \sum_{\omega_{jk}=\tau;\ E_{j,k}\in I(\hbar)} |a_{jk}|^2.$$

It is known that classical ergodicity (resp. classical mixing) entail quantum ergodicity (rep. quantum mixing) ([148, 37]). In the high energy case Zelditch asked the following questions: does quantum ergodicity (rep. quantum mixing) entail classical ergodicity (resp. classical mixing)? The answer is still unknown. Sunada[137] and Zelditch[148] have proven that quantum ergodicity (rep. quantum mixing) plus a condition $(\star)$ entails classical ergodicity (resp. classical mixing).
The following properties are proved in [37].

Theorem 4.18 *1. If the classical system is ergodic on Σ_E then the quantum evolution $U(t)$ is semi-classically-quantum-ergodic at the energy level E and furthermore we have, for all $A \in \mathcal{S}_0(E)$, $\forall\epsilon > 0\ \exists\delta_\epsilon > 0$, $\hbar_\epsilon > 0$ such that*

$$(\star)\quad \frac{1}{\#\Lambda(\hbar)} \sum_{E_k\in I(\hbar),\ |\omega_{jk}|\leq\delta_\epsilon} |a_{jk}|^2 \leq \epsilon,\ \forall\hbar \in]0, \hbar_\epsilon].$$

2. *If the classical system is weak mixing on Σ_E then the quantum evolution $U(t)$ is semi-classically-quantum weak mixing at the energy level E and furthermore we have, for all $A \in \mathcal{S}_0(E)$, for all $\tau \in \mathbb{R}$, $\forall\epsilon > 0\ \exists\delta_\epsilon > 0$, $\hbar_\epsilon > 0$ such that*

$$(\star\star)\quad \frac{1}{\#\Lambda(\hbar)} \sum_{E_k\in I(\hbar),\, |\omega_{jk}-\tau|\le\delta_\epsilon} |a_{jk}|^2 \le \epsilon,\ \forall\hbar \in]0,\hbar_\epsilon].$$

The following result is a semi-classical translation of Sunada [137] and Zelditch [148].

Theorem 4.19 *1. The condition $(\star)$ holds if and only if the classical system is ergodic on the energy level E.*

2. *The condition $(\star\star)$ holds if and only if the classical system is weak mixing on the energy level E.*

Proof:
Let us assume $(\star)$ holds. From [37] we get

$$\frac{1}{\#\Lambda(\hbar)} \sum_{E_j\in I(\hbar),\, E_k\in J} |a_{jk}|^2 \left|\frac{\sin\omega_{jk}T}{\omega_{jk}T}\right|^2 = \frac{1}{\#\Lambda(\hbar)} \sum_{E_j\in I(\hbar)} \langle A_T^* A_T\varphi_j, \varphi_j\rangle + o(1), \tag{4.21}$$

where $o(1)$ is for $\hbar \to 0$ (depending on T).
For every $\delta > 0$ we have

$$\sum_{E_j\in I(\hbar),\, E_k\in J; |\omega_{jk}|\ge\delta} |a_{jk}|^2 \left|\frac{\sin\omega_{jk}T}{\omega_{jk}T}\right|^2 \le \frac{1}{T\delta} \sum_{E_j\in I(\hbar),\, E_k\in J} |a_{jk}|^2. \tag{4.22}$$

From the corollary (4.3), we have

$$\limsup_{\hbar\to 0} \left\{ \sum_{E_j\in I(\hbar),\, E_k\in J; |\omega_{jk}|\ge\delta} |a_{jk}|^2 \left|\frac{\sin\omega_{jk}T}{\omega_{jk}T}\right|^2 \right\} \le \frac{C}{T\delta}, \tag{4.23}$$

where C is a constant independent on T. Now using (4.21) and corollary (4.3) again, choosing $\delta = \delta_\epsilon$, we get

$$\int_{\Sigma_E} \left|\frac{1}{2T}\int_{-T}^{T} A(\Phi^t)dt\right|^2 d\nu_E \le \epsilon + \frac{C}{T\delta}.$$

So, $\forall A \in C^\infty(\Sigma_E)$ such that $\langle A\rangle = 0$ we have proven

$$\lim_{T\to+\infty} \int_{\Sigma_E} \left|\frac{1}{2T}\int_{-T}^{T} A(\Phi^t)dt\right|^2 d\nu_E = 0. \tag{4.24}$$

By an easy smoothing argument we can extend (4.24) for $A \in L^2(\Sigma_E)$ such that $\langle A \rangle = 0$. Now we conclude using the spectral characterization of ergodicity. If $A \in L^2(\Sigma_E)$ such that $A(\Phi^t) = A$ and $\langle A \rangle = 0$, then by (4.24) we have $A = 0$, a.e on Σ_E so Φ^t is ergodic. ∎

Now let us assume $(\star\star)$ and prove that the system is weak mixing. We already know that the system is ergodic i.e. 1 is a simple eigenvalue for the Koopman operator.
As in [37] let us introduce the function θ such that

$$\hat{\theta}(\lambda) = \left(\frac{\sin\lambda}{\lambda}\right)^2, \quad \theta_T(t) = \frac{1}{T}\theta(\frac{t}{T}),$$

so we have

$$\sum_{E_k \in J} |a_{jk}|^2 \hat{\theta}_T(\omega_{jk} - \lambda) = \int e^{it\tau}\theta_T(t)\langle\varphi_j, A(t)A^*\varphi_j\rangle dt + O(\hbar), \tag{4.25}$$

uniformly in $T > 0$, $\tau \in \mathbb{R}$, $E_j \in I(\hbar)$.
So, as in the ergodic case, we get easily, for every $A \in C^\infty(\Sigma_E)$, $\tau \neq 0$,

$$\int e^{it\tau}\theta_T(t)C_A(t)dt = 0, \tag{4.26}$$

where $C_A(t)$ is the autocorrelation function

$$C_A(t) = \int_{\Sigma_E} A(\Phi^t(z))\bar{A}(z)d\nu_E(z).$$

As above, we can extend (4.26) to every $A \in L^2(\Sigma_E)$. Let us consider now an eigenfunction A of the Koopman operator with eigenvalue $e^{-it\tau}$, $\tau \neq 0$, $A \in L^2(\Sigma_E)$, $A(\Phi^t) = e^{-it\tau}A$, $\forall t \in \mathbb{R}$.
Using (4.26) we get $A = 0$ a.e on Σ_E. ∎

Before closing this section let us mention here three other interesting subjects concerning semi-classical asymptotics for bound states. We refer to the original papers for statements and proofs.

- Hamiltonians invariant with respect to a symmetry group (finite or compact) [51, 50].
- Integrable Hamiltonians and systems of several quantum commuting observables [34, 27].
- Semi-classical limit of the Berry's phase [11, 60].

Let us remark that it is an interesting open question to study the Berry phase and its semi-classical limit for chaotic systems [15].

5 Semi-classical approximation in Quantum Scattering Theory

In this section we want to report on some results concerning semi-classical spectral analysis of long range perturbations of momentum dependent Hamiltonians on $\mathbb{R}^n$ such that their difference is short range. Typical examples are Schrödinger Hamiltonians: $\hat{H}_j = -\hbar^2\Delta + V_j$ with $V_j(x) = O(|x|^{-\delta})$, $j = 1, 2$, $V_2(x) - V_1(x) = O(|x|^{-\rho})$ with $\delta > 0$, $\rho > n$. We can also consider perturbations by magnetic fields and cases where Δ is the Laplace-Beltrami operator for asymptotically flat metrics on $\mathbb{R}^n$.
For the scattering pair $(\hat{H}_2, \hat{H}_1)$ a natural time delay operator can be defined and also an average time-delay, $\tau^D(\hbar, \lambda)$, depending on the energy λ and the semi-classical parameter $\hbar$. It is related to the spectral shift function and also to the scattering phase. We shall consider here asymptotics for these spectral functions. We shall follow essentially the paper [127].
There are many other interesting results known in semi-classical scattering: behaviour of the scattering cross sections, many body problems, resonances. We choose here to report only on one subject more or less related to some trace perturbation formulas. Let us begin by introducing some of the quantum scattering notions involved.

5.1 Time Delay - Spectral Shift - Scattering Phase

Let us consider two quantum Hamiltonians $\hat{H}_1$ and $\hat{H}_2$ acting in the Hilbert space $\mathcal{H}$. $\hat{H}_1$ and $\hat{H}_2$ being self-adjoint operators, they generate unitary groups: $U_j(t) = \exp(-it\hat{H}_j)$, $j = 1, 2$.
Let us consider a family of bounded operators in $\mathcal{H}$: $\{P_R\}_{R\geq 0}$ such that $\lim_{R\to+\infty} P_R = 1\!\!1_{\mathcal{H}}$, strongly on $\mathcal{H}$; $1\!\!1_{\mathcal{H}}$ being the identity on $\mathcal{H}$ (P_R are used to localize quantum particles).
For ψ in $\mathcal{H}$, the local sojourn time of $\hat{H}_j$ in P_R is defined by

$$\langle T_{j,R}\psi, \psi\rangle = \int_{-\infty}^{+\infty} \|P_R U_j(t)\psi\|^2 dt. \tag{5.1}$$

Assume now that $\hat{H}_2$ is a short range perturbation of $\hat{H}_1$ in the sense that the wave operators:

$$\Omega_\pm = \lim_{t\to\pm\infty} U_2(-t)U_1(t)\Pi_{ac}(\hat{H}_1)$$

exist and are complete, where $\Pi_{ac}(\hat{H}_1)$ denotes the projection on the absolutely continuous subspace of $\hat{H}_1$.
In [120], Jauch-Misra-Sinha gave the following definition of Time-Delay for the pair $(\hat{H}_2, \hat{H}_1)$:
Let us assume that: $\langle T_{1,R}\psi, \psi\rangle < +\infty$ and $\langle T_{2,R}\Omega_-\psi, \Omega_-\psi\rangle < +\infty$.
The local time-delay in P_R, for the system in the state ψ, is defined as the difference:

$$\langle T_R^D\psi, \psi\rangle = \langle T_{2,R}\Omega_-\psi, \Omega_-\psi\rangle - \langle T_{1,R}\psi, \psi\rangle. \tag{5.2}$$

Using the intertwining property of the wave operators:

$\Omega_- U_1(t) = U_2(t)\Omega_-$, we have also (Amrein-Cibils [6])

$$T_R^D = \int_{-\infty}^{+\infty} U_1(-t)\left(\Omega_-^\star . P_R^2 \Omega_- - P_R^2\right) U_1(t)dt. \tag{5.3}$$

