Remarks on time dependent Schrödinger equation, bound states and coherent states

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ABSTRACT It is well known from the beginning of quantum theory that there exist deep connections between the time evolution of a classical Hamiltonian system and the bound states for the Schrödinger equation in particular in the semi-classical régime. These connections are well understood for integrable systems (Bohr-Sommerfeld quantization rules). But for more intricated systems (like classically chaotic Hamiltonian) the mathematical analysis of the bound states is much more difficult and there are few rigorous mathematical results.
In this paper our goal is to revisit some of these results and to show that they can be proven, and sometimes improved, by using essentially two technics: the Wigner-Weyl calculus and the propagation of observables on one side, the propagation of coherent states on the other side. We want to put emphasis in our approach that we get rather explicit estimates in terms of classical dynamics.
The main ideas explained here, in particular the use of coherent states, are the results of several years of collaboration with Monique Combescure.

0 Introduction

One of the most important problem in quantum mechanics is to compute matrix elements $A_{jk}(\hbar) = \langle \hat{A}\varphi_j, \varphi_k\rangle$ (transition amplitudes), where $\hat{A}$ is an observable and $\{\varphi_j\}$ is an orthonormal system of normalized bound states of a given quantum Hamiltonian $\hat{H}$. $\hat{H}$ is supposed to be a self-adjoint operator in the Hilbert space in $L^2(\mathbb{R}^d)$ for a system with d degrees of freedom.

In the semiclassical régime considered here, $\hat{H}$ is obtained as the $\hbar$-Weyl quantization of a classical Hamiltonian H. We have $\hat{H}\varphi_j = E_j\varphi_j$, where E_j is the eigenenergy of φ_j.
The diagonal matrix elements $A_{jj}(\hbar)$ are clearly related with trace formu-

las. Assume for simplicity in a first step that $\hat{H} = -\frac{\hbar^2}{2}\triangle + V$ where V is a smooth confining electric potential i.e $\lim_{|q|\to+\infty} V(q) = +\infty$ (like a polynomial). $A(q,p)$ can be any smooth classical observable on the phase space with polynomial behaviour in (q,p) at ∞.
Let be $\{\varphi_j\}_{j\geq 0}$ an orthonormal basis of bounded states. So we have

$$\mathrm{Tr}(\hat{A}f(\hat{H})) = \sum_{j\geq 0} f(E_j)A_{jj}(\hbar)$$

Consider, for example, the Gibbs states at temperature $T = \beta^{-1}$, $\hat{G}(\beta) = \frac{\mathrm{e}^{-\beta\hat{H}}}{\mathrm{Tr}\left(\mathrm{e}^{-\beta\hat{H}}\right)}$ By standard application of Weyl-Wigner calculus, it is easily proved that

$$\mathrm{Tr}\left(\hat{A}\mathrm{e}^{-\beta\hat{H}}\right) \asymp (2\pi\hbar)^{-d}\sum_{j\geq 0} g_{\beta,j}\hbar^{2j} \text{ with } g_{\beta,0} = \int_{\mathbb{R}^{2d}} A(z)\mathrm{e}^{-\beta H(z)}dz \quad (1)$$

and

$$\lim_{\hbar\to 0}\mathrm{Tr}(\hat{A}\hat{G}(\beta)) = \langle A\rangle_\beta \text{ where } \langle A\rangle_\beta = \frac{\int_{\mathbb{R}^{2d}} A(z)\mathrm{e}^{-\beta H(z)}dz}{\int_{\mathbb{R}^{2d}} \mathrm{e}^{-\beta H(z)}dz} \quad (2)$$

and $H(z) = \frac{p^2}{2} + V(q)$, $z = (q,p)$.
These two asymptotics give a rough average behaviour for the energies E_j and the matrix elements $\hat{A}_{jj}(\hbar)$. To get more accurate informations, as it is well known, we need to work in a small window in the energy spectrum, $E_j \in [E-\delta, E+\delta]$ where E is a fixed classical energy and $\delta > 0$ is as small as possible. But doing that, time dependent phenomena occur, as it is expected from the time-energy uncertainty principle. More precisely the classical dynamics of the Hamiltonian H enter the game when δ is of the same order as $\hbar$. This is transparent with the Gutzwiller trace formula which displays a semiclassical asymptotic for

$$\Xi_{\rho,A}(\hbar) = \sum_{j\geq 0}\rho\left(\frac{E_j - E}{\hbar}\right)A_{jj}(\hbar) \quad (3)$$

where the Fourier transform $\tilde{\rho}$ of ρ is a smooth function with bounded support. Only periodic trajectories of energy E of the classical Hamiltonian contribute in the asymptotic expansion of $\Xi_{\rho,A}(\hbar)$. This is also true for the average of an observable in the Gibbs state if the temperature is low, of the same order of the Planck constant $\hbar$ (see [6]).
A closely related problem is to estimate the counting function of the eigenenergies in a fixed real intervall $I = [E', E]$. Let us denote by $N_I(\hbar)$ the number of bound states of $\hat{H}$ in I. Under generic assumptions (E', E are not critical for V) we have the Weyl law

$$N_I(\hbar) = (2\pi\hbar)^{-d}\int_{H(z)\in I} dz + O(\hbar^{1-d})$$

As we shall see later, a more difficult problem is to find a second term and to estimate the error. Some properties of the classical flow at large time are also needed because periodic trajectories give oscillatory contributions. This is already obvious for the harmonic oscillator ($V(q) = q^2$).
When the classical dynamics is chaotic (ergodic) on the energy shell $\Sigma_E := H^{-1}(E)$ (E non critical), we shall also discuss the quantum ergodic theorem, whose meaning is the following. Let be $I_\hbar = [E - \delta_\hbar, E + \delta_\hbar]$ shrinking to E in a suitable way. Then, except for a negligible set of eigenenergies in $I_\hbar$, we have

$$\lim_{\hbar\to 0,\ E_j(\hbar)\in I_\hbar} A_{jj}(\hbar) = \int_{\Sigma_E} A(z) d\nu_E(z) \tag{4}$$

where $d\bar{\nu}_E$ is the normalized Liouville measure on Σ_E.

The links between time dependent and time independent phenomena appear also clearly in the following question. It is conjectured that the behaviour of $\hat{A}_{jk}(\hbar)$ resemble a random matrix model. (see for example[28, 29]) For classically chaotic systems, Wilkinson [28] conjectures that the matrix elements $A_{jk}(\hbar)$ are independent, Gaussian, with mean zero when $j \neq k$. The last statement is supported by results proved in ([4]). The variance introduced by Wilkinson is

$$\mathcal{V}_{(f,g)}(\hbar, E, \tau) = \sum_{[E_j(\hbar), E_k(\hbar)\in I_\hbar]} |A_{jk}(\hbar)|^2 f_\hbar\left(E - \frac{1}{2}(E_j(\hbar) + E_k(\hbar)\right).g\left(\tau - \omega_{jk}(\hbar)\right) \tag{5}$$

where E is inside the interval $I_\hbar$, $\omega_{jk}(\hbar) = \frac{E_j(\hbar)-E_k(\hbar)}{\hbar}$, f, g are Gaussian regularizations of the Dirac δ_0 distribution. $f_\hbar(u) := \frac{1}{\hbar} f(\frac{u}{\hbar})$ with $f(u) = \frac{1}{\sigma_1\sqrt{2\pi}} \mathrm{e}^{\frac{u^2}{2\sigma_1^2}}$ and $g(u) = \frac{1}{\sigma_2\sqrt{2\pi}} \mathrm{e}^{\frac{u^2}{2\sigma_2^2}}$, $\sigma_1, \sigma_2 > 0$.

