Distribution of Matrix Elements and Level Spacings for Classically Chaotic Systems

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Abstract

For quantum systems obtained by quantization of chaotic classical systems we prove some rigorous results concerning the semi-classical behaviour of matrix elements of observables on an orthonormal system of bound states of the Hamiltonian.

1 Introduction

Our aim in this paper is to study the energy levels and the corresponding eigenstates for quantum Hamiltonians like Schrödinger: $P(\hbar) = -\hbar^2\Delta + V$ on the configuration space $X = \mathbb{R}^n$ (our proofs can be easily translated on some Riemannian compact manifold X (a torus, see [25] for examples, or a compact manifold with constant negative curvature) such that the corresponding classical system is chaotic on some energy shell of the phase space (ergodic or mixing).
Let $I_{c\ell} \subset \mathbb{R}$ be a classical energy interval such that the spectrum of $P(\hbar)$ is purely discrete in $I_{c\ell}$. So we have $P(\hbar)\varphi_j = E_j(\hbar)\varphi_j$ where $\{\varphi_j\}_j$ is an orthonormal system of bound states of energies $E_j(\hbar) \in I_{c\ell}$. Let us denote by $p(x,\xi) \in C^\infty(T^*(X))$ the corresponding classical Hamiltonian and assume that on some energy shell $\Sigma_E := \{(x,\xi) \in T^*(X);\ p(x,\xi) = E\}$, $E \in I_{c\ell}$, the classical motion is ergodic (or mixing). Let us introduce a classical smooth observable $a(x,\xi) \in C^\infty(T^*(X))$, $A(\hbar)$ its quantum counterpart and the matrix elements $A_{jk}(\hbar) :=< A(\hbar)\varphi_j, \varphi_k >$ (scalar product in $L^2(X)$)
The matrix elements are important at least for two reasons: firstly, in quantum mechanics they measure the transition probabilities between the states j and k; secondly they appear naturally in the stationary perturbation theory (see any text book in quantum theory for details). Let us briefly recall here how do they appear. Let us consider in the abstract Hilbert space $\mathcal{H}$ a self adjoint operator P with a discrete spectrum: $\{E_j\}_{j\in\mathbb{N}}$, without multiplicities for simplicity. We have an orthormal basis of eigenfunctions: $\{\varphi_j\}_{j\in\mathbb{N}}$, $P\varphi_j = E_j\varphi_j$. Let us

consider a small perturbation $P_\gamma := P + \gamma A$ of P where A is a bounded operator in $\mathcal{H}$ and $\gamma \in \mathbb{R}$, small. For a fixed $j \in \mathbb{N}$ we try to solve the eigenvalue problem: $P_\gamma \varphi_j^\gamma = E_j^\gamma \varphi_j^\gamma$ by the "ansatz":

$$
\begin{aligned}
E_j^\gamma &= E_j + \gamma\varepsilon_1 + \gamma^2\varepsilon_2 + \cdots && (1)\\
\varphi_j^\gamma &= \varphi_j + \gamma\psi_1 + \gamma^2\psi_2 + \cdots && (2)
\end{aligned}
$$

Asking that ψ_1 is orthogonal to φ_j, we get easily:

$\boxed{\varepsilon_1 = \langle A\varphi_j, \varphi_j\rangle}$

$\boxed{\varepsilon_2 = \sum_{k\neq j} \frac{|\langle A\varphi_j, \varphi_k\rangle|^2}{E_k - E_j}}$

So we see that the diagonal elements give the first order approximation and the non diagonal elements give the second order approximation.

Now we come back to the quantum mechanics case in the configuration space $\mathbb{R}^n$. There is a huge physicist literature discussing the behaviour of the $A_{jk}(\hbar)$ as the Planck constant $\hbar \searrow 0$ and $\mathrm{E_j(\hbar),\ E_k(\hbar) \to E \in I_{c\ell}}$, in connexion with the chaotic properties of the classical dynamics on Σ_E. (see references [23, 24, 19, 22, 17]). In particular, if the classical dynamics is ergodic on Σ_E, then it is claimed that for the diagonal elements we have:

$$
\lim_{\hbar\searrow 0} A_{jj}(\hbar) = < a >_E \quad \text{(the average of } a \text{ for the Liouville measure on } \Sigma_E) \tag{3}
$$

and for the non diagonal elements:

$$
\lim_{[\hbar\searrow 0,\, j\neq k]} A_{jk}(\hbar) = 0 \tag{4}
$$

Untill now theses claims are not completly proved. Following the works by Shnirelmann [1], Zelditch [3], Colin de Verdière [2], Helffer-Martinez-Robert [5] it can be proved that (3) is true "almost everywhere". One of the main goals of this paper is to discuss the claim (4) and in particular to extend and improve some results obtained by Zelditch [4]. We will also discuss the variance of the statistical distribution of the series $\{A_{jk}(\hbar)\}_{jk}$ according to a definition proposed by Wilkinson [9]. We will give a rigorous proof of the semi-classical $\hbar$-expansion which appeared in [9].

The unifying theme of our paper is the role of different "sum rules" (see [24, 17]). The idea is to consider sums like:

$$
S_{\theta,j}(\hbar) = \sum_k |A_{jk}(\hbar)|^2 \theta\left(\frac{E_j(\hbar) - E_k(\hbar)}{\hbar}\right) \tag{5}
$$

We first transform this sum using Parseval relation and try to control the classical limit by direct estimates or by the WKB method. We get in this way different results, according to the choice of the test functions θ, which generally will depend on some extra parameters. In a forthcoming paper we will apply these techniques to check rigorously the classical limit of the geometrical Berry's phase for chaotic systems [20] (for integrable systems see [21]).

2 A Semi-Classical Analysis Background

In this section we introduce our technical assumptions and recall some more or less well known mathematical facts about semi-classical analysis in the phase space. For details see for exemple the book [6].

On the configuration space $\mathbb{R}^n$ it is convenient to choose the so called Weyl quantization which is defined by the formula:

$$(op_\hbar^w b)\psi(x) = (2\pi\hbar)^{-n} \int \int \mathrm{e}^{\frac{i}{\hbar}<x-y,\xi>} b(\frac{x+y}{2}, \xi)\psi(y) dy d\xi \tag{6}$$

We shall use as well the notations $op_\hbar^w b := b_\hbar^w := B(\hbar)$; b is by definition the $\hbar$-Weyl symbol of the operator $B(\hbar)$. (b is also the classical observable corresponding to the quantum observable $B(\hbar)$).

We start with a quantum Hamiltonian $P(\hbar)$ of $\hbar$-Weyl symbol $p(\hbar, x; \xi)$. We assume that $p(\hbar, x; \xi)$ has an asymptotic expansion:

$$p(\hbar, x; \xi) \asymp \sum_{0 \le j < +\infty} \hbar^j p_j(x, \xi) \tag{7}$$

with the following properties:

(H_1) *$p(\hbar, x, \xi)$ is real valued , $p_j \in C^\infty(\mathbb{R}^{2n})$*

(H_2) *There exist $C > 0$; $M \in \mathbb{R}$ such that:*

$$(1 + p_0(x, \xi)^2) \le C(1 + p_0(y, \eta)^2)(1 + |x - y| + |\xi - \eta|)^M \quad \forall x, y, \xi, \eta, \in \mathbb{R}^n$$

(H_3) *$\forall j \ge 0$ $\forall \alpha$, β multiindices $\exists c > 0$ such that: $|\partial_x^\alpha \partial_\xi^\beta p_j| \le c(1 + p_0^2)^{1/2}$*

(H_4) *$\forall N \ge N_0$, $\forall \alpha, \beta$ $\exists c(N, \alpha, \beta) > 0$ such that $\forall \hbar \in]0, 1]$, $\forall (x, \xi) \in \mathbb{R}^{2n}$ we have:*

$$|\partial_x^\alpha \partial_\xi^\beta \{p(\hbar; x, \xi) - \sum_{0 \le j \le N} \hbar^j p_j(x, \xi)\}| \le c(N, \alpha, \beta)\hbar^{N+1}$$

Under these assumptions it is well known that $P(\hbar)$ has a unique self-adjoint extension in $L^2(\mathbb{R}^n)$ (see for example[6]) and the propagator:

$$U(t, \hbar) := \exp\left(-\frac{it}{\hbar} P(\hbar)\right)$$

is well defined as a unitary operator in $L^2(\mathbb{R}^n)$, for every real number t. In what follows the function and operator norms in $L^2(\mathbb{R}^n)$ will be denoted by $\|.\|$.

Because we are interested in bound states, let us consider a classical energy interval $I_{c\ell} =]\lambda_-, \lambda_+[$; $\lambda_- < \lambda_+$ and assume:

(H_5) *$p_0^{-1}(I_{c\ell})$ is a bounded set of the phase space $\mathbb{R}^{2n}$.*

This imply that for every closed interval $J_{c\ell} := [E_-, E_+] \subset I_{c\ell}$, and for $\hbar > 0$ small enough, the spectrum of $P(\hbar)$ in $J_{c\ell}$ is purely discrete ([28]). In what follows we fix such an interval $J_{c\ell}$.

For a fixed energy level $E \in]E_-, E_+[$, we assume:
(H_6) *E is a regular value of p_0. That means: $p_0(x,\xi) = E \Rightarrow \nabla_{(x,\xi)} p_0(x,\xi) \neq 0$)*
So, the Liouville measure $d\sigma_E$ is well defined on the energy shell

$$\Sigma_E := \{(x,\xi) \in \mathbb{R}^{2n},\ p_0(x,\xi) = E\}$$

Let us recall that:

$$d\sigma_E = \left(\int_{\Sigma_E} \frac{d\Sigma_E}{|\nabla p_0|} \right)^{-1} \frac{d\Sigma_E}{|\nabla p_0|}$$

where $d\Sigma_\lambda$ is the Euclidean measure on Σ_λ.