The total time-delay of the system in $\mathcal{H}$ is defined by:

$$\langle T^D \psi, \psi\rangle = \lim_{R\to+\infty} \langle T_R^D \psi, \psi\rangle, \tag{5.4}$$

whenever the limit exists.
For the usual Schrödinger pair, we have: $\hat{H}_1 = \hat{H}_0 \stackrel{\text{def}}{=} -\frac{\hbar^2}{2m}\triangle$ and $\hat{H}_2 = \hat{H}_0 + V$ acting in the Hilbert space $L^2(\mathbb{R}^n)$ where V is supposed to be smooth and such that for a $\rho > 1$ we have: $|\partial_x^\alpha V(x)| \leq C_\alpha(1+|x|)^{-\rho-|\alpha|}$.
It was proved independently by Wang [140] and Nakamura [108] that, taking for the localization operator: $P_R\psi(x) = \chi(\frac{|x|}{R})\psi(x)$ with χ smooth with compact support on $\mathbb{R}$ and $\chi(r) = 1$, for $|r| \leq 1$, the time-delay T^D exists as a self-adjoint operator in $L^2(\mathbb{R}^n)$ (unbounded, with a dense domain) commuting with $\hat{H}_0$. Furthermore they proved that in the spectral representation of $\hat{H}_0$, T^D is related with the scattering matrix $S(\lambda)$ of the pair $(\hat{H}_2, \hat{H}_0)$ by the Eisenbud-Wigner formula

$$T^D(\lambda) = -iS(\lambda)^\star \frac{dS(\lambda)}{d\lambda}. \tag{5.5}$$

Amrein-Cibils [6] considered also the case when χ is not smooth.
The local time-delay operator T_R^D commutes with $\hat{H}_0$ (see (1.3)) so it has a diagonal form in the spectral representation of $\hat{H}_0$ and the local-average time-delay can be defined by:

$$\tau_R^D(\lambda) = \mathrm{tr}\left(T_R^D(\lambda)\right), \tag{5.6}$$

tr being the trace functional in $L^2(\mathbb{S}^{n-1})$ ($\mathbb{S}^{n-1}$is the unit sphere in $\mathbb{R}^n$) Furthermore, if V decreases quickly enough ($\rho > n$), we know that $T^D(\lambda)$ is a trace-class operator on $L^2(\mathbb{S}^{n-1})$, so that we can define the average time-delay at energy λ for the scattering process $(\hat{H}_2, \hat{H}_1)$, by:

$$\tau^D(\lambda) = \mathrm{tr}\left(T^D(\lambda)\right).$$

As it is expected, we have : $\lim_{R\to+\infty} \tau_R^D(\lambda) = \tau^D(\lambda)$. Moreover the average time-delay $\tau^D(\lambda)$ is connected with the spectral shift function of Krein and also with the scattering phase for $(\hat{H}_2, \hat{H}_1)$. The spectral shift function $s(\hbar, \lambda)$ is defined as a distribution on $\mathbb{R}$ by :

$$\mathrm{tr}\left(f(\hat{H}_2) - f(\hat{H}_1)\right) = -\int_{-\infty}^{+\infty} f'(\lambda)s(\hbar,\lambda)d\lambda, \tag{5.7}$$

$\forall f \in C_0^\infty(\mathbb{R})$.
The (total) scattering phase: $\theta(\hbar, \lambda)$, is defined by

$$\det(S(\lambda)) = \exp(2i\theta(\hbar, \lambda)). \tag{5.8}$$

A famous result of Birman-Krein [16] (see also the book by Yafaev [145] for complete and accessible proofs) says that on $]0, +\infty[$ we have: $\theta' = \pi s'$

From the Eisenbud-Wigner formula we have: $\tau_D(\hbar,\lambda) = -2\theta'(\hbar,\lambda)$.
So the following three notions: *average time-delay, spectral shift function and scattering phase*, coïncide with different physical meanings.
Several papers stated results about the asymptotics for $\tau^D(\hbar,\lambda)$ in the usual Schrödinger case $(\hat{H}_0, \hat{H}_2)$ in the high energy régime ($\lambda \nearrow +\infty$) or in the semiclassical régime ($\hbar \searrow 0$) (see [22, 31, 61, 117, 129, 122, 123]).
In the next section we shall give a unified presentation and extensions of these results when $\hat{H}_0$ is replaced by a long range perturbation $\hat{H}_1$ of $\hat{H}_0$ and $\hat{H}_2$ is a short range perturbation of $\hat{H}_1$. The detailed proofs appeared in [127].

5.2 Perturbations of the Laplace operator

Let us consider long range perturbations of the Laplace operator in $\mathbb{R}^n$: $\hat{H}_0 = -h^2\Delta$ obtained with a Riemannian metric g, a magnetic potential A and an electric potential V. g and A are determined by their coefficients: $g = \{g_{jk}\}$, $A = (A_1, A_2, ..., A_n)$. As usual we denote $G = \det(g)$, $\{g^{jk}\} = \{g_{jk}\}^{-1}$.
The natural quantum Hamiltonian to compare with $\hat{H}_0$ in $L^2(\mathbb{R}^n)$ is

$$\hat{H}(g,A,V) = -G^{-1/4}. \sum_{\substack{1\leq j\leq n\\ 1\leq k\leq n}} (\hbar\partial_j + iA_j)G^{1/2}g^{jk}(\hbar\partial_k + iA_k)G^{-1/4} + V. \tag{5.9}$$

The data g, A, V are supposed to be smooth and satisfy the following decay assumptions:

$$\exists\delta > 0\,\text{such that}\,\forall\alpha, \text{multiindex}, \exists C_\alpha \quad \text{such that} \quad \forall x \in \mathbb{R}^n,$$
$$|\partial_x^\alpha\left(g(x) - g_0(x)\right)| + |\partial_x^\alpha A(x)| + |\partial_x^\alpha V(x)| \leq C_\alpha(1+|x|)^{-\delta-|\alpha|}, \tag{5.10}$$

where g_0 is the flat Euclidean metric. Let us consider the two Hamiltonians:
$\hat{H}_k = \hat{H}(g^k, A^k, V^k)$, $k = 1, 2$. We assume that g^k, A^k, V^k satisfy (5.10) and that:

$$\exists\rho > 1\,\text{such that}\,\forall\alpha, \text{multiindex}, \exists C_\alpha\,\text{such that}\,\forall x \in \mathbb{R}^n,$$
$$|\partial_x^\alpha\left(g^2(x) - g^1(x)\right)| + |\partial_x^\alpha\left(A^2(x) - A^1(x)\right)|$$
$$+|\partial_x^\alpha\left(V^2(x) - V^1(x)\right)| \leq C_\alpha(1+|x|)^{-\rho-|\alpha|}. \tag{5.11}$$

For all results stated below we shall assume that the pair $(\hat{H}_1, \hat{H}_2)$ satisfies (5.10) and (5.11) for $\delta > 0$ and $\rho > n$. Let us denote by $\tau^D(\hbar,\lambda)$ the relative time-delay for this pair. To prove pointwise energy asymptotic results for $\tau^D(\hbar,\lambda)$ in the high energy limit ($\lambda \nearrow +\infty$) or in the semiclassical limit ($\hbar \searrow 0$) is a rather difficult problem. It is well known that the same problem is much easier after some regularization procedure in the energy variable λ is applied. The point is, if we want to fix the energy, we have to get information on the propagator for every time, due to the time-energy uncertainty principle.
As a preliminary result we begin with asymptotics in weak sense in the energy variable. Under the previous assumptions, we have:

Theorem 5.1 (weak asymptotic trace formula) *For every f in the Schwartz space $\mathcal{S}(\mathbb{R})$, $f(\hat{H}_2) - f(\hat{H}_1)$ is a trace class operator and we have the full asymptotics:*
(i) as $h \searrow 0$

$$tr\left(f(\hat{H}_2) - f(\hat{H}_1)\right) \asymp \hbar^{-n} \sum_{j\geq 0} c_{2j}(f)\hbar^{2j}. \tag{5.12}$$

The coefficients $c_{2j}(f)$ are distributions in f, in principle computable in terms of the symbols of $\hat{H}_2$ and $\hat{H}_1$.
(ii) Assume $h = 1$. Then as $\beta \searrow 0$ we have:

$$tr\left(f(\beta\hat{H}_2) - f(\beta\hat{H}_1)\right) \asymp \beta^{-n/2} \sum_{j\geq 0} C_j(f)\beta^j. \tag{5.13}$$

The coefficients $C_{2j}(f)$ and $C_j(f)$ are distributions in f, in principle computable in terms of the symbols of $\hat{H}_2$ and $\hat{H}_1$.

This preliminary result is a direct consequence of the functional calculus for pseudodifferential operators, as presented in [73, 44, 122](see section 3). An interesting approach concerning Schrödinger operators is due to Melin [106].

Let us state some more accurate results:
In what follows, $\sigma_{pp}(L)$ denotes the set of eigenvalues of $\hat{H}$; $\sigma(\hat{H})$; $\sigma_{ac}(\hat{H})$; $\sigma_{sc}(\hat{H})$ will denote respectively the whole spectrum; the absolutely continuous spectrum and the singular continuous spectrum of $\hat{H}$.

Theorem 5.2 (High energy asymptotics) *i) The relative time-delay $s(\hbar, \lambda)$ is C^∞ in $]0, +\infty[\setminus(\sigma_{pp}(\hat{H}_1) \cup \sigma_{pp}(\hat{H}_2))$.*
ii) Assume $\hbar$ fixed i.e. $\hbar = 1$. If the metrics g^k, $(k = 1, 2)$, have no trapped geodesics, then there exists $\lambda_0 > 0$ such that $s(\hbar, \cdot)$ is C^∞ in $]\lambda_0, +\infty[$ and $\forall k \in \mathbb{N}$, $\frac{d^k s}{d\lambda^k}(\lambda)$ has a complete asymptotic expansion for $\lambda \nearrow +\infty$

$$\frac{d^k s}{d\lambda^k}(\lambda) \asymp \lambda^{n/2-k-1}\left(\sum_{j\geq 0} \alpha_j^{(k)}\lambda^{-j}\right). \tag{5.14}$$

In particular we have:

$$\alpha_0^{(0)} = c(n)\int_{\mathbb{R}^n} (dv_{g^2} - dv_{g^1}),$$

where dv_g denotes the volume form defined by g and $c(n)$ is a universal constant depending only on the dimension n:

$$c(n) = \frac{4\pi^{(n+1)/2}}{\Gamma(n/2+1)}.$$

Let us consider now the case when $\lambda > 0$ is fixed and $\hbar \searrow 0$. To formulate the next result we consider the $\hbar$-principal-symbol H_k of $\hat{H}_k$ which is given by $H_k(x, \xi) = \langle g^k(x)(\xi + A^k(x)), \xi + A^k(x)\rangle + V^k(x)$.

An energy interval $J \subset]0, +\infty[$ is said to be non trapping for the classical Hamiltonian H if for every $\lambda \in J$, every classical path for the flow Φ_H^t on the surface of energy λ escapes to infinity as times goes to plus or minus infinity (see below for a more precise definition).