This variance has a nice semiclassical limit. If the Fourier transform $\tilde{f}$ of f has a small support around zero then

$$\lim_{\hbar\to 0} (2\pi\hbar)^d \mathcal{V}_{(f,g)}(\hbar, E, \tau) = \tilde{f}(0) \int \tilde{g}(t) \mathrm{e}^{it\tau} C_A(E,t) dt$$

where $\tilde{f}$ (Fourier transform of f) has a small support around zero and $C_A(E,t)$ is the classical autocorrelation function

$$C_A(E,t) = \int_{\Sigma_E} A(z) A(\Phi_H^t(z)) d\nu_E(z)$$

If the support of f contains some non zero periods of the classical flow we have oscillatory terms, like in the Gutzwiller trace formula as we shall see later.

It seems much more difficult to prove a similar result for Gaussians test functions. The main difficulty comes from f: we need some control of the

large periods of the classical flow which are not well kown up to now. Concerning g one can use recent results obtained in [1] where accurate estimates for longtime propagation of observables are proved.
Our main goal in this paper is to revisit some already kown connections between time dependent properties and time independent one for Shrödinger equations by adding when possible explicit estimates. We will give some ideas about proofs showing that they can be deduced essentially from two basic long time dependent accurate results: propagation of observables and propagation of coherent states. This last technics will be used instead of the BKW method to avoid the well known caustic problem. Moreover this way we can get time dependent estimates up to the Ehrenfest time (of order $|\log \hbar|$ in the chaotic case, $\hbar^{-\kappa}$, $\forall \kappa < 1/8$, in the integrable case. These time dependent estimates are useful, for exemple, to improve the remainder estimate in Weyl formula with 2 terms or to control the speed of convergence in the quantum ergodic theorem.
The content of the paper is the following.
We first recall from [1] the results concerning propagation of observables. Then we recall from [6, 25] the mains facts concerning coherent states and their propagation by the time dependent Schrödinger equation.
We will explain how to apply these tools to different spectral problems. We discuss the trace Gutzwiller formula and the main steps to prove it according the method used in [3]. Then we apply this to the Weyl law with two terms and remainder estimate. We also discuss the proof of the semiclassical expansion for the Wilkinson variance.
In the last section we explain some results concerning diagonal and non diagonal matrix elements $A_{jk}(\hbar)$, in particular the quantum ergodic theorem and related topics.

1 Propagation of observables

Let us denote by $X = \mathbb{R}^d$ the configuration space of a classical mechanical system with d degrees of freedom. The corresponding phase space Z is identified with $\mathbb{R}^{2d}$ equipped with the symplectic form σ defined by

$$\sigma(z, z') = Jz \cdot z' \tag{6}$$

where $\cdot$ is the Euclidean scalar product and J is the $2d \times 2d$ matrix

$$J = \begin{pmatrix} 0 & \mathbb{I}_d \\ -\mathbb{I}_d & 0 \end{pmatrix} \tag{7}$$

A generic point in Z is denoted z and its coordinates by (q, p) where $q, p \in \mathbb{R}^d$.
A classical Hamiltonian is a smooth real function $H : Z \to \mathbb{R}$. Our basic example will be $H(q, p) = \frac{|p|^2}{2m} + V(q)$ $(m > 0)$ where $|p|^2 = p \cdot p$.

The motion of the classical system is determined by the system of Hamilton's equations

$$\frac{dq_t}{dt} = \frac{\partial H}{\partial p}(q_t, p_t), \quad \frac{dp_t}{dt} = -\frac{\partial H}{\partial q}(q_t, p_t) \ ; (q_0, p_0) = (q, p). \tag{8}$$

The equations (8) generate a flow Φ_H^t on the phase space Z, defined by $\Phi_H^t(q,p) = (q_t, p_t)$. Let us consider a classical observable A, i.e A a smooth real valued function defined on Z. The time evolution of A is given by

$$\frac{d}{dt}A(\Phi^t(z)) = \{H, A\}(\Phi^t(z)), \tag{9}$$

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

$$\{H, A\} = \partial_q H \cdot \partial_p A - \partial_p H \cdot \partial_q A. \tag{10}$$

Here we have used the notation $\partial_q = \frac{\partial}{\partial q}$. By Weyl quantization of H and A, we get quantum observables $\hat{H}$ and $\hat{A}$ in in $L^2(X)$ with $\hat{H}$ self-adjoint. So we can define the one parameter group of unitary operators $U(t) = \exp\left(-\frac{it}{\hbar}\hat{H}\right)$. The quantum time evolution of the observable $\hat{A}$ is given by $\hat{A}(t) = U(-t)\hat{A}U(t)$ which satisfies the Heisenberg-von Neumann equation:

$$\frac{d\hat{A}(t)}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}], \tag{11}$$

where $[K, B] = KB - BK$ is the commutator of K, B. Let us recall the $\hbar$-Weyl quantization formula, for $A \in \mathcal{S}(Z)$ (the space of Schwartz functions) and for $\psi \in \mathcal{S}(X)$, we have:

$$Op_\hbar^w A\psi(x) = \hat{A}\psi(x) = (2\pi\hbar)^{-d} \iint_Z A\left(\frac{x+y}{2}, p\right) \mathrm{e}^{i\hbar^{-1}(x-y)\cdot p}\psi(y)dydp. \tag{12}$$

This definition can be extended to the following classes of observables.

Definition 1.1. *(i) A weight function on the phase space Z is a positive continuous function μ on Z such that there exist $C > 0$, $M \geq 0$ such that for every $z, z' \in Z$,*

$$\mu(z) \leq C(1 + |z - z'|)^M \mu(z')$$

(ii) $A \in \mathcal{O}(\mu)$, where μ is a weight, if and only if $Z \xrightarrow{A} \mathbb{C}$ is C^∞ in Z and for every multi-index $\gamma \in \mathbb{N}^{2d}$ there exists $C_\gamma > 0$ such that

$$|\partial_z^\gamma A(z)| \leq C_\gamma \mu(z), \ \forall z \in Z.$$

(iii) We say that A is a semiclassical observable of weight μ if there exist $\hbar_0 > 0$ and a sequence $A_j \in \mathcal{O}(\mu)$, $j \in \mathbb{N}$, such that for every $N \in \mathbb{N}$ and

every $\gamma \in \mathbb{N}^{2d}$ there exists $C_N > 0$ such that for all $\hbar \in]0, \hbar_0[$ we have

$$\sup_Z \mu^{-1}(z) \left| \partial_z^\gamma \left(A(\hbar, z) - \sum_{0 \le j \le N} \hbar^j A_j(z) \right) \right| \le C_N \hbar^{N+1}. \qquad (13)$$

A_0 is called the principal symbol, A_1 the sub-principal symbol of $\hat{A}$. The set of semi-classical observables of weight μ is denoted by $\mathcal{O}_{sc}(\mu)$. Its range by the $\hbar$-Weyl quantization is denoted $\widehat{\mathcal{O}}_{sc}(\mu)$.
If $\mu(z) = \mu_m(z) = (1 + |z|)^m$, $m \in \mathbb{R}$, we say that the observable is of weight m.