Let us introduce also the Hamiltonian vector field $\mathcal{H}_{p_0} := (\nabla_\xi p_0, -\nabla_x p_0)$ and the Hamiltonian flow: $\Phi^t(x,\xi) := \exp(t\mathcal{H}_{p_0}(x,\xi))$. We are mainly concerned here by the dynamical system $(\Sigma_E, d\sigma_E, \Phi^t)$ and its connections with the spectrum of $P(\hbar)$ close to E. There is a huge litterature on this subject in physics and in mathematics; but there are rather few mathematical rigorous result about quantum consequences of classical chaos.
For later purpose, let us recall some well established results concerning semi-classical asymptotics of bound states:
(R_1) <u>the general Weyl formula</u> [28, 8])
Under the assumptions (H_1) to (H_5), if $\lambda,\ \mu \in I_{c\ell},\ \lambda < \mu$, are regular values for p_0, then we have:

$$\#\{j,\ E_j(\hbar) \in [\lambda, \mu]\} = (2\pi\hbar)^{-n} Vol_{\mathbb{R}^{2n}}\{p_0^{-1}[\lambda,\mu]\} + O(\hbar^{1-n}) \tag{8}$$

(R_2) <u>the "generic" Weyl formula</u> [7, 8])
Furthermore, under the same assumptions as above, if we add the following condition (H_7), for $E = \lambda$ and $E = \mu$:
(H_7) *The Liouville measure of the closed trajectories on Σ_E is zero.*
(that means: $\sigma_E\{(x,\xi) \in \Sigma_E,\ \exists t \neq 0,\ \Phi^t(x,\xi) = (x,\xi)\} = 0$).
Then we have a two terms asymptotic expansion:

$$\#\{j,\ E_j \in [\lambda, \mu]\} = (2\pi\hbar)^{-n} Vol_{\mathbb{R}^{2n}}\{p_0^{-1}[\lambda,\mu]\} + c_1\hbar^{1-n} + o(\hbar^{1-n}) \tag{9}$$

where c_1 was computed in [7] (c_1=0 if $p_1 = 0$)
The result (R_2) can be seen as a weak form of chaos! (see also section 6 for a weaker form)
A more suggestive result is the following: let us consider $\hbar$-dependent energy intervals: $I(\hbar) = [\alpha(\hbar), \beta(\hbar)]$, $\alpha(\hbar) < E < \beta(\hbar)$ with $\lim_{\hbar\to 0}(\beta(\hbar) - \alpha(\hbar)) = 0$, $\beta(\hbar) - \alpha(\hbar) \geq \epsilon_2\hbar$, for some $\epsilon_2 > 0$.
Let us denote: $\Lambda(\hbar) = \{j,\ E_j(\hbar) \in I(\hbar)\}$ and by $\mathcal{B}_\infty$ the space of smooth functions a: $\mathbb{R}^{2n} \to \mathbb{C}$ such that all derivatives $\partial_x^\alpha \partial_\xi^\beta a(x,\xi)$ are bounded in $\mathbb{R}^{2n}$. Under the same assumptions as in (R_2), we have:
(R_3) (see [5])

$$\lim_{\hbar \searrow 0} \frac{\sum_{j\in\Lambda(\hbar)} A_{jj}(\hbar)}{\#\Lambda(\hbar)} = \int_{\Sigma_E} a\, d\sigma_E \tag{10}$$

Moreover we have the following asymptotic formula for the number of bound states of $P(\hbar)$ in $I(\hbar)$, under the assumption (H_7) (see Appendix (A)),

$$\lim_{\hbar\searrow 0}\left(\frac{(2\pi\hbar)^n(\#\Lambda(\hbar))}{\beta(\hbar)-\alpha(\hbar)}\right)=\int_{\Sigma_E}\frac{d\Sigma_E}{|\nabla p_0|}:=|\Sigma_E| \tag{11}$$

The above asymptotic result is an easy corollary of [5] (Théorème 1.1, p.315). For a particular case see also ([15])
Let us remark here that if we have

$$\lim_{\hbar\searrow 0}\left(\frac{\hbar}{\beta(\hbar)-\alpha(\hbar)}\right)=0$$

then (11) is still valid without (H_7), simply by using the general Weyl formula (R_1).
Let us introduce a first chaotic assumption:
(H_8) *The dynamical system* $(\Sigma_E, d\sigma_E, \Phi^t)$ *is* ergodic *which means: for every continuous function a on* Σ_E*, we have, for almost all* $(x,\xi)\in\Sigma_E$*:*

$$\lim_{T\nearrow+\infty}\frac{1}{T}\int_0^T a(\Phi^t(x,\xi))dt=\int_{\Sigma_E} a d\sigma_E$$

We will use in this paper the following basic result about the semi-classical behaviour of the diagonal matrix elements:

Theorem 2.1 *([5]) Under the assumptions* (H_1) *to* (H_8)*,* $n\geq 2$*, for every* $\hbar>0$*, there exists* $M(\hbar)\subseteq\Lambda(\hbar)$*, depending only on the Hamiltonian* $P(\hbar)$*, such that:*

$$\lim_{\hbar\searrow 0}\left(\frac{\#M(\hbar)}{\#\Lambda(\hbar)}\right)=1,\ \ \text{and}\ \ \lim_{[\hbar\searrow 0,\, j\in M(\hbar)]}A_{jj}(\hbar)=\int_{\Sigma_E} a d\sigma_E,\ \ \forall a\in\mathcal{B}_\infty \tag{12}$$

Remark 2.2 *The following question is still open: can we take* $M(\hbar)=\Lambda(\hbar)$ *in the conclusion of the above therem, if* $n\geq 2$*?*

3 New Results for the Non Diagonal Matrix Elements

We begin with a crude estimate but it explains further restrictions on energy localization.

Proposition 3.1 *Under the assumptions* (H_1) *to* (H_5)*, for every* $a\in\mathcal{B}_\infty$ *there exists* $c_0>0$ *such that we have:*

$$|A_{jk}(\hbar)|\leq c_0\frac{\hbar}{|E_k(\hbar)-E_j(\hbar)|}\quad\forall E_j,\ E_k\in J_{c\ell},\ E_j(\hbar)\neq E_k(\hbar) \tag{13}$$

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

$$\langle [A(\hbar), \chi(P(\hbar)).P(\hbar)]\varphi_j, \varphi_k\rangle = (E_j(\hbar) - E_k(\hbar))\langle A(\hbar)\varphi_j, \varphi_k\rangle$$

But from the $\hbar$-Weyl calculus (see for example [6]) we have the well known commutator estimate:

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

The proposition follows. ∎

Remark 3.2 *(i) The proof of the proposition (3.1) 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 $A_{jk}(\hbar)$ for level spacings of order $\hbar$ (only this case is considered in the physics litterature).

Let us formulate a second crude result coming easily from Theorem(2.1):

Proposition 3.3 *Let us assume (H_1) to (H_7) and $n \geq 2$. Then for every $\hbar > 0$ there exists $\Box(\hbar) \subseteq \Lambda(\hbar) \times \Lambda(\hbar)$ such that*

$$\lim_{\hbar \searrow 0} \frac{\#\Box(\hbar)}{\#\Lambda(\hbar)^2} = 1, \quad \text{and} \lim_{[\hbar \searrow 0,\ (j,k) \in \Box(\hbar)]} A_{jk}(\hbar) = 0 \tag{14}$$

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

$$\begin{aligned} \sum_{(j,k)\in\Lambda(\hbar)^2} |A_{jk}(\hbar)|^2 &= \sum_{j\in\Lambda(\hbar)} \langle \Pi_P(I(\hbar)).A\varphi_j, A\varphi_j\rangle \\ &\leq \sum_{j\in\Lambda(\hbar)} \langle A^2\varphi_j, \varphi_j\rangle \end{aligned} \tag{15}$$

But we know that $\lim_{\hbar\searrow 0} \#\Lambda(\hbar) = +\infty$ (see [7] and (11)) So, using (R_3), we get:

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

and we get the proposition using the following lemma whose proof is implicit in [5] (part.3-p.319) ∎

Lemma 3.4 *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 finite part of integers, and finite families of complex numbers: $\{a_j(\hbar)\}_{j\in\Omega(\hbar)}$ 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*

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

Now we can formulate our main results concerning the non diagonal matrix elements.