Theorem 5.3 (Semi-classical Asymptotics) *If J is a compact interval, $J \subset]0, +\infty[$, non trapping for H_j, $j = 1, 2$, then for $\hbar$ small enough we have:*

$$s(\hbar, \lambda) \asymp \hbar^{-n}. \sum_{j \geq 0} c_j(\lambda)\hbar^j \text{ as } \hbar \searrow 0, \text{ uniformly for } \lambda \in J. \tag{5.15}$$

Furthermore this expansion can be differentiated in λ to any order.

Remark 5.4 1. *It follows from the non trapping condition and virial theorem that for $\hbar$ small enough $\hat{H}_j$ has no eigenvalues in J.*

2. *The above asymptotics in the high energy case and semi-classical case above were proven in this form in [125]. For $\hat{H}_1 = -\hbar^2\Delta$ the asymptotic have been proven in [33, 61, 117, 100, 124] under various assumptions on the perturbation, in the high energy case. The semi-classical case was proven the first time in [130] for g equal to the flat metric g_0 and $A = 0$.*

The particular case $\hat{H}_1 = -h^2\Delta$ shows that full asymptotics as in Theorem 1.1 and 1.2 cannot hold in general if some classical path is trapped. In particular it was proved in [59] that a Breit-Wigner formula holds for $\frac{ds}{d\lambda}$. We shall come back to this point below. However, even if there are classically trapped rays, we still get estimates for the scattering phase $s(\hbar, \lambda)$ similar to Weyl estimates, well known for the number of bound states (see section 3).
It is also interesting to formulate the result for the Riesz means of the average time-delay which are defined as we did for the discrete spectrum in section 3. The Riesz mean of order γ for $s(\hbar)$ is defined by :

$$s_\gamma(\hbar, \lambda) = \int_{-\infty}^{\lambda} (\lambda - \mu)^\gamma ds(\hbar, \mu).$$

To state the next results we replace the non trapping assumption by weaker control of the resolvent close to the continuous spectrum. So, let us introduce the resolvent: $R_j(z) = (\hat{H}_j - z)^{-1}$, and the following conditions:
There exists positive numbers s_0, S, k, C, such that for $0 < |\tau| \leq 1$, $\lambda \in J$, $\hbar \in]0, 1]$, we have:

$$\| < x >^{-s_0} R_j(\lambda + i\tau) < x >^{-s_0} \| \leq C \exp(S\hbar^{-k}) \tag{5.16}$$

and, for $\hbar = 1$, $0 < |\tau| \leq 1$, $\lambda \geq 1$, we consider:

$$\| < x >^{-s_0} R_j(\lambda + i\tau) < x >^{-s_0} \| \leq C \exp(S\lambda^k). \tag{5.17}$$

Theorem 5.5 (Riesz means Asymptotics) *For every $\gamma \geq 0$, we have:*
i) Let us assume that J is a non critical compact interval for H_j, and (5.16) holds for

$j = 1,\ 2$. *Then we have the following finite asymptotic expansion as* $\hbar \searrow 0$ *and uniformly for* $\lambda \in J$:

$$s_\gamma(\hbar, \lambda) = \hbar^{-n} \sum_{j=0}^{j=[\gamma]+} c_{j,\gamma}(\lambda)\hbar^j + O(\hbar^{-n+\gamma+1}). \tag{5.18}$$

Furthermore if on the energy surfaces: $\{\hat{H}_j = \lambda\}$ *for j=1, 2, the set of closed trajectories is of measure 0 for the Liouville measure, then the remainder term can be improved to* $o(\hbar^{-n+\gamma+1})$ *and we get a term more if* $\gamma \in \mathbb{N}$.
In particular, for $\gamma = 0$, *we have the Weyl law:*

$$s(\hbar, \lambda) = w(\lambda)\hbar^{-n} + O(\hbar^{1-n}), \tag{5.19}$$

where:

$$w(\lambda) = (2\pi)^{-n} \int_{\mathbb{R}^n} \left(\int_{H_2(x,\xi)\leq\lambda} d\xi \ - \int_{H_1(x,\xi)\leq\lambda} d\xi \right) dx. \tag{5.20}$$

ii) Assume that $\hbar$ *is fixed,* $\hbar = 1$ *and (5.17) holds for* $\hat{H}_j,\ j = 1,\ 2$. *Then we have the finite asymptotics as* $\lambda \nearrow +\infty$:

$$s_\gamma(\hbar, \lambda) = \lambda^{n/2+\gamma} \sum_{j=0}^{j=[\gamma]+} \alpha_{j,\gamma}\lambda^{-j} + O\left(\lambda^{(n-1)/2}\right). \tag{5.21}$$

Furthermore if the set of closed geodesics for g^j, $j = 1, 2$ *is of measure 0 for the Liouville measure, then the remainder term in (5.21) can be improved to* $o(\lambda^{(n-1)/2})$ *and we get a term more if* $\gamma \in \mathbb{N}$.
In particular, for $\gamma = 0$, *we get that* $s(\lambda)$ *satisfies the following Weyl law:*

$$s(\lambda) = W_e\lambda^{\frac{n}{2}} + O(\lambda^{\frac{n-1}{2}}). \tag{5.22}$$

We have:

$$W_e = d(n) \int_{\mathbb{R}^n} (dv_{g^2} - dv_{g^1}), \tag{5.23}$$

where dv_g *denotes the volume form defined by* g *and* $d(n)$ *is a universal constant depending only on the dimension* n:

$$d(n) = \frac{2\pi^{n/2+1}}{n\Gamma(n/2+1)}.$$

Remark 5.6 *For* $\hat{H}_1 = \hat{H}_0 = -\hbar^2\Delta$ *it is proved in [129] that the above results hold without assumptions (5.16) or (5.17). Even so, conditions (5.16) and (5.17) seem to be very weak conditions. In particular they are satisfied for* $\hat{H}_2 = -\hbar^2\Delta + V$ *when we are in the situation of the "well in an island" (see [59]).*
In the high energy case the first proof of a Weyl estimate for the scattering phase was given by Melrose [105], for compactly support perturbations in odd dimensions, using his estimate on the number of scattering poles.

The above results are corollaries of a more general result which is an $\hbar$-asymptotic trace formula proved in [127]. Before stating this result let us introduce some notations and definitions. In scattering theory we need to control the observables when the particle escapes at ∞, so we have to introduce suitable classes of observables involving some control at infinity in position variable.

Definition 5.7 *(i)If Ω is an open set in $\mathbb{R}^{2n}$, k, $\mu \in \mathbb{R}$, we shall say that $A \in S_\Omega(\mu, k)$ if $A \in C^\infty(\Omega)$ and satisfies there, for every multiindex α, β,*

$$|\partial_x^\alpha \partial_\xi^\beta A(x, \xi)| = O\left(< x >^{\mu-|\alpha|} < \xi >^k\right). \tag{5.24}$$

We shall use the simpler notations: $S_\Omega(\mu) = S_\Omega(\mu, -\infty)$, $S(\mu) = S_{\mathbb{R}^{2n}}(\mu)$.
As usual, $S_\Omega(\mu, k)$ is endowed with the structure of Frechet space defined by the natural seminorms.
(ii) We shall say that a formal series in $\hbar$: $A(\hbar) \asymp \sum_{j\geq 0} \hbar^j A_j$ is a $\hbar$-admissible symbol of weight μ if the following properties hold:
$\forall j \in \mathbb{N}$, $A_j \in S(\mu-j)$; $\forall N \geq 1$; $\hbar^{-N}\left(A(\hbar) - \sum_{j\leq N-1} \hbar^j A_j\right)$ *is uniformly bounded in* $S(\mu-N)$, *as* $\hbar \in]0, 1]$. *We shall denote by $S_{ad}(\mu)$ the set of h-admissible symbols of weight μ.*

Now we can state the trace formula which essentially reduces the study of the gobal average of the time-delay to a local one in the configuration space $\mathbb{R}^n_x$. We sketch a proof of this theorem in section 5.5.

Theorem 5.8 (Asymptotic Representation Formula) *Let $J \subset]0, +\infty[$ be a compact interval. There exists $b_0 > 0$ large enough such that for every $\zeta \in C_0^\infty(\mathbb{R}^n)$ satisfying: $\zeta(x) = 1$ for $|x| \leq b_0$ we can find h-admissible symbols $K_\pm \in S_{ad}(-\rho)$ (ρ was defined in 5.11) such that for every $\lambda \in J$ we have:*

$$\begin{aligned} s'(\hbar, \lambda) &= \operatorname{tr}\left(\zeta\left(E'_{\hat{H}_2}(\lambda) - E'_{\hat{H}_1}(\lambda)\right)\zeta\right) \\ &\quad + \operatorname{tr}\left(\hat{K}_+ R_0(\lambda + i0)\right) + \operatorname{tr}\left(\hat{K}_- R_0(\lambda - i0)\right) \\ &\quad + \operatorname{tr}\left(X_1^\pm R_1(\lambda \pm i0) Y_1^\pm R_0(\lambda \pm i0) Z_1^\pm\right) \\ &\quad + \operatorname{tr}\left(X_2^\pm R_2(\lambda \pm i0) Y_2^\pm R_0(\lambda \pm i0) Z_2^\pm\right), \end{aligned} \tag{5.25}$$

in the two last lines we mean that we have a (+) and a (-) term.
$X_j^\pm$, $Y_j^\pm$, $Z_j^\pm$, are negligible operators in the following sense: $\forall M$,$\forall N$, we have for $j = 1, 2$,

$$\begin{aligned} \| < x >^M Y_j^\pm R_0(\lambda \pm i0) Z_j^\pm < x >^M \|_{\mathrm{tr}} &= O(\hbar^N), \\ \| < x >^M X_j^\pm < x >^M \| &= O(\hbar^N), \end{aligned} \tag{5.26}$$

$O(\hbar^N)$ being uniform in the energy parameter $\lambda \in J$. Furthermore formula (5.25) can be differentiated in λ to any order and we have also estimates like (5.26).

Remark 5.9 *For short range perturbations of the Laplace operator the above result can be replaced by a much simpler one which was introduced in Robert-Tamura [129]*

$$s'(\hbar,\lambda) = \frac{1}{2\lambda}\mathrm{tr}[(2V(x) + x\cdot\nabla V(x))\frac{\partial E_\lambda}{\partial\lambda}],$$

using the generator of the dilation group. Notice that this formula has to be interpreted correctly because the operator involved is not trace class.

Comments

First, by a standard scaling argument, it is not difficult to see that the high energy asymptotics ($\lambda\nearrow+\infty$) is a particular case of the semiclassical asymptotics ($h\searrow 0$) for another pair of Hamiltonians. So we will consider only the semi-classical case for a more general pair of Hamiltonians coming from long range perturbations of a fixed momentum dependent Hamiltonian.

The second and third term of the r.h.s of (5.25) clearly have $\hbar$-asymptotics because they essentially involve the free resolvent.

The first term is compactly supported in the configuration space and will be checked by the well known method of Hörmander-Levitan ([83, 123]) explained in section 3.

The last term will be considered as a remainder term and for checking it we need estimates on the boundary values of resolvents close to the absolutely continuous spectrum.