Notation : For any A and A_j satisfying (13), we will write : $A(\hbar) \asymp \sum_{j \ge 0} \hbar^j A_j$ in $\mathcal{O}_{sc}(\mu)$.

Let us now recall from [1] a statement for the propagation of observable which will be useful for applications to bound states.
Assume that $H \in \mathcal{O}_{sc}(\mu)$. Let Ω be a bounded* open set in the phase space Z. We assume that the closure $\overline{\Omega}$ of Ω is invariant by the flow $\Phi^t := \Phi^t_{H_0}$ ($\forall t \in \mathbb{R}$) and that there exists an increasing function s from $]0, \infty[$ in $[1, +\infty[$ satisfying $s(T) \ge T$ and such that the following estimates are satisfied:

$$\sup_{z \in \Omega, |t| \le T} \left| \partial_z^\gamma \Phi^t(z) \right| \le C_\gamma s(T)^{|\gamma|} \qquad (14)$$

where C_γ depends only on $\gamma \in \mathbb{N}^{2d}$. Then we have:

Theorem 1.2. *For every smooth observable A, with compact support in Ω, $\widehat{A}(t)$ is a semiclassical observable of weight $-\infty$, with semiclassical symbol supported in Ω, such that*

$$A(t, \hbar) \asymp \sum_{j \ge 0} A_j(t) \hbar^j$$

where

$$A_0(t, z) = A(\Phi^t(z)), \quad A_1(t, z) = \int_0^t \{A(\Phi^\tau), H_1\}(\Phi^{t-\tau}(z)) d\tau \qquad (15)$$

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

$$A_j(t, z) = \sum_{\substack{|(\alpha,\beta)| + k + \ell = j+1 \\ 0 \le \ell \le j-1}} C(\alpha, \beta) \int_0^t [(\partial_p^\alpha \partial_q^\beta H_k)(\partial_q^\alpha \partial_p^\beta A_\ell)(\tau)](\Phi^{t-\tau}(z)) d\tau, \ (16)$$

$$\text{with } \ C(\alpha, \beta) = \frac{(-1)^{|\beta|} - (-1)^{|\alpha|}}{\alpha! \beta! 2^{|\alpha| + |\beta|}} i^{-1-|(\alpha,\beta)|}. \ (17)$$

Furthermore we have the following estimates in L^2 operator-norm of the remainder term.

$$\|\hat{A}(t) - \sum_{0 \le j \le N} \hbar^j \hat{A}_j(t)\|_{L^2} \le C_N \hbar^{N+1} (1 + |t|)^{N+1} s(|t|)^{(2N + \epsilon_d)|t|}. \qquad (18)$$

where C_N is independent on t and $\hbar$, ϵ_d is a universal constant ($\epsilon_d = 5d+10$).

Remark 1.3. *Using classical result on ODE (Gronwall inequality), we always have estimates with exponential time: $s(T) = \mathrm{e}^{\Lambda T}$ for some $\Lambda > 0$. If the classical system is integrable, non singular in $\overline{\Omega}$, then we can choose $s(T) = 1+T$ ([1]). In particular the semiclassical régime is still valid in time intervals $[-T_\hbar, T_\hbar]$ where $T_\hbar = \frac{1-\varepsilon}{2\Lambda}|\log \hbar|$ for the general case and $T_\hbar = \hbar^{\varepsilon - 1/3}$ in the integrable case, for arbitrary $\varepsilon > 0$.*

Remark 1.4. *If the expansion of H in $\hbar$ is even (in particular if H is "classical" : $H = H_0$) then the $\hbar$-expansion of $A(t)$ is even and in the remainder estimate (18) the term $2N$ in the exponent becomes $3N/2$. This kind of improvement may be useful for some applications, as one can see in [9].*

2 Propagation of Gaussian Coherent States

Let us consider in this section the time dependent Schrödinger equation

$$i\hbar \frac{\partial \psi_{z,t}}{\partial t} = \widehat{H}\psi_{z,t}, \quad \psi_{z,0} = \psi_z, \tag{19}$$

where $\hat{H}$ is a semiclassical self-adjoint Hamiltonian of weight $m \in \mathbb{R}$ and ψ_z is a coherent state peacked at $z \in Z$. So we have

$$\psi_{z,t} = U(t)\psi_z, \text{ with } U(t) = \mathrm{e}^{\frac{-it}{\hbar}\hat{H}} \tag{20}$$

A well known method to construct asymptotic solutions of (19) is the WKB expansion. One the main difficulty of WKB methods comes from the occuring of caustic so that the shape of WKB approximations change dramatically when time increases (caustics may appear at times of order 1 in the Planck scale $\hbar$, as we can see, for example for the harmonic oscillator propagator). To get rid of the caustics we can replace the real phase of the WKB method by complex valued phases. Here we shall report on a related but more explicit approach using elementary properties of coherent states. Coherent states are used in partial differential equations from a long time, starting with Schrödinger himself and following by many authors (see [14, 6, 3, 20, 25, 19] for applications and historical comments).

We shall follow the presentation given in [25]. Let us now recall some basic definitions concerning coherent states. We start with the ground state of the harmonic oscillator,

$$g_0(x) = \pi^{-d/4} \exp\left(-|x|^2/2\right). \tag{21}$$

For $z = (q, p) \in \mathbb{R}^{2d}$, the Weyl-Heisenberg operator of translation by z in phase space is

$$\mathcal{T}_\hbar(z) = \exp\left(\frac{i}{\hbar}(p\cdot x - q\cdot \hbar D_x)\right) \tag{22}$$

Let us define the dilation operator $\Lambda_\hbar\psi(x) = \hbar^{-d/4}\psi\left(x\hbar^{-1/2}\right)$. So the coherent state picked on z is defined by $\psi_z = \mathcal{T}_\hbar(z)g_0$. A more explicit expression for ψ_z is

$$\psi_z(x) = \mathrm{e}^{\frac{i}{\hbar}(p\cdot x - \frac{q\cdot p}{2})}\psi_0(x-q) \tag{23}$$

For $\hbar = 1$ we shall denote $\psi_z = g_z$ and $\mathcal{T}_\hbar(z) = \mathcal{T}(z)$.
It is well known that $\{\psi_z\}_{z\in\mathbb{R}^{2d}}$ is an "overcomplete basis" in $L^2(\mathbb{R}^d)$. So for every trace-class observable $\hat{B}$ in $L^2(\mathbb{R}^d)$ we have

$$\mathrm{Tr}(\hat{B}) = (2\pi\hbar)^{-d}\int_Z \langle \hat{B}\psi_z, \psi_z\rangle dz \tag{24}$$

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

Under rather general assumptions, an asymptotic expansion for the quantum evolution of coherent states, $U(t)\psi_z$, was obtained in [6], with an error term of order $O(\hbar^\infty)$, with some control for large time of order $O(\log(\hbar^{-1}))$ (Ehrenfest time).