Theorem 3.5 *We assume that the assumptions* (H_1) *to* (H_8) *are fufilled.*
(i) For every $\varepsilon > 0$ *there exists* $T_\varepsilon > 0$ *and* $\hbar_\varepsilon > 0$ *such that:*

$$\forall j \in M(\hbar),\ \forall k \in \Lambda(\hbar),\ 0 < \hbar \leq \hbar_\varepsilon;\ |E_j(\hbar) - E_k(\hbar)| \leq \frac{\pi\hbar}{2T_\varepsilon} \Rightarrow |A_{jk}(\hbar)| \leq \varepsilon \tag{16}$$

(ii) For every family of matrix elements $\{A_{jk}(\hbar)\}_{(j,k)\in\Omega(\hbar)}$ *such that:*
(α) $\Omega(\hbar) \subseteq \Lambda(\hbar)^2$ *and* $(j,k) \in \Omega(\hbar) \Rightarrow j \neq k$
(β) $\displaystyle\lim_{[\hbar \searrow 0,\, (j,k)\in\Omega(\hbar)]} \left(\frac{E_j(\hbar) - E_k(\hbar)}{\hbar}\right) = 0$
(γ) $\displaystyle\liminf_{\hbar \searrow 0} \left(\frac{\#\Omega(\hbar)}{\#\Lambda(\hbar)}\right) > 0$
there exists $\tilde{\Omega}(\hbar) \subseteq \Omega(\hbar)$ *such that:*

$$\lim_{\hbar \searrow 0} \frac{\#\tilde{\Omega}(\hbar)}{\#\Omega(\hbar)} = 1;\ \lim_{\hbar \searrow 0} A_{jk}(\hbar) = 0, \text{ uniformly for } (j,k) \in \tilde{\Omega}(\hbar) \tag{17}$$

The above statement means: for all $\epsilon > 0$*, there exits* $\hbar_\epsilon > 0$*, such that for every* $0 < \hbar < \hbar_\epsilon$ *and for every* $(j,k) \in \tilde{\Omega}(\hbar)$ *we have* $|A_{jk}(\hbar)| \leq \epsilon$*.*
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 3.6 *(1)There exists a lot of non diagonal families satisfying the assumptions of Theorem (3.5) (ii) (see Appendix (A))*
(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* $a(x,\xi) = x \text{ for } |x| \leq \sqrt{E+1}$ *). We can compare this fact with (16)*

To give further results we introduce a stronger chaotic assumption:
(H_9) *The dynamical system* $(\Sigma_E, d\sigma_E, \Phi^t)$ *is mixing, that means:*

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

Theorem 3.7 *Let us assume* (H_1) *to* (H_9)*.*
(i) There exists $M(\hbar) \subseteq \Lambda(\hbar)$ *(*$M(\hbar)$ *is the same as in Theorems (2.1) and (3.5)) such that:*

$$\lim_{\hbar \searrow 0} \frac{\#M(\hbar)}{\#\Lambda(\hbar)} = 1, \quad \lim_{[\hbar \searrow, 0\ j \in M(\hbar),\, k \in \Lambda(\hbar),\, j \neq k]} A_{jk}(\hbar) = 0, \ \ \forall aJ \in \mathcal{B}_\infty$$

(ii) For every family of matrix elements $\{A_{jk}(\hbar)\}_{(j,k)\in\Omega(\hbar)}$ *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:*

$$\lim_{\hbar\searrow 0} \frac{\#\tilde{\Omega}(\hbar)}{\#\Omega(\hbar)} = 1 \text{ and } \lim_{\hbar\searrow 0} A_{jk}(\hbar) = 0, \quad \text{uniformly for } \ (j,k) \in \tilde{\Omega}(\hbar) \tag{18}$$

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

Remark 3.8 *The results given in Theorems (3.5) and (3.7) can be extended in two directions as we can see in Appendix.*
Firstly the assumption "$a \in \mathcal{B}_\infty$*" is not essential for the validity of the above results (and also for the following ones). Because we consider the action of* $op_\hbar^w(a)$ *on states essentially localized in a compact set of the phase space we can take as well unbounded observables satisfying, for some* $m \in \mathbb{N}$, $\partial_x^\alpha \partial_\xi^\beta a \in \mathcal{B}_\infty$ *for* $|\alpha+\beta| \geq m$*. This can be applied for example to the position or momentum observables (conductivity). We will give in the appendix B the technical details.*
Secondly, some results hold also for non smooth symbols (in the Borel class may be sufficient) by replacing Weyl quantization by anti-Wick quantization (which coincides with an error $O(\hbar)$ *in the smooth case see Appendix (C)).*

COMPARAISON WITH PREVIOUS RESULTS ([4])
In [4], S.Zelditch proved analogous results in the high energy "régime", for the Laplace-Beltrami operator Δ *on Riemannian compact manifold* M*. Our results are more acurate for the following reasons. In the case considered in [4] the semi-classical parameter is* $\hbar = \lambda_j^{-1/2}$*, the* λ_j *being the eigenvalues of* Δ*. Our methods can be applied also to this case, using known results in spectral analysis on manifolds ([31, 8]). In [4], theorems A and B, the order of magnitude of eigenvalues families considered is at least* $O(\hbar^{-n})$ *but ours is at least* $O(\hbar^{1-n})$*, which is the order of the mean level spacing in quantum mechanics (in agreement with the remainder term in the Weyl formula). Furthermore our proofs show that the number of non controlled non diagonal matrix elements is independent of the observable* A *.*

Let us remark now that the Proposition (1.1) of [4] concerning the so called "coherent non vanishing families" $A_{jk}(\hbar)$ can also be extended in our setting:
$\mathcal{B}_\infty \ni a \to A_{jk}(\hbar)$ is a Schwartz distribution on the phase space $T^*(\mathbb{R}^n)$. By modifying the quantification, we can replace $A(\hbar)$ by $\tilde{A}(\hbar)$ (anti-Wick procedure, see[11, 5] and Appendix (C)), such that $\|A(\hbar) - \tilde{A}(\hbar)\| = O(\hbar)$ and $\mathcal{B}_\infty \ni a \stackrel{\mu_{jk}}{\to} \tilde{A}_{jk}(\hbar)$ define complex valued Radon measures $d\mu_{jk}$ on $\mathbb{R}^{2n}$. It is proved in [5] that $d\mu_{jj}$ are positive bounded Radon measures and the non diagonal case follows easily by the parallelogram identity (Appendix (C)). Following [4] we have:

Proposition 3.9 *Let assume (H_1) to (H_7) If $\Omega(\hbar) \subseteq \Lambda(\hbar)^2$ is such that there exists a non vanishing Radon measure μ on $T^*(\mathbb{R}^n)$ satisfying:*

$$\forall a \in C_0^\infty(\mathbb{R}^{2n}) \quad \lim_{[\hbar \searrow 0\ (j,k)\in\Omega(\hbar)]} \int_{\mathbb{R}^{2n}} a(z) d\mu_{jk}(z) = \int_{\mathbb{R}^{2n}} a(z) d\mu(z)$$

then we have:
(i)

$$\lim_{[\hbar \searrow 0,\ (j,k)\in\Omega(\hbar)]} \left(\frac{E_k(\hbar) - E_j(\hbar)}{\hbar} \right) = \tau \ \text{ with } \tau := i^{-1} \frac{\int \{a, p_0\}(z) d\mu(z)}{\int a(z) d\mu(z)}$$

Moreover the limiting value τ is also an eigenvalue of the Hamiltonian flow i.e:

$$\forall t \in \mathbb{R},\ \forall a \in C_0^\infty(\mathbb{R}^{2n}),\ \int_{\mathbb{R}^{2n}} a(\Phi^t(z)) d\mu(z) = \mathrm{e}^{it\tau} \int_{\mathbb{R}^{2n}} a(z) d\mu(z)$$

and:
(ii) $\#\Omega(\hbar) = O(\#\Lambda(\hbar))$

Proof: Using the rules on calculus for $\hbar$-admissible operators, in particular the connections between commutators and Poisson bracket, and between the quantum flow and the classical flow (semi-classical Egorov Theorem, see[6]), we get:

$$\begin{aligned} \langle \frac{1}{\hbar}[A(\hbar), P(\hbar)]\varphi_j, \varphi_k \rangle &= \left(\frac{E_j(\hbar) - E_k(\hbar)}{\hbar} \right) A_{jk}(\hbar) \\ &= i \langle op_\hbar^w(\{a, p_0\}).\varphi_j, \varphi_k \rangle + O(\hbar) \qquad (19) \\ \langle A(\hbar, t)\varphi_j, \varphi_k \rangle &= \exp\left(\frac{it}{\hbar}(E_k(\hbar) - E_j(\hbar)) \right) A_{jk}(\hbar) \\ &= \langle op_\hbar^w(a(\Phi^t))\varphi_j, \varphi_k \rangle + O(\hbar) \qquad (20) \end{aligned}$$

So, if we choose $a \in C_0^\infty(\mathbb{R}^{2n})$ such that $\int_{\mathbb{R}^{2n}} a(z) d\mu(z) \neq 0$ we get:

$$\lim_{[\hbar \searrow 0,\ (j,k)\in\Omega(\hbar)]} \left(\frac{E_k(\hbar) - E_j(\hbar)}{\hbar} \right) = i^{-1} \frac{\int \{a, p_0\} d\mu}{\int a d\mu}$$

The part (i) of the proposition follows.
Proof of (ii): Let a be such as above. There exists $\kappa > 0$ and a $\hbar_\kappa > 0$ such that for $0 < \hbar \leq \hbar_\kappa$ we have:

$$\lim_{\hbar \searrow 0} \frac{1}{\#\Omega(\hbar)} \sum_{(j,k)\in\Omega(\hbar)} |A_{jk}(\hbar)|^2 \geq \kappa \qquad (21)$$

But we have:

$$\begin{aligned} \frac{1}{\#\Lambda(\hbar)} \sum_{(j,k)\in\Lambda(\hbar)^2} |A_{jk}(\hbar)|^2 &= \frac{1}{\#\Lambda(\hbar)} \sum_{j\in\Lambda(\hbar)} \langle \Pi_{P(\hbar)}(I(\hbar)).A\varphi_j, A\varphi_j \rangle \\ &\leq \frac{1}{\#\Lambda(\hbar)} \sum_{j\in\Lambda(\hbar)} \langle A^2(\hbar)\varphi_j, \varphi_j \rangle \qquad (22) \end{aligned}$$

then, using a variant of Théorème (1.3) in[5] we get:

$$\lim_{\hbar\searrow 0}\frac{1}{\#\Lambda(\hbar)}\sum_{(j,k)\in\Lambda(\hbar)^2}|A_{jk}(\hbar)|^2\leq\int_{\Sigma_E}|a|^2 d\sigma_E \tag{23}$$