The main ingredient in the proof is a construction of a long time parametrix by a method initiated by Isozaki-Kitada [86] for time dependent Schrödinger equations. By following carefully the estimates in the Isozaki-Kitada construction it is possible to control the difference of two propagators, obtained by long range perturbations of the same free translation invariant Hamiltonian. We shall explain these points in more details in subsection 5.5 .

5.3 Long Range Scattering and Propagation Estimates

Let us consider scattering theory with a free Hamiltonian $\hat{H}_0 = \omega(\hbar D)$ on $\mathbb{R}^n$, $n\geq 1$. Let $\hat{H} = \hat{H}_0 + \hat{Q}$ be a perturbation of $\hat{H}_0$. We make the following assumptions on ω,

($\mathbf{A_0}$) ω is non negative on $\mathbb{R}^n$ and $\lim_{|\xi|\to+\infty}\omega(\xi) = +\infty$.

($\mathbf{A_1}$) ω is smooth on $\mathbb{R}^n$ and for each multiindex α there exists c_α such that:

$$|\partial_\xi^\alpha\omega(\xi)| \leq c_\alpha(1+\omega(\xi)),\ \forall\xi\in\mathbb{R}^n.$$

($\mathbf{A_2}$) There exists $c>0$ and some $M>0$ such that:

$$\omega(\eta)\leq c(1+\omega(\xi)) <\xi-\eta>^M,\ \forall\xi\in\mathbb{R}^n,\ \text{and}\,\forall\eta\in\mathbb{R}^n.$$

This generalized kinetic energy term ω is sometimes called *dispersive* ([134]). The perturbation term $\hat{Q}$ is assumed to be an $\hbar$-admissible pseudodifferential operator, that means that it is the Weyl quantization of the $\hbar$-asymptotic symbol:

$$Q(\hbar;x,\xi)\asymp\sum_{j\geq 0}\hbar^j.Q_j(x,\xi),$$

where (x, ξ) is a point in the classical phase space.
Let us introduce the following assumptions:
$(\mathbf{A_3})$ There exist $c_0 > 0$ and $\epsilon_0 > 0$ such that:

$$Q_0(x,\xi) + \omega(\xi) + c_0 \geq \epsilon_0 \left(1 + \omega(\xi)\right), \ \forall x, \ \xi \in \mathbb{R}^n.$$

$(\mathbf{A_4})$ There exists $\delta > 0$ such that for every multiindex α, β and every $j \geq 0$ there exists $C(j, \alpha, \beta)$ such that for all $\xi \in \mathbb{R}^n$, we have:

$$|\partial_x^\alpha \partial_\xi^\beta Q_j(x,\xi)| \leq C(j,\alpha,\beta) < x >^{-\delta-|\alpha|} (1 + \omega(\xi)).$$

The asymptotic expansion holds in the following sense:
$(\mathbf{A_5})$ For every integer $N \geq 1$, every multiindex α, β there exists $C(N, \alpha, \beta) > 0$ such that $\forall (x, \ \xi) \in \mathbb{R}^{2n}$ $\forall \hbar \in]0, 1]$ we have:

$$\left|\partial_x^\alpha \partial_\xi^\beta \left(Q(\hbar; x, \xi) - \sum_{0\leq j\leq N-1} \hbar^j Q_j(x,\xi)\right)\right| \leq$$
$$C(N,\alpha,\beta)\hbar^N < x >^{-\delta-|\alpha|} (1 + \omega(\xi)). \tag{5.27}$$

Remark 5.10 *(i) Assumptions* $(\mathbf{A_1})$ *to* $(\mathbf{A_5})$ *are clearly satisfied by the pair defined in subsection (5.2),* $\hat{H} = \hat{H}(g, A, V)$; $\hat{H}_0(h) = -\hbar^2\Delta$.
(ii) If f *is a non negative, smooth real function such that:*

$$\left|\frac{d^j f}{d\lambda^j}(\lambda)\right| \leq c(1 + |\lambda|)^{-j}(1 + f(\lambda)),$$

then the pair $(f(\hat{H}); f(\hat{H}_0))$, *also satisfies* $(\mathbf{A_1})$ *to* $(\mathbf{A_5})$ *with* $\tilde{\omega}(\xi) = f(\omega(\xi))$. *This is an easy consequence of the functional calculus for h-admissible operators established in [73].*

Under the above assumptions $\hat{H}$ is essentially self-adjoint for $\hbar$ small enough. So, the propagator $U(t) = \exp(-it\hbar^{-1}\hat{H})$ is well defined for every t in $\mathbb{R}$. Furthermore, it is easy to see that the difference of resolvents, $\left(\hat{H} - i\right)^{-1} - \left(\hat{H}_0 - i\right)^{-1}$ is compact, hence, by the Weyl perturbation theorem, the essential spectrum of $\hat{H}$ coïncides with the essential spectrum of $\hat{H}_0$, which is equal to the range of ω.
Scattering theory is related to the absolutely continuous part of the spectrum of quantum Hamiltonians. So, let us consider an energy band $I =]a, b[$, an open non critical interval for ω. Then it is well known that $I \cap \sigma(\hat{H}_0) \subseteq \sigma_{ac}(\hat{H}_0)$. Thus we can get some preliminary spectral information using the conjugate operator method of Mourre [89]. It is convenient here to introduce the following operator (see also [134]):

$$\mathcal{D} = (2i)^{-1}(1 + \omega(\hbar D))^{-1} \left(x \cdot \nabla_\xi \omega(\hbar D) + \nabla_\xi \omega(\hbar D) \cdot x\right) (1 + \omega(\hbar D))^{-1},$$

which is the analogue of the usual dilation generator for Laplace operator. To apply Mourre's results the main point is to have a Mourre's inequality. In this context it is an easy consequence of $\hbar$-functional calculus ([73] and section 2), stated in the following lemma.

Lemma 5.11 *Let I be an open, bounded, non critical interval for ω. Then: $\forall\chi \in C_0{}^\infty(I)$ it exists $\gamma_0 > 0$ and some $\hbar$-admissible operator $\hat{A}$ satisfying $(\mathbf{A_4})$ and $(\mathbf{A_5})$ such that, for all $\hbar \in]0,1[$, we have:*

$$\chi(\hat{H})i^{-1}\left[\hat{H},\mathcal{D}\right]\chi(\hat{H}) \geq \hbar\chi(\hat{H}).(\gamma_0+\hat{A})\chi(\hat{H}).$$

In particular, $\chi(\hat{H})\hat{A}\chi(\hat{H})$ is a compact operator in $L^2(\mathbb{R}^n)$.

From the above Lemma and [89] we easily get the following :

Proposition 5.12 *With the notation of the Lemma 2.2, for every compact interval $J \subset I$, and every $\hbar \in]0,1]$, $\sigma(\hat{H}) \cap J$ is absolutely continuous with at most a finite number of eigenvalues for $\hat{H}$ (with multiplicities).*

Furthermore applying the full results of [89] we get propagation estimates for each fixed $\hbar$:

Proposition 5.13 *Let J be such that $J \cap \sigma_{pp}(\hat{H}) = \emptyset$.*
(i) For every real $s > 1/2$, $< x >^{-s} (\hat{H}-\lambda \pm i0)^{-1} < x >^{-s}$ exists in the operator norm on $L^2(\mathbb{R}^n)$, for every λ in J. In particular $\sigma_{sc}(\hat{H}) = \emptyset$.
(ii) For every $s > \frac{1}{2}+k$, $< x >^{-s} (\hat{H}-\lambda \pm i0)^{-1} < x >^{-s}$ is of class C^k of λ in J and

$$\frac{d^k}{d\lambda^k}\{< x >^{-s} (\hat{H}-\lambda \pm i0)^{-1} < x >^{-s}\} = k! < x >^{-s} (\hat{H}-\lambda \pm i0)^{-k-1} < x >^{-s}.$$

(iii) For every $\chi \in C_0^\infty(J)$ and $0 < \tau < s$ there exists $c_J(\chi,\tau,s)$ such that

$$\| < x >^{-s} \chi(\hat{H}).U(t). < x >^{-s} \| \leq c(\chi,\tau,s) < t >^{-\tau},\ \forall t \in \mathbb{R}.$$

Now we consider two perturbations Q_1 and Q_2 of $\hat{H}_0$ satisfying $(\mathbf{A_3})$, $(\mathbf{A_4})$,$(\mathbf{A_5})$, and such that Q_2 is a short range perturbation of Q_1 in the following sense:

$(\mathbf{A_6})$ There exists $\rho > 1$ such that for every multiindex α and β, and for every $N > 1$, there exists $c > 0$ such that for every h in $]0,1]$ and (x,ξ) in $\mathbb{R}^{2n}$, we have:

$$|\partial_x^\alpha\partial_\xi^\beta\left(Q_{2,j}(x,\xi)-Q_{1,j}(x,\xi)\right)| \leq c < x >^{-\rho-|\alpha|} (1+\omega(\xi)). \tag{5.28}$$

$$\left|\partial_x^\alpha\partial_\xi^\beta\left(Q_2(\hbar,x,\xi)-Q_1(\hbar,x,\xi)-\sum_{1\leq j\leq N-1}\hbar^j(Q_{2,j}(x,\xi)-Q_{1,j}(x,\xi))\right)\right| \leq c\hbar^N < x >^{-\rho-|\alpha|} (1+\omega(\xi)). \tag{5.29}$$

Let us introduce the propagators: $U_j(t) = \exp(-i\hbar^{-1}\hat{H}_j)$ where $\hat{H}_j = \hat{H}_0 + \hat{Q}_j$. The last proposition and Cook's method imply the following corollary (see [89]):

Corollary 5.14 *Under the above assumptions , for every interval J such that $J \cap \sigma_{pp}(\hat{H}_1) = \emptyset$, the wave operators :*

$$\Omega_\pm(J) = \lim_{t \to \pm\infty} U_2(-t)U_1(t)E_{\hat{H}_1}(J)$$

exist and are complete. ($E_A(J)$ denotes the spectral projector of the self-adjoint operator A on the interval J).

Because we are interested here in semiclassical asymptotics, a first step is to state *the propagation estimates controlled in the semiclassical parameter.* For that, we need a basic assumption on the classical systems. With $H(x,\xi)$ a classical Hamiltonian on the phase space $\mathbb{R}^{2n}$, let us consider the flow defined by it,

$$\Phi_H^t(x,\xi) = (q(t,x,\xi); p(t,x,\xi)).$$

Definition 5.15 *We say that an energy interval $J \subset \mathbb{R}$ is non trapping for H if for every $R > 0$ there exists $T_R \geq 0$ such that:*

$$\text{If } H(x,\xi) \in J,\ |t| > T_R,\ |x| < R \text{ then } |q(t,x,\xi)| > R.$$

In the following we denote by $H_j(x,\xi)$ the $\hbar$-principal symbol of $\hat{H}_j$, i.e $\hat{H}_j(x,\xi) = \omega(\xi) + Q_{j,0}(x,\xi)$. When the index j is fixed we drop it. Then the following results hold.