Recall that $z_t = (q_t, p_t)$ is the solution of (8) starting from $z = (q, p)$. For simplicity it is assumed that $z \in \Omega$, where Ω is like in section.1 and the flow satisfies 14. let us define

$$\delta_t(z) = S(t,z) - \frac{q_t\cdot p_t - q\cdot p}{2} \quad \text{where} \quad S(t,z) = \int_0^t p_s\cdot \dot{q}_s ds - tH_0(z) \tag{25}$$

is the classical action. The Jacobi stability matrix, F_t, is the linearized flow associated with (8) at the point z_t of the classical trajectory. F_t is also the Hamiltonian flow defined by the quadratic Hamiltonian $K_2(t,\zeta) = \frac{1}{2}\partial^2_{z,z}H(z_t)\zeta\cdot\zeta$ for $\zeta \in \mathbb{R}^{2d}$, where $\partial^2_{z,z}H$ is the Hessian matrix of $H(z)$ in the variables z. We have $F_0 = \mathbb{I}$ and F_t is a symplectic, $2d\times 2d$ matrix. It can be written as four $d\times d$ blocks :

$$F_t = \begin{pmatrix} A_t & B_t \\ C_t & D_t \end{pmatrix}. \tag{26}$$

We also need to introduce the quantization of F_t which can be defined as the quantum propagator $\mathcal{M}[F_t]$, *with Planck constant equal 1*, for the quadratic Hamiltonian $Op_1^w[K_2(t)]$. In particular we have the following useful formulas

$$\mathcal{M}[F_t]g_0(x) = \pi^{-d/4}\left(\det(A_t + iB_t)\right)^{-1/2}\mathrm{e}^{i\Gamma_t x\cdot x/2} \tag{27}$$

$$\mathcal{M}[F_t]^{-1}Op_1^w[L]\mathcal{M}[F_t] = Op_1^w[L\circ F_t] \tag{28}$$

where $\Gamma_t = (C_t + iD_t)(A_t + iB_t)^{-1}$ and L is any classical (smooth) observable defined on Z. Γ_t is a complex symmetric, $d \times d$ matrix, with positive definite imaginary part given as follows

$$\mathrm{Im}\,\Gamma_t = (AA' + BB')^{-1} \tag{29}$$

where A' denote the transposed matrix of A.

Let us now state the following result [6, 25]

Theorem 2.1. *Under the above assumptions, there exists a family of polynomials $\{b_j(t,x)\}_{j\in\mathbb{N}}$ in d real variables $x = (x_1, \cdots, x_d)$, with time dependent coefficients, such that for every $|t| \le T$, $\hbar \in]0,1]$, $N \in \mathbb{N}$, we have*

$$\left\| U(t)\psi_z - \exp\left(\frac{i\delta_t(z)}{\hbar}\right) \mathcal{T}(z_t)\Lambda_\hbar \mathcal{M}[F_t] \left(\sum_{0\le j\le N} \hbar^{j/2} b_j(t) g_0\right)\right\|_{L^2(\mathbb{R}^d)} \le$$
$$C_N s(T)^{(3N+\epsilon_d)}(1+T)^{N+1}\hbar^{(N+1)/2} \tag{30}$$

where $s(T)$ can be choosen like en section.2, formula 14, and the constant C_N is independent on T and $\hbar$.

Remark 2.2. *1) This result is proved in [6]. Theorem 2.1 and applied at finite time to give a proof of the Gutzwiller trace formula.*
In [25] Gevrey type estimates for C_N, N large, have been computed

2) The polynomials $b_j(t,x)$ can be explicitly computed by induction along the classical trajectories $z(t)$. In particular $b_0(t,x) = \exp\left(-i\int_0^t H_1(z_s)ds\right)$.
3) As for evolution of observable we get a critical time $T'_\hbar$ for the validity of semiclassical approximation. In the general case $\sigma(T) = \mathrm{e}^{\Lambda T}$ and $T'_\hbar = \frac{1-\varepsilon}{6\Lambda}|\log\hbar|$. In the integrable case we can choose $T'_\hbar = \hbar^{\varepsilon-1/8}$. These validity times are smaller than those found for propagation of observables.

3 Semiclassical Trace Asymptotics

All Hamiltonians considered here satisfy the following general technical assumptions:
(TA1) $\mu_0(z) := 1 + |H_0(z)|$ is a weight function on Z and H is a semiclassical observable with weight μ_0 and principal symbol H_0.
(TA2) E is a fixed energy such there exist $a < E < b$ and $H_0^{-1}[a,b]$ is a bounded closed set in the phase space Z. Moreover E is non critical for H_0 i.e $\nabla H_0(z) \ne 0$ for every $z \in \Sigma_E$ where $\Sigma_E = H_0^{-1}(E)$. So the Liouville measure is well defined on Σ_E,

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

where $d\Sigma_E$ is the canonical measure on the hypersurface Σ_E.
Our main goal in this section is to revisit the following spectral distribution:

$$\Xi_{\rho,A}(E,\hbar) = \sum_{j\geq 0} \rho\left(\frac{E_j - E}{\hbar}\right) A_{jj}(\hbar) \tag{31}$$

where the Fourier transform $\tilde{\rho}$ of ρ has a compact support. The ideal ρ should be the Dirac delta function, which need too much informations. So we will try to control large support for $\tilde{\rho}$. To do that we take
$\rho_T(t) = T\rho_1(tT)$ with $T \geq 1$, where ρ_1 is non negative, even, smooth real function, $\int_{\mathbb{R}} \rho_1(t)dt = 1$, $\mathrm{supp}\{\tilde{\rho}_1\} \subset [-1,1]$, $\tilde{\rho}_1(t) = 1$ for $|t| \leq 1/2$.
By applying the propagation theorem for coherent states stated in section.3, we can write $\Xi_{\rho_T,A}(E,\hbar)$ as a Fourier integral with an explicit complex phase. The classical dynamics enter the game in a second step, to analyse the critical points of the phase. Let us describe the steps (see [3] for the details).
(i) modulo a negligible error, we can replace $\hat{A}$ by $\hat{A}_\chi = \chi(\hat{H})\hat{A}\chi(\hat{H})$ where χ is smooth with support in a small neighborhood of E like $]E-\delta_\hbar, E+\delta_\hbar[$ such that $\lim_{\hbar\to 0} \delta_\hbar = 0$.
(ii) using inverse Fourier formula we have the following time dependent representation:

$$\Xi_{\rho_T,A}(E,\hbar) = \frac{1}{2\pi}\int_{\mathbb{R}} \tilde{\rho}_1\left(\frac{t}{T}\right) \mathrm{Tr}\left(\hat{A}_\chi \mathrm{e}^{\frac{it}{\hbar}(E-\hat{H})}\right) dt \tag{32}$$