So, we get that for $\hbar$ small enough, there exists $K>0$ such that:

$$K(\#\Lambda(\hbar))\geq\sum_{(j,k)\in\Lambda(\hbar)^2}|A_{jk}(\hbar)|^2\geq\sum_{(j,k)\in\Omega(\hbar)}|A_{jk}(\hbar)|^2\geq\kappa(\#\Omega(\hbar)) \tag{24}$$

and (ii) of the proposition follows. ∎

Our third main result in this paper is a mathematically rigorous version of a Wilkinson's result concerning the variance of the statistical distribution of the matrix elements $A_{jk}(\hbar)$ ([9]).
In physics literature (see for example [9, 18]) it is conjectured that for classically chaotic systems, the matrix elements $A_{jk}(\hbar)$ are independent, Gaussian, with mean zero when $j\neq k$. The last statement is corroborated by our above theorems. Wilkinson[9] proposed the following definition for the variance:

$$\begin{aligned} S_{(f,g)}(\hbar,E,\Delta E) &= \\ \sum_{[E_j(\hbar),E_k(\hbar)\in J_{c\ell}]}|A_{jk}(\hbar)|^2 f_\hbar\left(E-\frac{1}{2}(E_j(\hbar)+E_k(\hbar)\right) & .g_\hbar\left(\Delta E-(E_j(\hbar)-E_k(\hbar))\right) \end{aligned} \tag{25}$$

where E is inside the interval $J_{c\ell}\subset I_{c\ell}$ and $f_\hbar,\ g_\hbar$ are Gaussian regularisations of the Dirac δ distribution. For technical convenience, we choose for $f_\hbar,\ g_\hbar$ smooth functions, compactly supported in Fourier variable. Let $f,\ g$ be smooth functions on $\mathbb{R}$ with Fourier transform of compact support: $\hat f(v)=\int_{\mathbb{R}}\mathrm{e}^{-iuv}f(u)du$. Then we define $f_\hbar(u):=\frac{1}{\hbar}f(\frac{u}{\hbar})$.

Theorem 3.10 *Let us assume that Supp($\hat f$) $\subseteq\ ]-T_0,T_0[$ with $T_0>0$ small enough and Supp(g) compact. Then under assumptions (H_1) to (H_6) we have the following asymptotic expansion, mod($O(\hbar^\infty)$), as $\hbar\searrow 0$:*

$$S_{(f,g)}(\hbar,E,\Delta E)\asymp\hbar^{-n-1}.\left(\sum_{j\geq 0}\Gamma_j\left(E,\frac{\Delta E}{\hbar}\right)\hbar^j\right) \tag{26}$$

where $\Gamma_j(E,\tau)$ is smooth in E and τ. In particular we have:

$$\Gamma_0(E,\tau)=\hat f(0)\int\hat g(t)\mathrm{e}^{it\tau}C_a(E,t)dt \tag{27}$$

where $C_a(E,t)$ is the classical auto-correlation function:

$$C_a(E,t):=\int_{\Sigma_E}a(z)a(\Phi^t(z))d\sigma_E(z)$$

Remark 3.11 *No chaotic assumption is needed for the validity of the above theorem because we choose Supp($\hat{f}$) small around 0. We could get an analogous of Gutzwiller trace formula [13] by taking Supp($\hat{f}$) compact but arbitrary large. In clear, if the flow Φ^t restricted to Σ_E is clean, that is to say:*
(i) $\mathcal{P}_E := \{(t,z) \in \mathbb{R} \times \Sigma_E, \Phi^t(z) = z\}$ is a smooth manifold
(ii) $\forall (t_0, z_0) \in \mathcal{P}_E$ the tangent space $T_{(t_0,z_0)}(\mathcal{P}_E)$ at (t_0, z_0) satifies

$$T_{(t_0,z_0)}(\mathcal{P}_E) = \{(\tau, \zeta) \in \mathbb{R} \times T_{z_0}(\Sigma_E),\ \tau \mathcal{H}_{p_0}(z_0) + D\Phi^{t_0}(z_0)(\zeta) = \zeta\}$$

then we can get:

$$S_{(f,g)}(\hbar, E, \Delta E) \asymp \sum_{j \geq 0} \hbar^{j-n-1} \gamma_j(\hbar; \hat{f}, \hat{g}, E, \Delta E)$$

where $\hat{f} \to \gamma_j(\hbar; \hat{f}, \hat{g}, E, \Delta E)$ are distributions on $\mathbb{R}$, supported by the set of periods of the flow Φ^t on Σ_E and can be made more explicit under a non degenerescence condition on the closed path of Φ^t on Σ_E. (for details see [14, 12]) But it seems difficult to get rigorous results for Supp($\hat{f}$) non compact even very fast decreasing!

4 Proofs for Theorems (3.5) and (3.7)

Let $a \in \mathcal{B}_\infty$ be such that $< a >_E = 0$ (for the proofs of Theorems (3.5) and (3.7) it is clearly sufficient to consider this case). With the notations of sections 1 and 2, we have:

$$\sum_{E_k \in J_{c\ell}} |A_{jk}(\hbar)|^2 = \|\Pi_{P(\hbar)}(J_{c\ell}) A(\hbar) \varphi_j\|^2 \leq \|A(\hbar)\varphi_j\|^2 \tag{28}$$

We apply this estimate replacing $A(\hbar)$ with $A_{\theta_T}(\hbar)$ which is defined by:

$$A_{\theta_T}(\hbar) = \int_{\mathbb{R}} \theta_T(t) A(\hbar, t) dt, \text{ with } A(\hbar, t) := U(-t, \hbar) A(\hbar) U(t, \hbar)$$

Let us choose $\theta_T = \frac{1}{2T} 1_{[-T,T]}$ so we have: $\hat{\theta}_T(\lambda) = \frac{\sin(T\lambda)}{T\lambda}$. It is known that $A(\hbar, t)$ is an $\hbar$-admissible operator (see for example [6]) with a $\hbar$-Weyl principal symbol $a(t; x, \xi) = a\left(\Phi^t(x, \xi)\right)$. In particular we have:

$$\|A(\hbar, t) - op_\hbar^w(a(t))\| = O(\hbar) \ \text{ as } \hbar \searrow 0 \text{ uniformly for } t \text{ in every bounded interval} \tag{29}$$

Let us denote: $\omega_{jk}(\hbar) = \frac{E_k(\hbar) - E_j(\hbar)}{\hbar}$ (energies transition). We have:

$$\langle A_{\theta_T}(\hbar)\varphi_j, \varphi_k\rangle = 2\pi \hat{\theta}_T(\omega_{jk}(\hbar)) A_{jk}(\hbar) \tag{30}$$

We shall use the elementary inequality: $\frac{\sin(u)}{u} \geq \frac{2}{\pi}$ for $0 \leq u \leq \frac{\pi}{2}$.(*)
Hence we get from (28)

$$\sum_{E_k \in J_{c\ell}} 4\pi^2 \left(\frac{\sin(T\omega_{jk})}{T\omega_{jk}}\right)^2 |A_{jk}(\hbar)|^2 \leq \langle A^*_{\theta_T} A_{\theta_T} \varphi_j, \varphi_j\rangle \tag{31}$$

Fix an $\varepsilon > 0$ and $T > 0$. Using Theorem(2.1), there exists $\hbar_{\varepsilon,T} > 0$ such that for $0 < \hbar < \hbar_{\epsilon,T}$ and $j \in M(\hbar)$ we have :

$$|\langle A^*_{\theta_T} A_{\theta_T}\varphi_j, \varphi_j\rangle - \int_{\Sigma_E} \left| \frac{1}{2T}\int_{-T}^{T} a(\Phi^t(z))dt \right|^2 d\sigma_E(z)| \leq 8\varepsilon^2 \tag{32}$$

Now, using that $< a >_E = 0$ and (H_8) we choose $T = T_\varepsilon$ large enough such that:

$$\int_{\Sigma_E} \left| \frac{1}{2T_\varepsilon}\int_{-T_\varepsilon}^{T_\varepsilon} a(\Phi^t(z))dt \right|^2 d\sigma_E(z) \leq 8\varepsilon^2$$

and $\hbar_\varepsilon$ small enough such that: $|\omega_{jk}(\hbar)| \leq \frac{\pi}{2T_\varepsilon}$ $\forall (j,k) \in \Omega(\hbar)$, $0 < \hbar \leq \hbar_\varepsilon$. Then the conclusions of the first part of theorem (3.5) follow.

For proving the second part we follow [4] by estimating the variances (we always assume $< a >= 0$) :

$$\mathcal{V}_{\Omega(\hbar)}(A) := \frac{1}{\#\Omega(\hbar)} \sum_{(j,k)\in\Omega(\hbar)} |A_{jk}(\hbar)|^2$$

Using $(*)$, for every $T > 0$ there exists $\hbar_T > 0$ such that:

$$\mathcal{V}_{\Omega(\hbar)}(A) \leq \frac{\pi^2}{4(\#\Omega(\hbar))} \sum_{\omega_{jk}(\hbar)T<\pi/2, E_j\in I(\hbar), E_k\in J_{c\ell}} |A_{jk}(\hbar)|^2 \left|\frac{\sin(\omega_{jk}T)}{\omega_{jk}T}\right|^2 \tag{33}$$

for $\hbar \in]0, \hbar_T[$.