Theorem 5.16 *1) If the open interval I is non critical for ω and non trapping for H then we have:*

$$(i_1)\forall s > k - 1/2,\ \| < x >^{-s} (\hat{H} - \lambda \pm i0)^{-k} < x >^{-s} \| = O(\hbar^{-k})$$

uniformly for λ in each compact subset of I, as $\hbar \searrow 0$.
(i_2) For every $\chi \in C_0^\infty(I)$ and $0 < \tau < s$ there exists $c(\chi,\tau,s)$ such that:

$$\| < x >^{-s} \chi(\hat{H})U(t) < x >^{-s} \| \leq c(\chi,\tau,s) < t >^{-\tau}$$

for every t in $\mathbb{R}$ and every h in $]0,1]$.
2) Conversely, if (i_1) holds with $k = 1$ or (i_2) holds with some $0 < \tau < s$ then I is non trapping for H.

Sketch of Proof:
The method to prove the direct part (which is due essentially to [56]), involves a modification $\mathcal{D}_1$ of the conjugate operator $\mathcal{D}$. By replacing $\mathcal{D}$ by $\mathcal{D}_1$ in the Lemma (5.11, then the Mourre inequality holds with $\hat{A} = 0$; i.e. we have:

$$\chi(\hat{H})i^{-1}\left[\hat{H},\mathcal{D}_1\right]\chi(\hat{H}) \geq \gamma_0\hbar\chi(\hat{H})^2. \tag{5.30}$$

Let us remark that by the virial theorem, [107], it follows from (5.30) that $\hat{H}$ has no eigenvalues in I for $\hbar$ small enough.

The main steps of the proof are the following.
First, using standard properties of the calculus for $\hbar$-pseudodifferential operators, it is sufficient to construct a function $F \in C^\infty(\mathbb{R}^{2n})$ such that the Poisson bracket $\{H, F\}$ is positive on $H^{-1}(J)$ where J is a compact subinterval of I and $H(x,\xi) = \omega(\xi) + Q_0(x,\xi)$. F is constructed as follows. Let us consider:
$\chi \in C_0{}^\infty(\mathbb{R})$, $0 \le \chi \le 1$, $\chi(x) = 1$ for $|x| < 1$ and $\chi(x) = 0$ for $|x| > 2$. Let us denote: $\chi_R(x) = \chi(\frac{x}{R})$ and

$$K_R(x,\xi) = -\int_0^{+\infty} \chi_R(q(t,x,\xi))dt.$$

The non trapping assumption easily ensures that K_R is a bounded, C^∞ function on $H^{-1}(J)$. Then we introduce:

$$F(x,\xi) = c_1 \chi_{MR}(x) K_R(x,\xi) + F_0(x,\xi),$$

where

$$F_0(x,\xi) = \frac{x.\nabla\omega(\xi)}{1+\omega(\xi)}.$$

So, we first choose R large enough such that there exists some $\delta_0 > 0$ with $\{H, F_0\} > 2\delta_0$ for $|x| > R$ and $H(x,\xi) \in J$. Then we choose $c_1 > 0$ and $M > 0$ large enough such that we have:

$$\{H, F\} > \delta_0 \text{ in } H^{-1}(J).$$

The method to prove the second part uses a nice trick due to Wang [140].
Let us repeat here the argument for it is rather simple and it is not so often that we have a non trivial necessary and sufficient condition in semi-classical analysis. Let us assume that (i_1) holds with $k = 1$. Then by H-smoothness techniques (see [121]), for $s > 1/2$ we can get a constant $\gamma > 0$ such that

$$\int_{\mathbb{R}} \|\langle x\rangle^{-s}\chi(\hat{H})U(t)\psi\|^2 dt \le \gamma\|\psi\|^2, \tag{5.31}$$

$\forall\psi \in L^2(\mathbb{R}^n)$, $\forall\hbar \in]0,1]$. It is convenient to transform this inequality using traces. Let us introduce

$$\hat{A}_{2s}(t) = U(-t)\chi(\hat{H})\langle x\rangle^{-2s}\chi(\hat{H})U(t),$$

then using (5.31), for every density operator $\hat{B}$ (i.e $\hat{B}$ is a non negative observable of trace class in $L^2(\mathbb{R}^n)$ with $\mathrm{tr}(\hat{B}) = 1$), we have

$$\int_{\mathbb{R}} \mathrm{tr}(\hat{A}_{2s}(t)\cdot\hat{B}) \le \gamma. \tag{5.32}$$

Let us remark that, using the semi-classical propagation theorem, the principal symbol of $\hat{A}_{2s}(t)$ is $A_{2s}(t,x,\xi) = \chi^2(H(x,\xi))\langle q(t,x,\xi)\rangle^{-2s}$. So for every $T > 0$ there exists $C_T > 0$ such that for every $B \in \mathcal{S}(\mathbb{R}^{2n})$, $B \ge 0$, and $\int_{\mathbb{R}^{2n}} B(x,\xi)dxd\xi = 1$, we have

$$\int_{-T}^{T}\int_{\mathbb{R}^{2n}} A_{2s}(t,x,\xi)B(x,\xi)dxd\xi dt \le \gamma + C_T\hbar. \tag{5.33}$$

Now, taking $B(x,\xi) = (\pi\hbar)^{-n}\exp(-\frac{1}{\hbar}((x-y)^2 + (\xi-\eta)^2))$ and making $\hbar \searrow 0$ we get

$$\chi^2(H(y,\eta))\int_{\mathbb{R}} \langle q(t,y,\eta)\rangle^{-2s} dt \le \gamma. \tag{5.34}$$

If $\lambda \in I$, we choose χ such that $\chi(\lambda) = 1$. Hence, for $(y, \eta) \in H^{-1}(\lambda)$ we get from (5.34) that

$$\limsup_{|t| \to +\infty} |q(t, y, \eta)| = +\infty.$$

We conclude by a well known argument in classical mechanics that

$$\lim_{|t| \to +\infty} |q(t, y, \eta)| = +\infty$$

(for more details see [124]). ∎

5.4 Long Time Approximations for Propagators

Let us consider a Hamiltonian of the form $\hat{H} = \omega(hD) + \hat{Q}$ satisfying assumptions (A_0) to (A_6) of subsection (5.3). We shall report here on the method introduced by Isozaki-Kitada [86] to construct accurate approximations for the propagator $U(t) = \exp\left(-it\hbar^{-1}\hat{H}\right)$ uniformly in time $t \in \mathbb{R}$. The semi-classical version of this construction is due to Robert-Tamura [129] where it is proved that the estimates are uniform in the semi-classical parameter $\hbar$. According Isozaki-Kitada we look for an approximation for $U(t)$ of the form:

$$U_M(t) = \mathcal{J}(\varphi, A) U_0(t),$$

where $\varphi(x, \xi)$ solves the time independent Hamilton-Jacobi equation:

$$H(x, \partial_x \varphi(x, \xi)) = \omega(\xi), \tag{5.35}$$

in outgoing or incoming areas of the phase space and $\mathcal{J}(\varphi, A)$ is a Fourier-Integral operator associated to the amplitude A according to the usual formula:

$$\mathcal{J}(\varphi, A)u(x) = (2\pi\hbar)^{-n} \int_{\mathbb{R}^{2n}} \exp\{\frac{i}{\hbar}(\varphi(x, \xi) - < y, \xi >)\} A(x, \xi) u(y) dy d\xi.$$

Following the Isozaki-Kitada method, we solve (5.35) by localization in outgoing and incoming region of the phase space. Let us introduce the speed vector field $v(\xi) = \nabla_\xi \omega(\xi)$ and the notations:

$$\cos(x, \xi) = \frac{< x, \xi >}{|x||\xi|}, \text{ for } x \neq 0, \ \xi \neq 0,$$

$$\Gamma^{\pm}(J, \sigma, R) = \{(x, \xi) \in \mathbb{R}^{2n} : |x| \geq R, \ \omega(\xi) \in J \ , \pm\cos(x, v(\xi)) \geq -\sigma\},$$

where $R > 0$, $\sigma \in]-1, 1[$, J is a compact interval such that $v(\xi) \neq 0$ if $\omega(\xi) \in I$, I being a neighborhood of J.

Following [124] we state an extension of theorem (2.5) in [86].

Proposition 5.17 *For every compact interval $J \subseteq I$ and every $-1 < \sigma < 1$ there exist $R > 0$ and $\varphi_\pm \in C^\infty(\mathbb{R}^{2n})$ such that:*

$$H(x, \partial_x \varphi_\pm(x,\xi)) = \omega(\xi) \text{ in } \Gamma^\pm(J, \pm\sigma, R). \tag{5.36}$$

Moreover the following estimates hold:

$$\begin{aligned} \left|\partial_x^\alpha \partial_\xi^\beta \left(\varphi_\pm(x,\xi) - < x, \xi >\right)\right| &\leq C_{\alpha,\beta} < x >^{1-\delta-|\alpha|}, & (5.37)\\ \left|\partial^2_{x,\xi}\varphi_\pm(x,\xi) - \mathbb{1}\right| &\leq 1/2, \ \forall (x,\xi) \in \mathbb{R}^{2n}, & (5.38) \end{aligned}$$

where δ is defined in the assumptions on H and $\partial^2_{x,\xi}\varphi$ denotes the hessian matrix of the function φ in the variables (x, ξ) .

An idea of the proof: Without going into the details of the proof let us recall here the strategy (see [127] for all the details).
We consider the time dependent Hamilton-Jacobi equation :

$$\begin{aligned} \frac{\partial S}{\partial t} &= H(x, \partial_x S(t, x, \xi)), \\ S(0, x, \xi) &= < x, \xi > . \end{aligned} \tag{5.39}$$

From classical Hamilton theory we know that the solution S of (5.39) is connected with the Hamiltonian flow generated by H:

$$\Phi^t(x, \xi) = (q(t, x, \xi); p(t, x, \xi)).$$

S being a generating function for Φ^t we have:

$$\begin{aligned} \nabla_\xi S(t, x, \xi) &= q(t, x, \nabla_x S(t, x, \xi), \\ \xi &= p(t, x, \nabla_x S(t, x, \xi). \end{aligned} \tag{5.40}$$

Assume for example that $(x, \xi) \in \Gamma^+(J, \sigma, R)$. Then we shall prove that:

$$\lim_{t\to+\infty} |\nabla_\xi S(t, x, \xi)| = +\infty \text{ and } \nabla_x \varphi(x, \xi) = \lim_{t\to+\infty} (\nabla_x S(t, x, \xi)) \text{ exists.}$$

By the energy conservation law we have:

$$\lim_{t\to+\infty} H(x, \nabla_x S(t, x, \xi)) = \lim_{t\to+\infty} H(\nabla_\xi S(t, x, \xi), \xi).$$

So we get: $H(x, \nabla_x \varphi(x, \xi)) = \omega(\xi)$. To make rigorous the previous formal computations, an important step is to study the inverse of the mapping: $\xi \to p(t, x, \xi)$.