(iii) if B is a symbol then we have $\hat{B}\psi_z = B(z)\psi_z + \cdots$ where the $\cdots$ are correction terms in half power of $\hbar$ which depend on the Taylor expansion of B at z
(iv) putting all things together, after some computations, we get for every $N \geq 1$:

$$\Xi_{\rho_1,A}(E,\hbar) = (2\pi\hbar)^{-d}\int_{\mathbb{R}_t\times\mathbb{R}^{2d}_z} \tilde{\rho}_1\left(\frac{t}{T}\right) a^{(N)}(t,z,\hbar)\mathrm{e}^{\frac{i}{\hbar}\Psi_E(t,z)} dtdz + \mathcal{R}_{N,T,\hbar}. \tag{33}$$

The phase Ψ_E is given by

$$\Psi_E(t,z) = t(E - H_0(z)) + \frac{1}{2}\int_0^t \sigma(z_s - z, \dot{z}_s)ds + \frac{i}{4}(\mathbb{I}_d - W_t)(\breve{z} - \breve{z}_t)\cdot\overline{(\breve{z} - \breve{z}_t)}, \tag{34}$$

with $\breve{z} = q + ip$ if $z = (q,p)$ and $W_t = Z_t Y_t^{-1}$ where $Y_t = C_t - B_t + i(A_t + D_t)$, $Z_t = A_t - D_t + i(B_t + C_t)$.
The amplitude $a^{(N)}$ has the following property

$$a^{(N)}(t,z,\hbar) = \sum_{0\leq j\leq N} a_j(t,z)\hbar^j, \tag{35}$$

where each $a_j(t,z)$ is smooth, with support in variable z included in the neighborhood $\Omega = H_0^{-1}[E-\delta_E, E+\delta_E]$ of Σ_E, and estimated in t as follows

$$|a_j(t,z)| \leq C_j s(T)^{6j}(1+T)^{2j} \tag{36}$$

In particular for $j=0$ we have

$$a_0(t,z) = \pi^{-d/2}\left[\det(Y_t)\right]^{-1/2}\exp\left(-i\int_0^t H_1(z_s)ds\right) \tag{37}$$

The remainder term satisfies

$$\mathcal{R}_{N,T,\hbar} \leq C_N s(T)^{6N+\epsilon_d}(1+T)^{2N+1}\hbar^{N+1} \tag{38}$$

Form the above computations we can easily see that the main contributions as $\hbar \to 0$ in $\Xi_{\rho_T,A}(E,\hbar)$ come from the periods of the classical flow as it is expected. Let us first remark that we have

$$2\mathrm{Im}\Psi_E(t,z) \geq \langle \mathrm{Im}\,\Gamma_t(\Gamma_t+i)^{-1}(\breve{z}-\breve{z}_t), \Gamma_t+i)^{-1}(\breve{z}-\breve{z}_t)\rangle$$

Here $\langle,\rangle$ is the Hermitean product on $\mathbb{C}$. Because of positivity of $\mathrm{Im}\,\Gamma_t$ we get the following lower bound: there exists $c_0>0$ such that for every T and $|t|\leq T$ we have

$$\mathrm{Im}\Psi_E(t,z) + |\partial_t\Psi_E(t,z)|^2 \geq c_0\left(|H_0(z)-E|^2 + s(T)^{-4}|z-z_t|^2\right). \tag{39}$$

The stationary phase theorem with complex phase [17], vol.1, gives easily the contribution of the 0-period.

Theorem 3.1. *If T_0 is choosen small enough, such that $T_0 < \sup\{t>0,\ \forall z\in\Sigma_E,\ \Phi^t(z)\neq z\}$, then we have the following asymptotic expansion:*

$$\Xi_{\rho_{T_0},A}(E,\hbar) \asymp (2\pi\hbar)^{-d}\sum_{j\geq 0}\alpha_{A,j}(E)\hbar^{j+1} \tag{40}$$

where the coefficient $\alpha_{A,j}$ do not depend on ρ. In particular

$$\alpha_{A,0}(E) = \int_{\Sigma_E} A(z)d\nu_E(z),\quad \alpha_{A,1}(E) = \int_{\Sigma_E} H_1(z)A(z)d\nu_E(z) \tag{41}$$

By using a Tauberian argument [24], a Weyl formula with an error term $\mathrm{O}(\hbar^{1-d})$ can be obtained from 40.
The contributions of periodic trajectories can be computed if we had some specific assumptions on the classical dynamics. However Petkov-Popov [22] succeed to give a very general trace formula modulo an error $\mathrm{o}(\hbar^{1-d})$ using the Hörmander's Fourier integral operator theory. With our coherent states analysis it is possible to recover their result. Let us recall that in [3] this

coherent states analysis is used to give a proof of the Gutzwiller trace formula. Let us recall now the rigorous statement.
The main assumption is the following. Let $\mathcal{P}_{E,T}$ be the set of all periodic orbits on Σ_E with periods T_γ, $0 < |T_\gamma| \le T$ (including repetitions and change of orientation). T_γ^* is the primitive period of γ. Assume that all γ in $\mathcal{P}_{E,T}$ are nondegenerate, i.e. 1 is not an eigenvalue for the corresponding "Poincaré map", P_γ. It is the same to say that 1 is an eigenvalue of F_{T_γ} with algebraic multiplicity 2. In particular, this implies that $\mathcal{P}_{E,T}$ is a finite union of closed path with periods T_{γ_j}, $-T \le T_{\gamma_1} < \cdots < T_{\gamma_N} \le T$.

Theorem 3.2 (Trace Gutzwiller Formula). *Under the above assumptions, for every smooth test function ρ such that* $\mathrm{supp}\{\tilde\rho\} \subset]-T, T[$ *, the following asymptotic expansion holds true, modulo $O(\hbar^\infty)$,*

$$\Xi_{\rho,A}(E,\hbar) \asymp (2\pi\hbar)^{-d}\tilde\rho(0)\sum_{j\ge 0} c_{A,j}(\tilde\rho)\hbar^{j+1}$$

$$+\sum_{\gamma\in\mathcal{P}_{E,T}} (2\pi)^{d/2-1}\exp\left(i\left(\frac{S_\gamma}{\hbar}+\frac{\sigma_\gamma\pi}{2}\right)\right)|\det(\mathbb{I}-P_\gamma)|^{-1/2}.$$

$$\left(\sum_{j\ge 0} d^\gamma_{A,j}(\tilde\rho)\hbar^j\right) \tag{42}$$

where σ_γ is the Maslov index of γ ($\sigma_\gamma \in \mathbb{Z}$), $S_\gamma = \oint_\gamma pdq$ is the classical action along γ, $c_{A,j}(\tilde\rho)$ are distributions in $\tilde\rho$ supported in $\{0\}$, in particular

$$c_{A,0}(\tilde\rho) = \tilde\rho(0)\alpha_{A,0}(E), \;\; c_{A,1}(\tilde\rho) = \tilde\rho(0)\alpha_{A,1}(E).$$