Using (32), (28) we can see easily that it exists $c > 0$ such that for $\hbar$ small enough we have:

$$\mathcal{V}_{\Omega(\hbar)}(A) \leq \frac{c}{\#\Lambda(\hbar)} \cdot \sum_{j\in\Lambda(\hbar)} \langle A^*_{\theta_T}.A_{\theta_T}, \varphi_j, \varphi_j\rangle + O(\hbar) \tag{34}$$

with $O(\hbar)$ uniform in T.

The proof of the second part of Theorem (3.5) follows from (34) by the same argument used in the first part (see 32) and using the lemma (3.4). To prove that we can choose $\tilde{\Omega}(\hbar)$ independently of $A(\hbar)$ we use the construction of [5], page 321.

∎

Now we begin the proof of the Theorem (3.7). We will use the following lemma concerning sum rules which appeared in the physics literature for example in Feingold-Peres [17] and in Prosen-Robnik [22].

Lemma 4.1 *Let $J_{m,c\ell} := [\alpha_m, \beta_m]$, $m = 1, 2$ two closed classical energy intervals such that: $\lambda_- < \alpha_1 < \alpha_2 < E < \beta_2 < \beta_1 < \lambda_+$ and $\chi \in C_0^\infty(]\alpha_1, \beta_1[)$, $0 \leq \chi \leq 1$, $\chi \equiv 1$ on $[\alpha_2, \beta_2]$. Then, for $E_j(\hbar) \in J_{2,c\ell}$, we have:*

$$\sum_{E_k(\hbar)\in J_{1,c\ell}} |A_{jk}(\hbar)|^2 \exp(-it\omega_{jk}(\hbar)) = \langle \varphi_j, A(t,\hbar)\chi(P(\hbar))A(\hbar)\varphi_j\rangle + O(\hbar) \tag{35}$$

the remainder term being uniform in $t \in \mathbb{R}$ as $\hbar \searrow 0$.

Proof of the lemma: using Parseval equality, for $E_j(\hbar) \in J_{2,c\ell}$ we have:

$$\sum_{E_k(\hbar)\in J_{1,c\ell}} |A_{jk}(\hbar)|^2 \exp(-it\omega_{jk}(\hbar)) = \langle \varphi_j, A(t,\hbar)\Pi_{P(\hbar)}(J_{1,c\ell})A(\hbar)\varphi_j\rangle \tag{36}$$

But we have from localization properties of χ:

$$\begin{aligned}\langle \varphi_j, A(t,\hbar)\Pi_{P(\hbar)}(J_{1,c\ell})A(\hbar)\varphi_j\rangle = \\ \langle \varphi_j, A(t,\hbar)\chi(P(\hbar))A(\hbar)\varphi_j\rangle + \langle \varphi_j, A(t,\hbar)\Pi_{P(\hbar)}(J)[A(\hbar),\chi(P(\hbar))]\varphi_j\rangle\end{aligned} \tag{37}$$

It is well known that: $\|[A(\hbar),\chi(P(\hbar))]\| = O(\hbar)$, so the second term of the r.h.s is $O(\hbar)$ for $j \in \Lambda(\hbar)$, uniformly in $t \in \mathbb{R}$. ∎

Let us introduce $\theta : \mathbb{R} \to \mathbb{R}$ such that:
(i) $\theta \in L^1(\mathbb{R})$, $\int \theta(t)dt = 1$
(ii) $\hat{\theta}(\lambda) \geq 0\ \forall \lambda \in \mathbb{R}$.
For $T > 0$ we denote $\theta_T(t) = \frac{1}{T}\theta(\frac{t}{T})$. Here we choose $\hat{\theta}(\lambda) = \left(\frac{\sin\lambda}{\lambda}\right)^2$

So from (35) we have:

$$\sum_{E_k\in J_{c\ell}} |A_{jk}(\hbar)|^2\hat{\theta}_T(\omega_{jk}(\hbar)-\tau) = \int_{\mathbb{R}} \mathrm{e}^{it\tau}\theta_T(t)\langle\varphi_j, A(t,\hbar))\chi(P(\hbar))A(\hbar)\varphi_j\rangle dt + O(\hbar) \tag{38}$$

with $O(\hbar)$ uniform in $T > 0$, $\tau \in \mathbb{R}$ and $j \in \Lambda(\hbar)$.
The calculus on $\hbar$-admissible operators ([6]) shows that $A(t,\hbar))\chi(P(\hbar))A(\hbar)$ has for principal symbol: $a(\Phi^t(x,\xi))\chi(p_0(x,\xi))a(x,\xi)$. Let us recall that $C_a(E,t) = \int_{\Sigma_E} a(z)a(\Phi^t(z))d\sigma_E(z)$ (autocorrelation function). So fixing $\varepsilon > 0$, $T > 0$ and using Theorem (2.1) again we get that for every $T > 0$ there exists $\hbar_{\varepsilon,T} > 0$ such that:

$$|\langle\varphi_j, A(t,\hbar))\chi(P(\hbar))A(\hbar)\varphi_j\rangle - C_a(E,t)| < \frac{\varepsilon}{2} \tag{39}$$

$$\forall \hbar \in]0,\hbar_{\varepsilon,T}[,\ \forall t \in [-T^2, T^2] \text{ and } j \in M(\hbar) \tag{40}$$

Then we use (38), splitting the integral according $|t| < T^2$ and $|t| > T^2$, and using (39) we get for some $\gamma > 0$, independent of $\hbar, \varepsilon, T$:

$$|A_{jk}(\hbar)|^2\hat{\theta}_T(\omega_{jk}(\hbar)-\tau) \ \leq \tag{41}$$

$$\int_{\mathbb{R}} |\theta(u).C_a(E,Tu)|du + \frac{\varepsilon}{2} \ + \ \gamma\int_{\{|u|\geq T\}} |\theta(u)|du; \quad \forall\hbar \in]0,\hbar_{\varepsilon,T}[,\ \forall\tau \in \mathbb{R}. \tag{42}$$

Now we will use the mixing assumption (H_9) and $< a >_E = 0$. That gives by dominated Lebesgue convergence theorem :

$$\lim_{T\nearrow+\infty}\int |\theta(u)C_a(E,uT)|du = 0,\ \lim_{T\nearrow+\infty}\int_{\{|u|\geq T\}} |\theta(u)|du = 0$$

hence there exits $T_\varepsilon > 0$

such that:

$$|A_{jk}(\hbar)|^2\hat{\theta}_{T_\varepsilon}(\omega_{jk}(\hbar)-\tau) \leq \varepsilon, \quad \forall \hbar \in]0,\hbar_\varepsilon[\ \ (\hbar_\varepsilon := \hbar_{\varepsilon,T_\varepsilon});\ \forall (j,k) \in M(\hbar)\times\Lambda(\hbar),\ \forall \tau \in \mathbb{R} \quad (43)$$

The estimates (43) being uniform in τ we can take $\tau = \omega_{jk}(\hbar)$ so we get

$$|A_{jk}(\hbar)|^2 \leq \epsilon, \quad \forall \hbar \in]0,\hbar_\epsilon[, \ \ \forall (j,k) \in M(\hbar) \times \Lambda(\hbar) \tag{44}$$

so that we have proved the first part of the theorem.
For the second part we use the same method as in Theorem (3.5). With the same notations, we have:

$$\mathcal{V}_{\Omega(\hbar)}(A) \leq \frac{\pi^2}{4}\frac{1}{\#\Omega(\hbar)}\sum |A_{jk}(\hbar)|^2 \left|\frac{\sin((\omega_{jk}(\hbar)-\tau)T)}{(\omega_{jk}(\hbar)-\tau)T}\right|^2 \tag{45}$$

for $\hbar \in]0,\hbar_T[$, where the sum is computed for $(\omega_{jk}(\hbar)-\tau)T < \pi/2, E_j \in I(\hbar), E_k \in J_{c\ell}$
Then we get, using again the lemma (4.1):

$$\mathcal{V}_{\Omega(\hbar)}(A) \leq c.\frac{1}{\#\Lambda(\hbar)}\sum_{j\in\Lambda(\hbar)}\int_{\mathbb{R}} \mathrm{e}^{it\tau}\theta_T(t)\langle\varphi_j, A(t,\hbar))\chi(P(\hbar))A(\hbar)\varphi_j\rangle dt + O(\hbar) \tag{46}$$

with $O(\hbar)$ uniform in T.
¿From (46) the second part of the theorem (3.7) is obtained using the arguments of the first part. ∎

By the same kind of estimates as those used in the proof of the Theorem (3.7), we can get something which seems connected with a well known phenomenon called the levels repulsion [30]. Let us introduce the following assumption on the autocorrelation function:
(H_9^*) $\Gamma_E := \int_{\mathbb{R}} |C_a(E,t)|dt < +\infty$
Indeed, using the function $\theta(t) = \mathrm{e}^{-\omega|t|}$, $\omega > 0$, we get, as above, that:

$$\forall\varepsilon > 0,\ \forall\omega > 0,\ \exists\hbar_{\varepsilon,\omega} > 0 \text{ such that}$$

$$|A_{jk}(\hbar)|^2\frac{\omega}{\omega^2+\omega_{jk}^2} \leq \pi\int_{\mathbb{R}}|C_a(E,t)|dt + \varepsilon, \ \ \forall\hbar \in]0,\hbar_{\varepsilon,\omega}[,\ \forall j \in M(\hbar),\ \forall k \in \Lambda(\hbar) \tag{47}$$

From (47) we get easily the proposition:

Proposition 4.2 *Under the conditions of (47), for every $K > \pi\Gamma_E - \epsilon$, we have:*

$$\{|A_{jk}(\hbar)|^2 \geq K\omega\} \Rightarrow \{|E_j(\hbar) - E_k(\hbar)|^2 \geq \left(\frac{K-\pi\Gamma_E-\epsilon}{(\pi\Gamma_E+\epsilon)}\right)(\hbar\omega)^2\} \tag{48}$$