∎

Now we come to the construction of Fourier-Integral operators to approximate propagators uniformly in time.

The starting point for the construction of approximations for $U(t)$ is the following Duhamel formula:

$$\frac{d}{dt}(U(-t)\mathcal{J}((\varphi,A)U_0(t)) = \\ i\hbar^{-1}U(-t)\left[\hat{H}\mathcal{J}(\varphi,A) - \mathcal{J}(\varphi,A)\hat{H}_0\right]U_0(t). \tag{5.41}$$

So we have to realize the following intertwining property modulo arbitrary large powers of the semiclassical parameter $\hbar$:

$$\hat{H}\mathcal{J}(\varphi,A) - \mathcal{J}(\varphi,A)\hat{H}_0 \asymp 0. \tag{5.42}$$

Let us remark that by choosing φ to be a solution of equation (5.35) and $A = 1$ we get a solution of (5.42) with error $O(1)$. According to the W.K.B method (section 2), we can get better and better approximations by solving transport equations to determine an $\hbar$-admissible symbol: $A \asymp \sum_{j\geq 0}\hbar^j A_j$. The final result is

Theorem 5.18 (Isozaki-Kitada parametrix) (*i*) *There exists an $\hbar$-admissible symbol of weight 0, $B \asymp \sum_{j\geq 0} h^j B_j$, such that: $B_j \in S(-j)$, $Supp(B_j) \subseteq \Gamma_0^+$ and:*

$$\chi^w(x,\hbar D) = \mathcal{J}(\varphi, A^{(N)})\mathcal{J}(\varphi,B^{(N)})^* + \hbar^N\chi_N(\hbar,x,\hbar D),\ \forall N\in\mathbb{N}, \tag{5.43}$$

where we have: $A^{(N)} \stackrel{\mathrm{def}}{=} \sum_{0\leq j\leq N}\hbar^j A_j$ and χ_N is a bounded family of symbols in $S(-N)$ for $\hbar \in]0,1]$.

(*ii*) *For every $N\in\mathbb{N}$ the following equality holds:*

$$U(t)\chi^w(x,\hbar D) = \mathcal{J}(\varphi,A^{(N)})U_0(t)\mathcal{J}(\varphi,B^{(N)})^* + \\ \hbar^N U(t)\chi_N(\hbar,x,\hbar D) + \hbar^{N+1}\hat{R}_N(t,\hbar), \tag{5.44}$$

where we have:

$$\hat{R}_N(t,\hbar) = \int_0^t U(t-s)\mathcal{J}(\varphi,R_{N+1})U_0(s)\mathcal{J}(\varphi,B^{(N)})^* ds \tag{5.45}$$

and $R_{N+1}(h)$ is in a bounded set of symbols in $S(-N-1)$ as $\hbar \in]0,1]$.

Remark on the Proof: All things have been prepared to get this theorem. It is now a straightforward extension of results proved in [130] for Schrödinger Hamiltonians. In particular we know from the computation rules for h-admissible-Fourier-Integral operators that $\mathcal{J}(\varphi,A^{(N)})\mathcal{J}(\varphi,B^{(N)})^*$ has an $\hbar$-admissible symbol which can be explicitely computed ([122]). In this way we can determine B so that (5.43) is satisfied, because A is elliptic in Γ_0^+ (i.e its principal symbol does not vanish).
The second part of the theorem is a consequence of (5.41), and the transport equations ∎

Let us recall here an application to the existence and completeness of modified wave operators. Applying the Enss method as in [52] we get:

Proposition 5.19 *Assume that I is an open, non critical interval for ω, without eigenvalues for $\hat{H}$ (here $\hbar$ is fixed). Then the modified wave operators*

$$\Omega^{\pm}(I) = s - \lim_{t\to\pm\infty}\left(U(-t)\mathcal{J}(\varphi,1)U_0(t)E_{\hat{H}_0}(I)\right) \tag{5.46}$$

exist and are complete i.e.:

$$Range\left(\Omega^{\pm}(I)\right) = E_{\hat{H}}\left(\mathcal{H}_{ac}(\hat{H}\right).$$

5.5 A Sketch of the proof of the Asymptotic representation formula for the spectral shift function

Let us recall the statement:

Theorem 5.20 (Asymptotic Representation Formula) *Assume that $\hat{H}_1$ and $\hat{H}_2$ satisfy the above hypotheses* (no assumptions on the classical flow are need here). *Then the spectral shift function $s(\hbar,\lambda)$ satisfies:*
(i) $s(\hbar,\cdot)\in C^\infty(I)$
(ii) There exists $\rho_0>0$ large enough such that for every $\zeta\in C_0^\infty(\mathbb{R}^n)$ satisfying: $\zeta(x)=1$ for $|x|\le\rho_0$, we can find h-admissible symbols $K_\pm\in S_{ad}(-\rho)$ such that:

$$\begin{aligned} s'(\hbar,\lambda) &= 2\pi\mathrm{tr}\left(\zeta\left(\frac{\partial E_2(\lambda)}{\partial\lambda}-\frac{\partial E_1(\lambda)}{\partial\lambda}\right)\zeta\right)\\ &\quad+\mathrm{tr}\left(\hat{K}_-R_0(\lambda-i0)\right)+\mathrm{tr}\left(\hat{K}_+(R_0(\lambda+i0)\right)\\ &\quad+\mathrm{tr}\left(X_1^{\pm}R_1(\lambda\pm i0)Y_1^{\pm}R_0(\lambda\pm i0)Z_1^{\pm}\right)\\ &\quad+\mathrm{tr}\left(X_2^{\pm}R_2(\lambda\pm i0)Y_2^{\pm}R_0(\lambda\pm i0)Z_2^{\pm}\right), \end{aligned} \tag{5.47}$$

in the two last lines we mean that we have a (+) and a (-) term.
$X_j^{\pm}$, $Y_j^{\pm}$, $Z_j^{\pm}$, are negligeable operators in the following sense: $\forall M$, $\forall N$, we have for $j=1,2$,

$$\begin{aligned} \| <x>^M Y_j^{\pm}R_0(\lambda\pm i0)Z_j^{\pm}<x>^M\|_{tr} &= O(\hbar^N),\\ \| <x>^M X_j^{\pm}<x>^M\| &= O(\hbar^N), \end{aligned} \tag{5.48}$$

$O(\hbar^N)$ is uniform in the energy parameter $\lambda\in J$, for every compact interval $J\subset I$. Furthermore formula (5.47) can be differentiated in λ to any order and we also have estimates like (5.48).

Beginning of the Proof: Let $\tilde{I}$ be a bounded, open subinterval of I and $f\in C_0^\infty(I)$; $f=1$ on $\tilde{I}$. In the distributional sense on $\tilde{I}$ we have:

$$s'(\hbar,\lambda)=\mathrm{tr}\left(f(\hat{H}_2)E_2'(\lambda)-f(\hat{H}_1)E_1'(\lambda)\right). \tag{5.49}$$

For $b > 0$, which will be chosen large enoug, and $b < 2R$, let us introduce $\zeta \in C_0^\infty(|x| < 2R)$ and $\zeta(x) = 1$ for $|x| < b$. Then we define the following distributions in $\tilde{I}$

$$\sigma_\zeta(\hbar, \lambda) = \mathrm{tr}\left(\zeta\left(f(\hat{H}_2)E_2'(\lambda) - f(\hat{H}_1)E_1'(\lambda)\right)\right), \tag{5.50}$$

$$\sigma_{1-\zeta}(\hbar, \lambda) = s'(\hbar, \lambda) - \sigma_\zeta(\hbar, \lambda). \tag{5.51}$$

By the cyclicity of the trace we have

$$\mathrm{tr}\left(\zeta f(\hat{H}_j)E_j'(\lambda)\right) = \mathrm{tr}\left(\zeta f(\hat{H}_j)E_j'(\lambda)\tilde{\zeta}\right), \tag{5.52}$$

with $\tilde{\zeta} \in C_0^\infty(\mathbb{R}^n)$, $\tilde{\zeta}\zeta \equiv 1$.
So using propagation estimates (proposition 2.2), we can see easily that σ_ζ is a smooth function in λ.
Checking the term $\sigma_{1-\zeta}$ is more difficult. We go through its $\hbar$-Fourier transform:

$$\begin{aligned}\hat{\sigma}_{1-\zeta}(t, \hbar) &= \int_{\mathbb{R}} \exp(-i\hbar^{-1}t\lambda)\sigma_{1-\zeta}(\lambda, \hbar)d\lambda \\ &= tr\left((1-\zeta)\left(f(\hat{H}_2)U_2(t) - f(\hat{H}_1)U_1(t)\right)\right).\end{aligned} \tag{5.53}$$

To use the constructions of subsection (5.4), we introduce a partition of unity on the following subset of the phase space: $\Gamma := \{(x, \xi) : |x| > R; \omega(\xi) \in I\}$. So, let us introduce $\chi^\pm \in C^\infty(\mathbb{R}^{2n})$, such that $Supp(\chi^\pm) \subseteq \Gamma^\pm(I, \sigma_\pm, R)$; $\chi^+ + \chi^- \equiv 1$ on Γ.
From the functional calculus (see section 2), we know that $f(\hat{H}_j)$ is an $\hbar$-admissible operator, with an essential support in the set : $\{(x, \xi) : \omega(\xi) + Q_j(x, \xi) \in \tilde{I}\}$. So, taking b large enough we can see easily that $(1-\zeta)f(\hat{H}_j)$ has its essential support in Γ.

We have the following decomposition:

$$\hat{\sigma}_{1-\zeta}(t, \hbar) = \hat{\sigma}_-(t, \hbar) + \hat{\sigma}_+(t, \hbar), \tag{5.54}$$

where

$$\hat{\sigma_\pm}(t, \hbar) = \mathrm{tr}\left(\left(f(\hat{H}_2)U_2(t) - f(\hat{H}_1)U_1(t)\right)\chi_\pm^w(x, \hbar D)\right). \tag{5.55}$$

We use the simpler notation: $F_j = f(\hat{H}_j)$.
In what follows, the lower index j refers to the Hamiltonian $\hat{H}_j$ and the upper index $(\pm)$ refers to the constructions in outgoing and incoming domains in region $\Gamma^\pm$.
The strategy consist in using the Isozaki-Kitada parametrix

$$\begin{aligned}U(t)\chi^w(x, \hbar D) &= \mathcal{J}(\varphi, A^{(N)}(h))U_0(t)\mathcal{J}(\varphi, B^{(N)})^* + \\ &\quad \hbar^N U(t)\chi_N(h, x, \hbar D) + \hbar^{N+1}\hat{R}_N(t, \hbar),\end{aligned} \tag{5.56}$$

with $U = U_j$, $j = 1, 2$ and $\chi = \chi_\pm$ for $\pm t \geq 0$. The main technical points are contained in the two following lemmas

Lemma 5.21 *With the above notations,the following identity holds:*

$$\begin{aligned}&\mathrm{tr}\left\{F_2\mathcal{J}(\varphi_2, A_2^\pm)U_0(t)\mathcal{J}(\varphi_2, B_2^\pm)^* - F_1\mathcal{J}(\varphi_1, A_1^\pm)U_0(t)\mathcal{J}(\varphi_1, B_1^\pm)^*\right\} = \\ &\quad \mathrm{tr}\left\{U_0(t)\left(\mathcal{J}(\varphi_2, B_2^\pm)^*F_2\mathcal{J}(\varphi_2, A_2^\pm) - \mathcal{J}(\varphi_1, B_1^\pm)^*F_1\mathcal{J}(\varphi_1, A_1^\pm)\right)\right\}\end{aligned}$$

and each term between brackets $\{\cdots\}$ is trace class.