$d_j^\gamma(\widetilde\rho)$ are distributions in $\widetilde\rho$ with support $\{T_\gamma\}$. In particular

$$d_0^\gamma(\tilde\rho) = \tilde\rho(T_\gamma)\exp\left(-i\int_0^{T_\gamma^*} H_1(z_u)du\right)\int_0^{T_\gamma^*} A(z_s)ds \tag{43}$$

Remark 3.3. *By the same method it is possible as well to consider integrable systems to get Berry-Tabor formula or more generally systems satisfying the clean intersection property [3].*

For larger time we can use the time dependent estimates given above to improve the remainder estimate in the Weyl asymptotic formula, like Volovoy did for elliptic operators on compact manifolds [27]. For that, let us introduce some control on the measure of the set of periodic path. We call this property condition (NPC). Let be $J_E =]E-\delta, E+\delta[$ a small neighborhood of energy E and $s_E(T)$ an increasing function like in 14 for the open set $\Omega_E = H_0^{-1}(J_E)$. We assume for simplicity here that s_E is either an exponential ($s_E(T) = \exp(\Lambda T^b)$, $\Lambda > 0, b > 0$) or a polynomial ($s_E(T) = (1+T)^a$, $a \ge 1$).

The condition is the following:
(NPC) $\forall T_0 > 0$, there exist positive constants $c_1, c_2, \kappa_1, \kappa_2$ such that for all $\lambda \in J_E$ we have

$$\nu_\lambda \left\{ z \in \Sigma_\lambda,\ \exists t,\ T_0 \le |t| \le T,\ |\Phi^t(z) - z| \le c_1 s(T)^{-\kappa_1} \right\} \le c_2 s(T)^{-\kappa_2} \tag{44}$$

The following result, proved with using stationary phase arguments, estimate the contribution of the "almost periodic points ":

Proposition 3.4. *For all $0 < T_0 < T$, Let us denote $\rho_{T_0 T}(t) = (1 - \rho_{T_0})(t)\rho_T(t)$, where $0 < T_0 < T$. Then we have*

$$\Xi_{\rho_{T_0 T}, A}(E, \hbar) \le C_3 s(T)^{-\kappa_3} \hbar^{1-d} + C_4 s(T)^{\kappa_4} \hbar^{2-d} \tag{45}$$

for some positive constants $C_3, C_4, \kappa_3, \kappa_4$.

Let us now introduce the integrated spectral density

$$\sigma_{A,I}(\hbar) = \sum_{E_j \in I} A_{jj}(\hbar) \tag{46}$$

where $I = [E', E]$ is such that for some $\lambda' < E' < E < \lambda$, $H_0^{-1}[\lambda', \lambda]$ is a bounded closed set in Z and E', E are regular for H_0. We have the following two terms Weyl asymptotics with a remainder estimate

Theorem 3.5. *Assume that there exist open intervals J_E and $J_{E'}$ satisfying the condition (NPC). Then we have*

$$\sigma_{A,I}(\hbar) = (2\pi\hbar)^{-d} \int_{H_0^{-1}(I)} A(z) dz - (2\pi)^{-d} \hbar^{1-d} \times$$
$$\left(\int_{\Sigma_E} A(z) H_1(z) d\nu(z) - \int_{\Sigma_{E'}} A(z) H_1(z) d\nu(z) \right) + O\left(\hbar^{1-d} \eta(\hbar)\right) \tag{47}$$

where $\eta(\hbar) = |\log(\hbar|^{-1/b}$ if $s_E(T) = \exp(\Lambda T^b)$ and $\eta(\hbar) = \hbar^\varepsilon$, for some $\varepsilon > 0$, if $s_E(T) = (1+T)^a$. Furthermore if $I_{E,\delta_1,\delta_2}(\hbar) = [E + \delta_1 \hbar, E + \delta_2 \hbar]$ with $\delta_1 < \delta_2$ then we have

$$\sum_{E + \delta_1 \hbar \le E_j \le E + \delta_2 \hbar} A_{jj}(\hbar) = (2\pi\hbar)^{1-d} (\delta_2 - \delta_1) \int_{\Sigma_E} A(z) d\nu_E + O\left(\hbar^{1-d} \eta(\hbar)\right) \tag{48}$$

Remark 3.6. *(i) Formula 48 was first proved in [2], without remainder estimate.*
(ii) Theorem 3.5 is deduced from proposition 3.4 by a tauberian argument like in [23, 27, 2]

As it was done in [5], by the same technics used above it is possible to give semiclassical asymptotic expansion for the Wilkinson variance introduced before. Let us first write the time dependent representation formula

$$\mathcal{V}_{(\rho,g,A)}(\hbar,E,\tau)=\frac{\hbar^{-1}}{4\pi^2}\int\int_{\mathbb{R}\times\mathbb{R}}\tilde{\rho}(t)\tilde{g}(u-t/2).$$
$$\mathrm{Tr}\left(\hat{A}_u\hat{A}\exp-\frac{it}{\hbar}\left(\hat{H}-E+\frac{\hbar\tau}{2}\right)\right)\mathrm{e}^{iu\tau}dtdu \tag{49}$$

We know from section.2 that $\hat{A}_u := U(-u)\hat{A}U(u)$ is a semiclassical observable, with uniform estimates for $|\tau|\leq C\log(\hbar^{-1})$. So for ρ like in 42 (smooth with compact support) we can choose g Gaussian. It is enough to assume that g is a smooth fonction such that $|\tilde{g}(\tau)|\leq C\mathrm{e}^{-|\tau|/\varepsilon}$, for $\varepsilon>0$ small enough (depending only on $s(T)$). Then under the same conditions as for the Gutzwiller trace formula we have

Theorem 3.7 (Wilkinson Trace Formula).

$$\mathcal{V}_{(\rho,g,A)}(\hbar,E,\tau)\asymp(2\pi\hbar)^{-d}\sum_{j\geq 0}c_{A,j}(\tau,\tilde{\rho},g)\hbar^j+$$
$$\sum_{\gamma\in\mathcal{P}_{E,T}}(2\pi)^{d/2-1}\exp\left(i\left(\frac{S_\gamma}{\hbar}+\frac{\sigma_\gamma\pi}{2}\right)\right)|\det(\mathbb{I}-P_\gamma)|^{-1/2}\left(\sum_{j\geq 0}d_{A,j}^{\gamma}(\tau,\tilde{\rho},g)\hbar^{j-1}\right) \tag{50}$$

where $c_{A,j}(\tau,\tilde{\rho},g)$ are distributions in $\tilde{\rho}$ supported in $\{0\}$, in particular

$$c_{A,0}(\tau,\tilde{\rho},g)=\tilde{\rho}(0)\int\tilde{g}(t)\mathrm{e}^{it\tau}C_A(E,t)dt \tag{51}$$

where $C_A(E,t)$ is the classical autocorrelation function

$$C_A(E,t)=\int_{\Sigma_E}A(z)A(\Phi^t(z)d\nu_E(z) \tag{52}$$

Moreover, $d_j^{\gamma}(\tau,\tilde{\rho},g)$ are distributions in $\tilde{\rho}$ with support $\{T_\gamma\}$. In particular

$$d_0^{\gamma}(\tau,\tilde{\rho},g)=\tilde{\rho}(T_\gamma)\exp\left(-i\int_0^{T_\gamma^*}(H_1(z_u)+\tau/2)du\right)\cdot$$
$$\int_{\mathbb{R}}C_A^{\gamma}(u)\tilde{g}\left(\frac{T_\gamma}{2}-u\right)\mathrm{e}^{iu\tau}du \tag{53}$$

where $C_A^{\gamma}(u)=\int_0^{T_\gamma^*}A(z_{u+t})A(z_t)dt$ is the autocorrelation function along γ.