Remark 4.3 *The assumption (H_9^*) is not completely absurd. In [26, 27] the authors consider dynamical systems such that the Fourier transforms of autocorrelation function have analytic extension in horizontal trips in the complex plane. The geodesic flow on constant negative curvature compact manifolds (like the Poincaré half plane) satisfies this property; so in this case the autocorrelations are exponentially fast decreasing ($O(\mathrm{e}^{-\delta|t|})$ for some $\delta > 0$).*

5 Asymptotic Sum Rule for the Variance of Matrix Elements

Let us assume that $\mathrm{Supp}(\hat{f}) \subseteq]-T_0, T_0[$ with $T_0 > 0$ small enough, and $\mathrm{Supp}(\hat{g})$ compact. We assume the $P(\hbar)$ satisfies (H_1) to (H_5). The variance considered by Wilkinson [9] is defined by:

$$S_{(f,g)}(\hbar, E, \Delta E) := \sum_{E_j, E_k \in J_{c\ell}} |A_{j,k}(\hbar)|^2 f_\hbar(E - \frac{1}{2}(E_j + E_k)) g_\hbar(\Delta E - (E_j - E_k))$$

In fact, Wilkinson considers the case where $\hat{f}$, $\hat{g}$ are Gaussians which seems difficult to treat mathematically (If $\mathrm{Supp}(\hat{f})$ is compact but not small see Remark (3.11)).
Let us begin by the following lemma which localizes the sum $S_{(f,g)}(\hbar, E, \Delta E)$ to energies which are close to E and replace the "abrupt" energy cut off in $J_{c\ell}$ by a smooth one.

Lemma 5.1 *Let $\varepsilon_0 > 0$ be such that $[E - \varepsilon_0, E + \varepsilon_0] \subset J_{c\ell}$ and $\chi \in C_0^\infty(J_{c\ell})$, $\chi = 1$ on $[E - \varepsilon_0, E + \varepsilon_0]$, $0 \le \chi \le 1$. Let us denote $A_\chi(\hbar) := \chi(P(\hbar))A(\hbar)\chi(P(\hbar))$ and by $A_{\chi,jk}(\hbar)$ the corresponding matrix elements. Then we have:*

$$S_{(f,g)}(\hbar, E, \Delta E) = \sum_{j,k} |A_{\chi,jk}(\hbar)|^2 f_\hbar(E - \frac{1}{2}(E_j + E_k) g_\hbar(\Delta E - (E_j - E_k)) + O(\hbar^\infty) \qquad (49)$$

Proof: We have:

$$S_{(f,g)}(\hbar, E, \Delta E) - \sum_{j,k} |A_{\chi,jk}(\hbar)|^2 f_\hbar(E - \frac{1}{2}(E_j + E_k)) g_\hbar(\Delta E - (E_j - E_k)) =$$

$$\sum_{j,k} (1 - \chi(E_j)^2 \chi(E_k)^2) |A_{jk}(\hbar)|^2 f_\hbar(E - \frac{1}{2}(E_j + E_k) g_\hbar(\Delta E - (E_j - E_k)) \qquad (50)$$

We split the r.h.s of the last equality into two terms according $|E_k - E_j| > \varepsilon_0$ or $|E_k - E_j| \le \varepsilon_0$. First, remark that, using the proposition 3.1 and the remark 3.2 , the contribution of $|E_k - E_j| > \varepsilon_0$ in the sum is $O(\hbar^\infty)$. We have $\chi(E_j)^2\chi(E_k)^2 < 1$. Assume for example that $\chi(E_j) < 1$. Then we have $|E - E_j| > \varepsilon_0$ hence if $|E_k - E_j| \le \varepsilon_0$ we have:

$$|E - \frac{1}{2}(E_j + E_k)| \ge |E - E_j| - \frac{1}{2}|E_j - E_k| \ge \varepsilon_0/2$$

But $f \in \mathcal{S}(\mathbb{R})$ (the Schwartz space) so we see that the contribution of $|E_k - E_j| \le \varepsilon_0$ is $O(\hbar^\infty)$ and (50) gives the lemma. ∎

We continue to denote by $S_{(f,g)}(\hbar, E, \Delta E)$ the approximation of the variance $\mathrm{mod}(O(\hbar^\infty))$ given by the above lemma.
By inverse Fourier transform, we get:

$$f_\hbar(E - \frac{1}{2}(E_j + E_k)) = \frac{1}{2\pi\hbar} \int_{\mathbb{R}} \hat{f}(\Delta t) \exp\left(i\frac{\Delta t}{\hbar}(E - \frac{1}{2}(E_j + E_k))\right) d\Delta t \qquad (51)$$

$$g_\hbar(\Delta E - (E_j - E_k)) = \frac{1}{2\pi\hbar} \int_{\mathbb{R}} \hat{g}(t) \exp\left(i\frac{t}{\hbar}(\Delta E - (E_j - E_k))\right) dt \qquad (52)$$

Now by plugging (51) and (50) in (50), and using Parseval relation for the orthonormal system $\{\varphi_j\}$, we get after computations:

$$S_{(f,g)}(\hbar, E, \Delta E) = \frac{1}{(2\pi\hbar)^2}\mathrm{tr}\left\{\int\int \hat{g}(t)\exp(\frac{i}{\hbar}t\Delta E)A_\chi(\hbar)\hat{f}(\Delta t)\,.\right.$$
$$\left. .\exp(\frac{-i\Delta t}{\hbar}(P(\hbar)-E))A_\chi(\hbar, \frac{\Delta t}{2}-t)(\hbar)dtd\Delta t\right\} \tag{53}$$

To achieve the proof of the theorem (3.10) we use the W.K.B method along the same lines as in [28, 6, 7] where similar quantities were studied (i.e a regularization of the Fourier transform of spectral density). So, we will give here only a sketchy proof. Let us first recall that the operators: $\chi(P(\hbar))A(\hbar)$ and $A_\chi(\hbar, \frac{\Delta t}{2}-t)$ are $\hbar$-admissible operators with weight 1 (see [6]). Secondly if $\tilde{\chi} \in C_0^\infty(J_{c\ell})$ is an other cut-off such that $\tilde{\chi}=1$ on $\mathrm{Supp}(\chi)$ then we have :

$$\chi(P(\hbar))\exp(\frac{i\tau}{\hbar}P(\hbar)) = \chi(P(\hbar))\exp(\frac{i\tau}{\hbar}\tilde{\chi}(P(\hbar)).P(\hbar))$$

So nothing is changed if we replace in the exponent $P(\hbar)$ by $\tilde{\chi}(P(\hbar)).P(\hbar)$ which satisfies the assumptions (H_1) to (H_5) with $\tilde{p}_0 \in \mathcal{B}_\infty$; this last property is important to have uniform estimates in W.K.B method when solving the eikonal equation:

$$\begin{aligned} \partial_\tau\phi(\tau,x,\eta) + p_0(x, \partial_x\phi(\tau,x,\eta)) &= 0 \\ \phi(0,x,\eta) &= x.\eta \end{aligned} \tag{54}$$

and the transport equations (see [6])
In this way we get, for $|\tau|$ small enough, accurate approximations $U_{app}(\tau,\hbar)$ for $U(\tau,\hbar)$ such that:

$$\|\exp\left(\frac{-i\tau}{\hbar}\tilde{\chi}(P(\hbar)).P(\hbar)\right) - U_{app}(\tau,\hbar)\| = O(\hbar^\infty)$$

where $U_{app}(\tau,\hbar)$ is constructed as oscillating integral kernel:

$$U_{app}(\tau,\hbar)(x,y) = (2\pi\hbar)^{-n}\int \exp\left(\frac{i}{\hbar}(\phi(\tau,x,\eta)-x.\eta\right)\left(\sum_{j\geq 0}\hbar^j u_j(\tau,x,\eta)\right)d\eta \tag{55}$$

Hence using the computation rules on $\hbar$-admissible operators [6], finally, the proof of the theorem (3.10) is achieved by applying the stationary phase theorem to integrals like:

$$\int\int\int_{\mathbb{R}_t\times\mathbb{R}^n_x\times\mathbb{R}^n_\xi} b_t(\tau,x;\xi)\exp\left(\frac{i}{\hbar}(\phi(\xi,x,\xi)-x.\xi\right)\hat{f}(\tau)d\tau dx d\xi$$

In particular, for the dominant term $S_0(\hbar, E, \Delta E)$, we have:

$$\begin{aligned} &S_0(\hbar,E,\Delta E) = \\ (2\pi\hbar)^{-n}\int\int\int &\hat{g}(t)\exp(\frac{i}{\hbar}t\Delta E)\chi^4(p_0(x,\partial_x\phi(\tau;x,\eta))) \\ &\times a(x,\partial_x\phi(\tau;x,\eta))a\left(\Phi^{\tau/2-t}(x,\partial_x\phi(\tau;x,\eta)\right) \\ &\times\hat{f}(\tau)\exp\left(\frac{i}{\hbar}(\phi(\tau,x,\eta)-x.\eta+\tau E)\right)d\tau dx d\eta dt \end{aligned} \tag{56}$$

$Supp(\hat{f})$ being small enough, the stationary points in the integral (56) in the variables (τ, x, η) are defined by the equations:

$$\{\tau = 0, \quad p_0(x, \eta) = 0\}$$

So, the computation of the first term in the stationary phase theorem [6] gives:

$$S_0(\hbar, E, \Delta E) = (2\pi\hbar)^{-n-1}\hat{f}(0)\int_{\mathbb{R}}\left(\int_{\Sigma_E} a(x,\eta)a(\Phi^t(x,\eta))d\sigma_E\right).$$
$$.\hat{g}(t)\exp\left(\frac{it}{\hbar}\Delta E\right)dt \quad + \quad \sum_{j\geq 1}\hbar^{-n-1+j}c_j\left(E, \frac{\Delta E}{\hbar}\right) \tag{57}$$

∎

6 Other related results

A-A very weak form of chaos

Here, we shall prove a quantum mechanical analog of a simple and beautiful result due to Helton [10] (see also [13]) for elliptic operators on compact manifolds.