Lemma 5.22 *The operators:*

$$\hat{K}^{\pm} := \mathcal{J}(\varphi_2, B_2^{\pm})^* F_2 \mathcal{J}(\varphi_2, A_2^{\pm}) - \mathcal{J}(\varphi_1, B_1^{\pm})^* F_1 \mathcal{J}(\varphi_1, A_1^{\pm})$$

are $\hbar$-admissible pseudodifferential operators, with $\hbar$-symbols: $K^{\pm} \in S_{ad}(-\rho)$.
So we have the asymptotics:

$$K^{\pm} \asymp \sum_{j \geq 0} \hbar^j K_j^{\pm}.$$

Moreover, there exists some $\epsilon_0 > 0$ and some compact set $\mathcal{M}$ of $\mathbb{R}^n$ such that: $Supp(K_j^{\pm}) \subseteq \{(x,\xi); \epsilon_0 < |v(\xi)|;\ \xi \in \mathcal{M}\}$. In particular if $\rho > n$, $\hat{K}^{\pm}$ are trace class operators.

Remark about the proof: This lemma is an accurate form of the semi-classical analogue of the Egorov theorem, in microlocal analysis ([84]), which states that the conjugate of a pseudodifferential operator by a Fourier-Integral operator is a pseudodifferential operator.
Now we carry on the proof of the representation formula. With the previous constructions we have:

$$\hat{\sigma_{\pm}}(t,\hbar) = \mathrm{tr}\left(U_0(t,\hbar)K^{\pm}\right) + \hbar^N \mathrm{tr}\left(D_N^{\pm}(t,\hbar)\right) + \hbar^{N+1}\mathrm{tr}(E_N^{\pm}(t,\hbar),$$

where:

$$\begin{aligned} D_N^{\pm}(t,h) &= F_2 U_2(t,h)\chi_{N,2}(h,x,hD) - F_1 U_1(t,h)\chi_{N,1}(h,x,hD) \\ E_N^{\pm}(t,h) &= F_2 R_{N,2}(t,h) - F_1 R_{N,1}(t,h). \end{aligned}$$

First of all, let us remark that using the above lemmas we have easily

$$tr(U_0(t)\hat{K}^{\pm}) = O_{\hbar}(< t >^{-\infty}).$$

So we get the estimate:

$$\hat{\sigma}_{\pm}(t,\hbar) = O_{\hbar}(< t >^{-\infty});$$

hence it follows that $s \in C^{\infty}(I)$.
Now we can get the representation formula by inverse Fourier transform:

$$\sigma_{1-\zeta}(\lambda,\hbar) = (2\pi\hbar)^{-1}\int_{\mathbb{R}} \exp(it\lambda\hbar^{-1})\hat{\sigma}_{1-\zeta}(t,\hbar)dt. \tag{5.57}$$

Let us remark that we cannot use (5.54) directly because we have information on $\hat{\sigma}_+$ only for $t \geq 0$ and on $\hat{\sigma}_-$ only for $t \leq 0$. But using that the trace is a C^*-homomorphism to get:

$$\begin{aligned} \overline{\hat{\sigma}_+(t)} &= \mathrm{tr}\left((1-\zeta)(F_2U_2(t) - F_1U_1(t))\chi_+(x,\hbar D)\right)^* \\ &= \mathrm{tr}\left((U_2(-t)F_2 - U_1(-t)F_1)\chi_+(x,\hbar D)\right). \end{aligned} \tag{5.58}$$

Thus (5.58) shows that for $\hat{\sigma}_+(t)$ we have the same information for $t < 0$. Of course the same property holds for $\hat{\sigma}_-(t)$ for $t > 0$. Thus the representation formula follows using inverse Fourier transform in the variable t, dividing the integration domain into $\{t \geq 0\} \cup \{t \leq 0\}$, using the progation estimates and the well known formula

$$R_j(z) = i\int_0^{+\infty} U_j(t)\exp(itz)dt, \quad \text{for } \Im(z) > 0.$$

∎

5.6 Application to the behavior of the scattering phase close to a resonance

In [59] the authors gave a mathematical proof for the Breit-Wigner formula concerning the derivative of the scattering phase for short range perturbations of $-\hbar^2\Delta$. The interesting physical consequence is that the scattering phase varies very quickly as $\hbar \searrow 0$ when the energy variable crosses a resonant energy (for a precise statement see [59][corollary 2.3]).
Now we shall present this result and its extension to the scattering phase related to long range perturbations of $-\hbar^2\Delta$.
Let us consider two C^∞ potentials V_j, $j = 1, 2$. Assume there exist $\delta > 0$, $\rho > n$ such that:

$$|\partial_x^\alpha V_j(x)| \leq c_\alpha < x >^{-\delta-|\alpha|}, \tag{5.59}$$

$$|\partial_x^\alpha (V_2(x) - V_1(x))| \leq c_\alpha < x >^{-\rho-|\alpha|}. \tag{5.60}$$

Let us denote $\hat{H}_j = -\hbar^2\Delta + V_j$ and $\lambda_0 > 0$ a fixed energy level.
As in [59], we introduce the following assumptions:
$(\mathbf{AR_0})$ There is an open interval I, $\lambda_0 \in I$, and I is non trapping for V_1.
$(\mathbf{AR_1})$ ("The well in the island") There exists a connected open set $\hat{O} \subset \mathbb{R}^n$ and a compact, connected set $U \subset \hat{O}$ such that: $V_2 < \lambda_0$ in U, $V_2 > \lambda_0$ in $\hat{O} \setminus U$ and $V_2 < \lambda_0$ in $\mathbb{R}^n \setminus \hat{O}$.
$(\mathbf{AR_2})$ V_2 is holomorphic in a set:
$\{z \in \mathbb{C}^n; |\Im z| \leq \epsilon_0 < \Re z >, \ \Re z$ in a neighborhood of $\mathbb{R}^n \setminus \hat{O}\}$
$(\mathbf{AR_3})$ λ_0 is non trapping for V_2, outside $\mathbb{R}^n \setminus \hat{O}$, i.e if $x(t, y, \eta)$ is a classical trajectory for V_2 with $y \in \mathbb{R}^n \setminus \hat{O}$ and $\eta^2 + V_2(y) = \lambda_0$ then
$\lim_{|t|\to+\infty} |q(t, y, \eta)| = +\infty$.

According to the resonance theory of Helffer-Sjöstrand([78]), we can define the set $\Gamma(\hbar)$ of resonances for $\hat{H}_2$ close to λ_0. We assume furthermore that we have only one resonance denoted by $r(\hbar)$:
$(\mathbf{AR_4})$ There exists a family of complex open sets $\Omega(\hbar)$ such that:
$\cap_{\hbar>0}\Omega(\hbar) = \{\lambda_0\}$, $I(\hbar) \stackrel{\text{def}}{=} \Omega(\hbar) \cap \mathbb{R} \neq \emptyset$, $\Omega(\hbar) \cap \Gamma(\hbar) = \{r(\hbar)\}$ and $\forall \epsilon > 0$, $\exists c_\epsilon > 0$ such that $\text{dist}(\Gamma(\hbar), \partial\Omega(\hbar)) \geq c_\epsilon e^{-\epsilon/\hbar}$.
Let us remark that $(\mathbf{AR_4})$ is satisfied if $\lambda_0 = Min V_2 = V_2(x_0)$ where x_0 is a unique non degenerate minimum for V_2.
Now we recall the main result of [58] which will be plugged in the above representation formula to proceed as in the proof of Corollary 2.3 of ([59]).

Let us denote by d the Agmon distance associated to the degenerate metric $(V_2(x) - \lambda_0)_+ dx^2$, $S_0 = d(U, \partial\hat{O})$ and introduce a modification $\tilde{H}_2$ of H_2 by plugging up the well: choose $W \in C_0^\infty\{x; d(x, U) < \eta\}$ with $\eta > 0$, small enough and such that $V_2 + W > \lambda_0$ in $\hat{O}$. Let us denote by $e_2(\lambda, \hbar; x, y)$, $\tilde{e}_2(\lambda, \hbar; x, y)$ the integral kernel of $E_{\hat{H}_2}$, $E_{\hat{\tilde{H}}_2}$.

Theorem 5.23 (Breit-Wigner formula) *[58]. Under assumptions (AR_1) to (AR_4) we have the following estimate as $h \searrow 0$, locally, uniformly in x,*

$$\frac{\partial e_2}{\partial \lambda}(\lambda, \hbar; x, x) = \frac{\partial \tilde{e}_2}{\partial \lambda}(\lambda, \hbar; x, x) - \frac{1}{\pi}\Im[(\lambda - r(\hbar))^{-1}\psi(x)^2] + O_\eta\left(e^{(-2S_0+\epsilon(\eta))/\hbar}\right), \tag{5.61}$$

with $\lim_{\eta\to 0}\epsilon(\eta) = 0$ *and* $\forall\epsilon > 0$, $\int_{\hat{O}} \psi(x)^2 dx = 1 + O_\epsilon\left(e^{(-2S_0+\epsilon)/\hbar}\right)$.

Now we can state the following result concerning the semi-classical behaviour of the total scattering phase for energy close to the bottom of a well.

Theorem 5.24 *[127]. Let us assume (AR_1) to (AR_4) and also (5.16) for $\hat{H}_2$ in a neighborhood of λ_0. For every $\hbar$-family $\delta(\hbar)$ of positive real numbers such that*
(i) $\Re(r(\hbar)) \pm \delta(\hbar) \in I(\hbar)$ $\forall\hbar > 0$, small enough,
(ii) $\lim_{\hbar\searrow 0}\hbar^{-n}\delta(\hbar) = 0$; $\lim_{\hbar\searrow 0}|\Im(r(\hbar))|^{-1}\delta(\hbar) = +\infty$,
we have the following result for the scattering phase θ ($\theta(\lambda) = \pi s(\lambda)$) of the pair $(\hat{H}_2, \hat{H}_1)$,

$$\lim_{\hbar\searrow 0} \theta(\Re r(\hbar) \pm \delta(\hbar)) - \theta(\Re r(\hbar)) = \pm\pi/2. \tag{5.62}$$

This theorem can be proved by a direct computation, using theorem (5.23) as in the proof of Corollary 2.3 of [59]. ∎

Theorem (5.24) shows that the scattering phase $\theta(\lambda)$ is varying very fast (exponentially fast in the scale $\hbar$) when λ is close to a resonant energy. Let us remark that if λ is a non trapping energy level then $\theta(\lambda)$ is slowly varying by theorem (5.3).