Remark 3.8. *In [7] a similar result was found in the theory of linear response. As a distribution in g, $d_0^{\gamma}(\tilde{\rho},g)$ can be conveniently writen with* *the Fourier coefficient of the T^*_γ-periodic function $C^\gamma_A(u)$. So we get*

$$\int_{\mathbb{R}} C^\gamma_A(u)\tilde{g}\left(u-\frac{T_\gamma}{2}\right)\mathrm{e}^{iu\tau}du = \frac{2\pi}{T^*_\gamma}\sum_{k\in\mathbb{Z}} C^\gamma_{A,k} g\left(\frac{2\pi k}{T^*_\gamma}+\tau\right)\exp\left(i\left(\frac{2\pi k}{T^*_\gamma}+\tau\right)\frac{T_\gamma}{2}\right) \tag{54}$$

with the Fourier decomposition $C^\gamma_A(u) = \frac{1}{T^*_\gamma}\sum_{k\in\mathbb{Z}} C^\gamma_{A,k}\exp\left(\frac{2i\pi k u}{T^*_\gamma}\right)$

This shows, in particular, that $d^\gamma_0(\tau,\tilde{\rho},g)$ is a distribution in g supported in the discrete set $\{\frac{2\pi k}{T^*_\gamma}+\tau,\ k\in\mathbb{Z}\}$.

4 Quantum Ergodicity and Mixing

This section revisits some results first proved par Sunada [26] and Zelditch[29] for compact manifolds. Our presentation is somehow different and some estimates are improved. Let us begin with a rough estimate concerning the matrix elements $A_{jk}(\hbar)$ and $\omega_{j,k}(\hbar)$. Let be an energy interval $I=[E',E]$, an observable $A\in\mathcal{O}(\mu)$ for some weight μ. Assume that for some $\lambda' < E' < E < \lambda$, $H_0^{-1}[\lambda',\lambda]$ is compact. Let us choose χ a smooth cutoff supported in $]\lambda',\lambda[$, such that $\chi = 1$ on I. Let us introduce the new observable $\hat{A}_\chi = \chi(\hat{H})\hat{A}\chi(\hat{H})$. Then starting from the equality

$$\frac{i}{\hbar}\langle[\hat{A}_\chi,\hat{H}]\varphi_j,\varphi_k\rangle = \omega_{j,k}(\hbar)A_{jk}(\hbar),$$

by induction, we get for every $N\geq 1$, $|\omega_{j,k}(\hbar)|^N|A_{jk}(\hbar)|\leq C_N$ where C_N is independent on $\hbar$.
The following result, proved in [5] and following Helton's trick, show that a single non periodical trajectory disturbs very much the energy spectrum.

Theorem 4.1. *Suppose that on Σ_E there exists at least one periodical classical trajectory. Let be $0<\hbar_n$ such that $\lim_{n\to 0}\hbar_n = 0$. Then for every $\varepsilon>0$ and $c>0$, the following set*

$$\left\{\omega_{j,k}(\hbar_n),\ n\in\mathbb{N},\ E_j,E_k\in[E-c\hbar_n^{1-\varepsilon},E+c\hbar_n^{1-\varepsilon}]\right\}$$

is dense in $\mathbb{R}$.

Sketch of proof: For every observables $A,B\in\mathcal{O}(0)$ and every integrable function f let us introduce $\hat{A}_f=\int_{\mathbb{R}} f(t)\hat{A}_t dt$ where $\hat{A}_t = U(-t)\hat{A}U(t)$. An easy formal computation, assuming for simplicity that φ_j is an orthonormal basis in $L^2(\mathbb{R}^d)$, gives

$$\mathrm{Tr}(\hat{A}_f\hat{B}) = \sum_{j,k} A_{jk}(\hbar)B_{kj}(\hbar)\tilde{f}(\omega_{j,k}(\hbar)) \tag{55}$$

Assume that $\tilde{f}(\omega_{j,k}(\hbar_n)) = 0$ for all j, k, n. Taking the limit $n \to +\infty$, we get $\int_Z A(\Phi^t(z)B(z)f(t)dtdz = 0$. Using existence of one non periodical trajectory we construct suitable observables such that for every smooth, with compact support function $k(t)$ we can get $\int_{\mathbb{R}} k(t)f(t)dt = 0$ hence $f \equiv 0$. □

We shall now consider some specific dynamical properties for the flow on the energy shell Σ_E, equipped with the flow invariant Liouville measure. For $A \in L^1(\Sigma_E)$, let us denote its average $\langle A \rangle_E = \int_{\Sigma_E} A(z)d\bar{\nu}_E(z)$.

Definition 4.2. *(i) Φ^t is ergodic on Σ_E if for every measurable function A on Σ_E we have*

$$\{\forall t \in \mathbb{R}, A \circ \Phi^t = A\} \Longleftrightarrow \{A = \text{constant a.e on } \Sigma_E\} \tag{56}$$

(ii) Φ^t is weakly mixing on Σ_E if for every $A \in L^2(\Sigma_E)$ we have

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} C_A(E, t)dt = \langle A \rangle_E^2 \tag{57}$$

Let us introduce the unitary group in $L^2(\Sigma_E)$ defined as $(\mathcal{U}(t)A)(z) = A(\Phi^t(z))$. A consequence of spectral theory is existence, for every $A \in L^2(\Sigma_E)$, of a finite Borel measure μ_A on the real axis $\mathbb{R}$ such that

$$\langle \mathcal{U}(t)A.A \rangle_E = \int_{\mathbb{R}} \mathrm{e}^{it\theta} d\mu_A(\theta).$$

Then we have the following spectral characterizations:

$$\{\Phi^t \text{ ergodic}\} \Longleftrightarrow \{\text{supp}\{\mu_A\} = \{0\} \Rightarrow A = \text{constant}\} \tag{58}$$

$$\{\Phi^t \text{ weakly mixing}\} \Longleftrightarrow \left\{A \in L^2(\Sigma_E), \langle A \rangle_E = 0 \Rightarrow \mu_A \text{ is continuous}\right\} \tag{59}$$