Theorem 6.1 *Under the assumptions (H_1) to (H_6) for $P(\hbar)$, assume furthermore that there exits on Σ_E a non periodical trajectory for the flow Φ^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 $f \in C_0^\infty(\mathbb{R})$ 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[10] we consider the operator:

$$A_{E,f}(\hbar) = \int \hat{f}(t)U(-t,\hbar)A_E(\hbar)U(t,\hbar)dt \tag{58}$$

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

$$A_{E,f}(\hbar) = 2\pi\sum_{j,k} f(\omega_{jk}(\hbar))\chi\left(\frac{E_j(\hbar) - E}{\hbar^{1-\delta}}\right)\chi\left(\frac{E_k(\hbar) - E}{\hbar^{1-\delta}}\right)\Pi_k A(\hbar)\Pi_j \tag{59}$$

where Π_k is the projection on the state φ_k.
¿From (58,59) we have:

$$\int \hat{f}(t)U(-t,\hbar)A_E(\hbar)U(t,\hbar)dt = 0,\ \forall a \in \mathcal{B}_\infty \tag{60}$$

¿From (60) 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 Egorov theorem[6] and functional calculus with parameter for pseudodifferential operators [32]. We test (60) with the trace functional of operators with an arbitary $op_\hbar^w(b)$, $b \in \mathcal{B}_\infty$. we get easily:

$$\lim_{\hbar \searrow 0} (2\pi\hbar)^n . Tr\left(A_{E,f}(\hbar).op_\hbar^w(b)\right) = \int\int \hat{f}(t) a\left(\Phi^t(z)\right).b(z)dzdt = 0, \ \forall b \in \mathcal{B}_\infty \tag{61}$$

So we get

$$\int \hat{f}(t) a\left(\Phi^t(z)\right) dt = 0, \ \forall z \in \Sigma_E \tag{62}$$

Now, choose $z_0 \in \Sigma_E$ such that $t \to \Phi^t(z_0)$ is not periodic, we should like to deduce from (62) that $\hat{f} \equiv 0$. Using the same arguments as in [29] (p.866-867) we can get easily the following:

Lemma 6.2 *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 $\mathcal{N}_\mathcal{T}$ 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 $z \in \mathcal{N}_\mathcal{T}$. We have clearly $a(\Phi^t(z_0)) = g(t)$ if $|t| \leq T$. For $|t| \geq T$ and $\Phi^t(z_0) \in \mathcal{N}_\mathcal{T}$ we have $\Phi^t(z_0) = \Phi_1^t(z)$ 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 notations, using the above lemma and 62 we get:

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

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

Remark 6.3 *Using very recent results obtained by S.Dozias [35] we can see that the theorem (6.1) admits a partial converse: if $p_1 = 0$ 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 exist $\gamma_0, \gamma_1, C \in \mathbb{R}$; $\varepsilon > 0$ such that:*

$$\text{spectrum}[P(\hbar)] \cap [E - c\hbar^{1-\delta}, E + c\hbar^{1-\delta}] \subseteq \bigcup_{k \in \mathbb{Z}} [\gamma_0 + \gamma_1 k\hbar - C\hbar^{1+\varepsilon}, \gamma_0 + \gamma_1 k\hbar - C\hbar^{1+\varepsilon}] \tag{63}$$

Clearly (63) entails that $\mathcal{T}_{E,\delta}$ is not dense in $\mathbb{R}$.

B-Sum rules and classical limits

We want here to revisit the physics literature on this subject and make the connection with the technique used in part **4** of this paper.

Under the assumptions (H_1) to (H_5), a useful distribution to consider is:

$$\mathcal{R}_{A,B;j,\hbar}(\Delta E) = \sum_{E_k(\hbar)\in J_{c\ell}} A_{jk}(\hbar)B_{kj}(\hbar)\delta(\omega_{jk}(\hbar) - \Delta E)$$

where $A(\hbar), B(\hbar)$ are two quantum observables, with $\hbar$-Weyl symbols in $\mathcal{B}_\infty$. For $A = B$, $\mathcal{R}_{A,A;j,\hbar}(\Delta)$ is the response function of some atomic kernel, in the state φ_j, to the action of A.

Let us denote by $\hat{\mathcal{R}}_{A,B;j,\hbar}(t)$ the Fourier transform in ΔE of $\mathcal{R}_{A,B;j,\hbar}(\Delta E)$. ¿From Parseval identity we have also:

$$\hat{\mathcal{R}}_{A,B;j,\hbar}(t) = \langle\varphi_j, A(t,\hbar)\Pi_{P(\hbar)}(J_{c\ell})B(\hbar)\varphi_j\rangle$$

As above (see part.4) it is convenient to smooth the spectral projector $\Pi_{P(\hbar)}(J_{c\ell})$.

Lemma 6.4 *Let us consider an interval $\tilde{J}_{c\ell} \subset J_{c\ell}$ and a smooth cutoff $\chi \in C_0^\infty(J_{c\ell})$, $\chi \equiv$ 1 on a neighborhood of $\tilde{J}_{c\ell}$. Then we have:*

$$\hat{\mathcal{R}}_{A,B;j,\hbar}(t) = \langle\varphi_j, (A(t,\hbar)\chi(P(\hbar))B(\hbar)\varphi_j\rangle + O(\hbar^\infty), \text{ for } E_j(\hbar) \in \tilde{J}_{c\ell}, \tag{64}$$

the $O(\hbar^\infty)$ being uniform in j such that $E_j(\hbar) \in \tilde{J}_{c\ell}$ and in t such that $|t| \leq T$ for some $T > 0$.

Proof: We denote $J_{c\ell} = [\alpha, \beta]$ and $\tilde{J}_{c\ell} = [\lambda, \mu]$ with $\alpha < \lambda < \mu < \beta$. We fix some $\varepsilon > 0$, small enough. Then we construct a family of smooth cutoff functions as follows: $\chi = \chi_0$, $\chi \equiv 1$ on $[\lambda-\varepsilon, \mu+\varepsilon]$ and for every $N \geq 1$ we construct χ_N such that $\chi_N \in C_0^\infty(]\lambda - \frac{\varepsilon}{2^{N-1}}, \mu + \frac{\varepsilon}{2^{N-1}}[)$, $\chi_N \equiv 1$ on $[\lambda - \frac{\varepsilon}{2^N}, \mu + \frac{\varepsilon}{2^N}]$

In what follows we skip the $\hbar$-dependence for simplicity, although it is everywhere present.

In the first step we have:

$$\langle\varphi_j, A(t)\Pi_P(J_{c\ell})B\varphi_j\rangle = \langle\varphi_j, A(t)\chi_0(P)B\varphi_j\rangle + \langle\varphi_j, A(t)\Pi_P(J_{c\ell})[B, \chi_0(P)]\varphi_j\rangle \tag{65}$$

the last term in (65) is $O(\hbar)$. To improve this estimate we apply (65) to it remarking that B is replaced by $[B, \chi_0(P)]$. So we get:

$$\begin{aligned}\langle\varphi_j, A(t)\Pi_P(J_{c\ell})[B, \chi_0(P)]\varphi_j\rangle = \langle\varphi_j, A(t)\chi_1(P)[B, \chi_0(P)]\varphi_j\rangle +\\ \langle\varphi_j, A(t)\Pi_P(J_{c\ell}[[B, \chi_0(P)], \chi_1]\varphi_j\rangle\end{aligned} \tag{66}$$

Using standard rules for the $\hbar$ admissible calculus [6] and property of supports for χ_0 and χ_1 we have $\chi_1(P)[B, \chi_0(P)] = O(\hbar^\infty)$ in the operator norm. Furthermore, thanks to the double commutator, the last term in (66) is $O(\hbar^2)$. Clearly, the procedure can be iterated and at the step N we get:

$$\langle\varphi_j, A(t)\Pi_P(J_{c\ell})B\varphi_j\rangle = \langle\varphi_j, A(t)\chi_0(P)B\varphi_j\rangle + O(\hbar^N) \tag{67}$$

∎

Let us introduce the classical correlation:

$$C_{a,b}(E,t) = \int_{\Sigma_E} \bar{b}(z) a\left(\Phi^t(z)\right) d\sigma_E(z)$$

By applying [5] we can get:

Theorem 6.5 *Under the assumptions (H_1) to (H_7), for every real $T > 0$ and every integer ℓ we have:*

$$\frac{d^\ell}{dt^\ell}\hat{\mathcal{R}}_{A,B;j,\hbar}(t) = \frac{d^\ell}{dt^\ell}C_{a,b}(E,t) + o(\hbar), \text{ as } \hbar \searrow 0 \text{ for } j \in M(\hbar) \text{ and uniformly in} t \in [-T,T] \tag{68}$$

Proof:
We have only to check the uniformity in $t \in [-T,T]$. It is sufficient to consider the case $\ell = 0$. The conclusion comes easily from the following elementary lemma whose proof is an exercise about application of compactness by an $\varepsilon/3$-argument!