6 Propagation of Coherent States

In this section we report briefly on a direct approach to the semiclassical approximation of the time-dependent Schrödinger equation with initial data localized at an arbitrary point in phase space.
The use of Gaussian coherent states in quantum mechanics and in partial differential equations is rather old. It probably goes back to Schrödinger (see [99] and its references). More recently (1974/75) Hepp [82] and Heller [79, 80] used this approach to study the time dependent Schrödinger equation. Later on more accurate mathematical results were proved, in particular by Hagedorn (1981)[66, 67] and Paul-Uribe (1995) [110, 111]. Recently Combescure-Robert [38] have proven that one can get semi-classical approximations by Gaussian wave packets, for the time dependent Schrödinger equation, valid in time intervals with lengths increasing to ∞ as the Planck constant $\hbar$ tends to 0. In particular the well known log-time limit (or Ehrenfest time) for the validity of semi-classical approximation is rigorously proved. For example, with this control of the remainder term in large time intervals, it is possible to prove the exponentially fast spreading of initial wave packets concentrated at an unstable fixed point of the classical system.

Let us consider the Schrödinger equation

$$i\hbar\frac{\partial\psi(t)}{\partial t} = \hat{H}(t)\psi(t), \quad \psi(0) = \varphi_\alpha, \tag{6.1}$$

where $\hat{H}(t)$ is a time dependent family of self-adjoint operators in the Hilbert space $L^2(\mathbb{R}^n)$. The typical example is $\hat{H}(t) = -\frac{\hbar^2}{2m}\Delta + V(x,t)$, where $V(x,t)$ is a smooth potential depending on the position variable $x \in \mathbb{R}^n$ and time $t \in \mathbb{R}$. The initial data φ_α is the Gaussian coherent state centred at the point $\alpha = (q,p)$ introduced in the section 1 of this paper. Let us recall that $\varphi_\alpha = W(\alpha)\Psi_0$,where Ψ_0 is the ground state of the usual harmonic oscillator K_0. More generally let us denote by Ψ_μ, for $\mu \in \mathbb{N}^n$ the orthonormal basis in $L^2(\mathbb{R}^n)$ of eigenfunctions of $K_0 = \frac{1}{2}(-\hbar^2\Delta + |x|^2)$. According to the correspondence principle, equation (6.1) is approximated by the following Hamiltonian system, since Planck's constant $\hbar$ is negligible relative to m,

$$\dot{q}(t) = \frac{\partial H}{\partial \xi}(q(t),p(t);t), \quad \dot{p}(t) = -\frac{\partial H}{\partial x}(q(t),p(t);t), \quad q(0) = q \quad p(0) = p. \tag{6.2}$$

It is well known that the stability of the system (6.2) is governed by the linear Hamiltonian system

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = JH''(\alpha_t,t)\begin{pmatrix} u \\ v \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 1\!\!1 \\ -1\!\!1 & 0 \end{pmatrix}; \tag{6.3}$$

$H''(z,t)$ denotes the Hessian matrix in the variable $z \in \mathbb{R}^{2n}$. Let us introduce the quadratic Hamiltonian $H_{qe}(x,\xi;t) = \frac{1}{2} < (x,\xi), H''(t)(x,\xi) >$, the quantum propagator, $U_{qe}(t,s)$ defined by $H_{qe}(x,\hbar D_x;t)$ and the numbers $\delta_t = \int_0^t (\dot{q}(s)\cdot p(s) - H(q(s),p(s);s)ds - \frac{q(t)\cdot p(t) - q\cdot p}{2}$.

Let us introduce also the linear flow $F(t)$ defined by (6.3), starting at time 0 ($F(0) = 1\!\!1$). We need also the notations $\Psi_{\mu,\alpha} = W(\alpha)\Psi_\mu$, $\Phi_\mu(t) = W(\alpha_t)U_0(t)\Psi_\mu$. The error term will be estimated by

$$\theta(\alpha,t) := \sup_{0\le s\le t}[\mathrm{tr}(F^\star(t)F(t))]^{1/2}; \quad \sigma(\alpha,t) := \sup_{0\le s\le t}(1 + |\alpha_s|) \tag{6.4}$$

$$\rho_\ell(\alpha,t,\hbar) = \sigma(\alpha,t)^{\ell M_1} \sum_{1\le j\le \ell} \left(\frac{|t|}{\hbar}\right)^j (\sqrt{\hbar}\theta(\alpha,t))^{2j+\ell}. \tag{6.5}$$

The constants $M_1, K_{H,T}$ depend on the following assumptions on the classical Hamiltonian H.
H is assumed to be a C^∞-smooth function in z and $t \in]-T,T]$ $(0 \le T \le +\infty)$, satisfying a global estimate

(A.0) there exists some non-negative constants $m, M, K_{H,T}$ such that

$$(1 + |z|^2)^{-M/2}|\partial_z^\gamma H(z,t)| \le K_{H,T},$$

uniformly in $z \in Z$ and $t \in [-T,T]$ for $|\gamma| \ge m$.
For example H may be a very general Hamiltonian including time-dependent magnetic fields or non Euclidean metrics.
Furthermore it is assumed that the classical and quantum evolutions exist from time zero to time t for t in some interval $]-T,T[$. More precisely :

(A.1) Given some $\alpha = (q_0,p_0) \in \mathbb{R}^{2n}$, there exists a positive T such that the classical

Hamilton's equations :

$$\begin{cases} \dot{q}_t = \dfrac{\partial H}{\partial p}(q_t, p_t, t), \\ \dot{p}_t = -\dfrac{\partial \partial H}{\partial q}(q_t, p_t, t), \end{cases}$$

have a unique solution starting from initial data (q_0, p_0) for any $t \in]-T, T[$. We call $\alpha_t = (q_t, p_t)$ the phase space point reached at time t by the so defined classical flow, starting from $\alpha_0 = \alpha$.

(A.2) There exists a unique quantum propagator $\{U(t,s), (t,s) \in]-T, T[^2\}$ satisfying some technical condiditions (see [38]). When H is time independent we only ask $\hat{H}$ to be essentially self-adjoint.

Theorem 6.1 ([38]) *Suppose that assumptions (A.0) to (A.2) on the quantum (6.1) and the classical (6.2) system, hold. Then for all integers $\ell \geq 1$, $J \geq 1$, for every real number $\kappa > 0$, there exists $\Gamma > 0$ such that for every finite family of complex numbers $\{c_\mu,\ \mu \in \mathbb{N}^n,\ |\mu| \leq J\}$ there exist $c_\nu(t,\hbar)$ for $\nu \in \mathbb{N}^n$, $|\nu| \leq 3(\ell-1)+J$, such that for $0 < \hbar + \sqrt{\hbar}\theta(\alpha,t) < \kappa$ the following L^2-norm estimate holds, uniformly in $|t| < T$,*

$$\|U(t,0)\left(\sum_{|j|=0}^{J} c_j \Psi_{j,\alpha}\right) - e^{i\delta_t/\hbar} \sum_{|\mu|=0}^{J+3(\ell-1)} c_\mu(t,\hbar)\Phi_\mu(t)\| \leq \tag{6.6}$$

$$\Gamma K_{H,T}\, \rho_\ell(\alpha,t,\hbar) \left(\sum_{0\leq\mu\leq J} |c_\mu|^2\right)^{1/2}. \tag{6.7}$$

Moreover the coefficients $c_\mu(t,\hbar)$ are polynomials in $\sqrt{\hbar}$ whose coefficients are given by the evolution of the classical system (6.2).

Remark 6.2 *Without control of the constants, this kind of results appeared many times in the literature (see [119] and the references there, concerning Gaussian beams, [66, 67, 111, 12]).*
This propagation theorem for coherent states can be used to prove semi-classical trace formulas and can replace the W.K.B method explained in section 4 (see [39]). The reader can find more details in the references concerning many works related to this subject. The starting point for the use of coherent states to prove trace asymptotic formula is the following

$$\mathrm{tr}\left(U(t)\hat{A}\right) = (2\pi\hbar)^{-n} \int_{\mathbb{R}^{2n}} \langle U(t)\hat{A}\varphi_\alpha, \varphi_\alpha\rangle d\alpha,$$

where $U(t)$ is the propagator for a time independent Hamiltonian and $A \in \mathcal{S}(\mathbb{R}^{2n})$.

Propagation from an equilibrium point

Let us assume that $\hat{H}$ is time independent and $\alpha_t = \alpha$, $\forall t \in \mathbb{R}$. If α is a stable equilibrium point then it is easily shown that there exists $C > 0$ such that

$$\rho_\ell(\alpha, t, \hbar) \leq C|t|^\ell \hbar^{\ell/2}. \tag{6.8}$$

It then follows that semi-classical approximation is valid for

$$|t| \leq \hbar^{\varepsilon - 1/2}, \ \forall \varepsilon > 0.$$

Let us assume now that α is an unstable equilibrium point. Then it exists $\lambda > 0$ (Lyapounov exponent) such that

$$\theta(\alpha, t) \leq e^{\lambda|t|}.$$

Hence it follows that semi-classical approximation is valid for

$$|t| \leq \gamma \log(\frac{1}{\hbar}), \ \forall \gamma < \frac{1}{2\lambda}.$$

More generally the last conclusion still holds for every time independent Hamiltonian and for α in a compact energy shell (i.e $H^{-1}(H(\alpha))$ is compact).
In the case of an unstable equilibrium point α it is possible to measure semi-classically the spreading starting with a wave packet localized at α. For simplicity we suppose here $n = 1$ (see [38] for details and more general results). Let us define the mean value localization of the wave packet at time t,

$$S(t) = \frac{2}{\hbar}\langle W(-\alpha)\psi(t), K_0 W(-\alpha)\psi(t)\rangle, \tag{6.9}$$

with $\psi(t) = U(t,0)\varphi_\alpha$ and $K_0 = \frac{1}{2}(-\hbar^2\Delta + |x|^2)$. The Hessian matrix here is $H''(\alpha) = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$. The instability assumption is $b^2 > ac$; $\lambda > 1$ and $\frac{1}{\lambda}$ denote the Lyapounov exponents of $JH''(\alpha)$ with

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

Theorem 6.3 ([38]) *With the above assumptions, for $\epsilon' > \epsilon$ small enough, we have*

$$s(t) - s(0) = \frac{4b^2 + (a-c)^2}{2(b^2 - ac)} \sinh^2(\lambda t) + O(\hbar^\varepsilon); \tag{6.10}$$

the estimate is uniform for

$$0 \leq t \leq \frac{1 - 2\varepsilon'}{6\lambda} \log(\frac{1}{\hbar}).$$

This theorem shows that the spreading of a wave packet localized at an unstable equilibrium point is exponentially fast, the exponent depending on the Lyapounov instability coefficient.

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