Let us consider a small slice of energy, $I_\hbar^\varepsilon = [E - c\hbar^{1-\varepsilon}, E - c\hbar^{1-\varepsilon}]$, where $\varepsilon \geq 0$. The quantum analogue of the Liouville measure and the spectral measures for a flow can be defined as follows.
We have $\text{Spec}[\hat{H}] \cap I_\hbar^\varepsilon = \{E_1 \leq E_2 \leq \cdots E_{N_\hbar^\varepsilon}\}$ with multiplicities and we introduce the spectral projectors $\Pi_\hbar^\varepsilon$ of $\hat{H}$ on $I_\hbar^\varepsilon$ so that $\text{Tr}(\Pi_\hbar^\varepsilon) = N_\hbar^\varepsilon$. Using Weyl asymptotics, it is not difficult to prove, for every $\varepsilon > 0$,

$$\lim_{\hbar\to 0} \frac{1}{N_\hbar^\varepsilon} \text{Tr}(\Pi_\hbar^\varepsilon \hat{A}) = \int_{\Sigma_E} A(z)d\bar{\nu}_E(z) \tag{60}$$

It is well known that we can modify the quantization $\hat{A}$ with an error $O(\hbar)$ such that $A \mapsto A_{jj}$ is a positive Radon measure. This is done by taking $A_{jj} = \langle Op_\hbar^{aw} A\varphi_j, \varphi_j \rangle$, where $Op_\hbar^{aw}$ is the antiWick quantization, easily defined using coherent states analysis of section.1:
$Op_\hbar^{aw}\eta(q) = (2\pi\hbar)^{-d} \int_Z A(z)\langle \eta, \psi_z \rangle \psi_z(q)dz$. So we can write $A_{jj}(\hbar) =$

$\int_Z A dv_j(z)$ where dv_j is a probability measure on Z. Then, for every $\varepsilon > 0$, we have for the weak convergence of measures

$$\lim_{\hbar \to 0} \frac{1}{N_\hbar^\varepsilon} \sum_{\{E_j \in I_\hbar^\varepsilon\}} dv_j = d\bar{\nu}_E \qquad (61)$$

We can also define, modulo $O(\hbar^\infty)$, the Borel measures $dm_{A,\hbar}$,

$$\int_{\mathbb{R}} f(\theta) dm_{A,\hbar}(\theta) = \frac{1}{N_\hbar^\varepsilon} \sum_{E_j, E_k \in I_\hbar^\varepsilon} f(\omega_{j,k}(\hbar)) |A_{jk}(\hbar)|^2 \qquad (62)$$

We also have

$$\int_{\mathbb{R}} f(\theta) dm_{A,\hbar}(\theta) = \frac{1}{N_\hbar^\varepsilon} \mathrm{Tr}(\Pi_\hbar^\varepsilon \hat{A}_f \Pi_\hbar^\varepsilon \hat{A}) \qquad (63)$$

Taking the classical limit we have the weak convergence of $dm_{A,\hbar}$ to $d\mu_A$

$$\lim_{\hbar \to 0} \int_{\mathbb{R}} f(\theta) dm_{A,\hbar}(\theta) = \int_{\mathbb{R}} f(\theta) d\mu_A(\theta) \qquad (64)$$

The ergodic quantum theorem can be stated as follows

Theorem 4.3. *Let us assume here $\varepsilon = 0$ and denote $N_\hbar^0 = N_\hbar$, $I_\hbar^0 = I_\hbar^0$. If the classical system is ergodic on Σ_E then we have*

$$\lim_{\hbar \to 0} \frac{1}{N_\hbar} \sum_{\{E_j \in I_\hbar\}} \left| \int A dv_j - \langle A \rangle_E \right|^2 = 0 \qquad (65)$$

Furthermore is we have some estimate on the rate of classical ergodicity, and if the (NPC) condition *is fulfilled, then we get a control of the quantum ergodicity. So let us assume that for some $0 < a \leq 1$ we have*

$$\int_{\Sigma_E} \left| \frac{1}{2T} \int_{-T}^{T} A(\Phi^t(z)) dt - \langle A \rangle_E \right|^2 d\nu_E(z) = O(T^{-a}) \qquad (66)$$

then there exists $C > 0$ such that

$$\frac{1}{N_\hbar} \sum_{\{E_j \in I_\hbar\}} \left| \int A dv_j - \langle A \rangle_E \right|^2 \leq C |\log(\hbar)|^{-a} \qquad (67)$$

The inverse problem was discussed by Sunada [26] and Zelditch [29]. It is still open. But a partial result can be proved by considering contribution of nearby non diagonal matrix elements.

Theorem 4.4. *Let us assume that the condition* (NPC) *is satisfied. Then the classical flow is ergodic on Σ_E if and only if for every $A \in \mathcal{O}(0)$*

such that $\langle A\rangle_E = 0$ *and every* $\alpha :]0,1] \mapsto]0,+\infty[$ *such that* $\lim_{\hbar\to 0}\alpha(\hbar) = 0$, $\lim_{\hbar\to 0}\alpha(\hbar)|\log(\hbar)| = +\infty$ *we have*

$$\lim_{\hbar\to 0}\frac{1}{N_\hbar}\sum_{\substack{\{E_j\in I_\hbar,\\ |\omega_{jk}(\hbar)|\le\alpha(\hbar)\}}}|A_{jk}(\hbar)|^2 = 0 \tag{68}$$

We can also get a similar result for weak-mixing systems.

Theorem 4.5. *Let us assume that the condition* (NPC) *is satisfied. Then the classical flow is weakly-mixing on* Σ_E *if and only if for every* $\lambda\in\mathbb{R}$, *every* $A\in\mathcal{O}(0)$ *such that* $\langle A\rangle_E = 0$ *and every* $\alpha :]0,1] \mapsto]0,+\infty[$ *such that* $\lim_{\hbar\to 0}\alpha(\hbar) = 0$, $\lim_{\hbar\to 0}\alpha(\hbar)|\log(\hbar)| = +\infty$ *we have*

$$\lim_{\hbar\to 0}\frac{1}{N_\hbar}\sum_{\substack{\{E_j\in I_\hbar,\\ |\omega_{jk}(\hbar)-\lambda|\le\alpha(\hbar)\}}}|A_{jk}(\hbar)|^2 = 0 \tag{69}$$

The starting points to prove these results are the following trace formulae. For the ergodic case we use

$$\sum_{\{E_j,E_k\in I_\hbar\}}\left|A_{jk}(\hbar)\widetilde{M_T}(\omega_{jk}(\hbar))\right|^2 = \mathrm{Tr}\left(\hat{A}_{M_T}\right)^2 \tag{70}$$

with $M_T(u) = \frac{1}{2T}\mathbb{I}_{[-T,T]}$

and for the weak-mixing case,

$$\sum_{\{E_j,E_k\in I_\hbar\}}|A_{jk}(\hbar)|^2\widetilde{M_T^{(2)}}(\omega_{jk}(\hbar)-\lambda)) = \mathrm{Tr}\left(\int_{\mathbb{R}}\mathrm{e}^{it\lambda}\hat{A}_t\hat{A}_{M_T^{(2)}}(t)dt\right) \tag{71}$$

with $M_T^{(2)} = M_T\star M_T$ ($\star$ denotes the convolution product). Then the two theorems are proved by computing carrefully the semiclassical limits of r.h.s □

Remark 4.6. *The definition of quantum ergodicity or quantum weak mixing proposed by Sunada and Zelditch is property 65 or 69 with* $a(\hbar)\equiv 0$. *It is not known if these definitions are equivalent to the classical ones.*

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