Lemma 6.6 *Let us consider a family of probability measures $(\mu_{\hbar,j})_{j\in M(\hbar)}$ on $\mathbb{R}^m$, weakly convergent to some probability measure μ as $\hbar \searrow 0$. Let us consider a continuous mapping: $t \mapsto g_t$ from $[-T,T]$ into the Banach space $\mathcal{C}_b(\mathbb{R}^m)$ (bounded and continuous functions on $\mathbb{R}^m$ with the supremum norm). Then we have:*

$$\lim_{[\hbar\searrow 0,\, j\in M(\hbar)]} \int_{R^m} g_t(z) d\mu_{\hbar,j}(z) = \int_{\mathbb{R}^m} g_t(z) d\mu(z), \text{ uniformly in } t \in [-T,T]$$

Remark 6.7 *The semi-classical sum rules [17, 22] concerning*

$$\sum_{E_k \in J_{c\ell}} \left(\frac{(E_k(\hbar) - E_j(\hbar))}{\hbar}\right)^\ell |A_{jk}(\hbar)|^2$$

are obvious consequences of (68) by computing $\frac{d^\ell}{dt^\ell}C_{a,b}(E,t)$. For example we have:

$$\frac{d}{dt}C_{a,b}(E,t) = \int_{\Sigma_E} \bar{b}(z)\{a,p_0\}(\Phi^t(z))d\sigma_E(z) \tag{69}$$

$$\frac{d^2}{dt^2}C_{a,b}(E,t) = -\int_{\Sigma} \overline{\{b,p_0\}}(z).\{a,p_0\}(\Phi^t(z))d\sigma_E(z) \tag{70}$$

where $\{a,p_0\}$ denotes the classical Poisson bracket.

Remark 6.8 *In [19] the authors consider the quantum correlation function:*

$$Q_j(t,\hbar) := \Re\left\{\frac{1}{2i}[\hat{\mathcal{R}}_{A,B;j,\hbar}(t) - \hat{\mathcal{R}}_{A,B;j,\hbar}(-t)]\right\}$$

We have also:

$$Q_j(t,\hbar) = \sum A_{jk}B_{jk}\sin(\omega_{jk}(\hbar)t)$$

They remark that all the moments: $\int t^r Q_j(t,\hbar)dt = 0,\ \forall r \in \mathbb{N}$. *These integrals indeed exist as generalized integrals. It is well known that we have:*

$$\int_0^{+\infty} t^r e^{it\omega} dt = i^{-r}\frac{d^r}{d\omega^r}\left(\pi\delta(\omega) + iPV(\frac{1}{\omega})\right)$$

where PV *is the Cauchy principal value.*
By considering the cases r *even and* r *odd we get easily that, for* $\omega \neq 0$, $\int_{-\infty}^{+\infty} t^r.\sin(\omega t)dt = 0$.
If the classical system is mixing in the classical limit, applying the theorem (6.5), we have:

$$\lim_{[\hbar\searrow 0,\, j\in M(\hbar)]} Q_j(t,\hbar) = \int_{\Sigma_E}(a\left(\Phi^t(z)\right)b(z) - b\left(\Phi^t(z)\right)a(z))d\sigma_E(z) := \Gamma_{a,b}(t,E) \tag{71}$$

$\Gamma_{a,b}(.,E)$ *is an odd function. If furthermore we have exponential decay for the correlations as in [26, 27] then the Fourier transform of* $\Gamma_{a,b}(.,E)$ *is analytic in a complex neighborhood of the real axis. So if for every* $r \in \mathbb{N}$ *we have* $\int t^r\Gamma_{a,b}(t,E)dt = 0$ *then* $\Gamma_{a,b}(.,E) \equiv 0$. *So, as claimed in [19], if* $\Gamma_{a,b}(t,E) \neq 0$ *for some time* t*, this shows that for very large times quantum and classical evolutions are very different.*

A Families of energy transitions with a classical limit

The aim of this section is to constuct examples of non diagonal matrix elements satisfying assumptions $(\alpha), (\beta), (\gamma)$ of Theorems (3.5) and (3.7). We assume that the quantum Hamiltonian $P(\hbar)$ satisfies the hypotheses (H_1) to (H_7) . Let us recall the following notations and assumptions:

$$\begin{aligned}
I(\hbar) &= [\alpha(\hbar),\beta(\hbar)],\ \text{with } \alpha(\hbar) < E < \beta(\hbar)\\
\lambda(\hbar) : &= \beta(\hbar) - \alpha(\hbar)\ \ \lim_{\hbar\searrow 0}\lambda(\hbar) = 0 \text{ and } \lambda(\hbar) \geq \epsilon_2\hbar,\ \text{for some } \epsilon_2 > 0\\
\Lambda(\hbar) &= \{j,\ E_j(\hbar) \in I(\hbar)\};\ \omega_{jk}(\hbar) = \left(\frac{E_k(\hbar) - E_j(\hbar)}{\hbar}\right)\\
|\Sigma_E| &= \int_{\Sigma_E}\frac{d\Sigma_E}{|\nabla p_0|}
\end{aligned}$$

We first give estimates as $\hbar \searrow 0$ for the size of the sets:

$$\Omega(\tau,\delta,\hbar) := \{(j,k); E_j(\hbar), E_k(\hbar) \in I(\hbar), |\omega_{jk}(\hbar) - \tau| \leq \frac{\delta}{2}\}$$

Our main tool will be the following result stated in [5]:

Theorem A.1 *(see also [7]). There exist* $\gamma > 0$*, depending only on the fixed energy* E *and on the classical Hamiltonian* p *such that:*

$$\begin{aligned}
\forall\varepsilon > 0,\quad &\exists\eta_\varepsilon > 0, \exists C_\varepsilon > 0,\ \text{such that for all interval } I \subseteq]E-\eta, E+\eta[, \forall\hbar \in]0,1], \text{we have :}\\
&|\#\{j; E_j(\hbar) \in I\} - (2\pi\hbar)^{-n}Vol_{\mathbb{R}^{2n}}p_0^{-1}(I)| \leq \gamma\varepsilon\hbar^{1-n} + C_\varepsilon\hbar^{2-n}
\end{aligned} \tag{72}$$

We first prove the following lemma:

Lemma A.2 *There exists $c_0 > 0$ small enough such that for every $0 < \delta < c_0\varepsilon_2$ there exists $\hbar_\delta > 0$ such that:*

$$\frac{1}{2}(2\pi\hbar)^{-2n}\delta\hbar\lambda(\hbar)|\Sigma_E|^2 \leq \#\Omega(\tau,\delta,\hbar) \leq \frac{3}{2}(2\pi\hbar)^{-2n}\delta\hbar\lambda(\hbar)|\Sigma_E|^2 \tag{73}$$

under the conditions:

$$0 \leq \hbar \leq \hbar_\delta,\ (|\tau| + \frac{\delta}{2})\hbar \leq \frac{4}{5}\lambda(\hbar)$$

Proof: We will establish the lower bound only and for $\tau > 0$. The other cases can be checked in the same way. We have:

$$\#\Omega(\tau,\delta,\hbar) \geq$$
$$\#\{(j,k); E_j(\hbar) \in I(\hbar) \cap [\alpha(\hbar) - (\tau - \frac{\delta}{2})\hbar, \quad \beta(\hbar) - (\tau + \frac{\delta}{2})\hbar], |\omega_{jk}(\hbar) - \tau| \leq \frac{\delta}{2}\} \tag{74}$$

In what follows γ is a "generic constant" independent of $\hbar$ and ε.
Using Theorem (A1) we have the following estimate:

$$\#\{k; |\omega_{jk}(\hbar) - \tau| \leq \frac{\delta}{2}\} \geq (2\pi\hbar)^{-n}(\delta\hbar|\Sigma_E| - \gamma\delta\hbar\lambda(\hbar) - \gamma\varepsilon\hbar) \tag{75}$$

under the conditions:

$$\hbar \in]0,\hbar_\varepsilon],\ E_j(\hbar) \in I(\hbar) \cap [\alpha(\hbar) - (\tau - \frac{\delta}{2})\hbar, \beta(\hbar) - (\tau + \frac{\delta}{2})\hbar]$$

where we have used that under the above conditions we have, by the fondamental theorem on calculus:

$$Vol_{\mathbb{R}^{2n}}(p_0^{-1}[E_j(\hbar) + (\tau - \frac{\delta}{2})\hbar, E_j(\hbar) + (\tau + \frac{\delta}{2})\hbar] \geq \delta\hbar|\Sigma_E| - \gamma\delta\hbar\lambda(\hbar)$$

In the same way we have also:

$$\#\{j; E_j(\hbar) \in [\alpha(\hbar), \beta(\hbar) - (\tau + \frac{\delta}{2})\hbar]\} \geq (2\pi\hbar)^{-n}(\lambda(\hbar)|\Sigma_E| - (\tau + \frac{\delta}{2})\hbar|\Sigma_E| - \gamma\lambda(\hbar)^2) \tag{76}$$

Now putting together (75) and (76) and choosing $\varepsilon = \frac{\delta}{\Gamma}$ with Γ large enough, we get the lower bound:

$$\#\Omega(\tau,\delta,\hbar) \geq \frac{1}{2}(2\pi\hbar)^{-2n}\delta\hbar\lambda(\hbar)|\Sigma_E|^2 \tag{77}$$

under the conditions of the lemma. ∎

By using the same technique as above (being a little bit more accurate in the estimates) it is not difficult to prove the following asymptotic result:

Proposition A.3 *Let us assume that* (H_1) *to* (H_7) *are fulfilled and furthermore that we have:* $\lim_{\hbar \searrow 0} \frac{\hbar}{\lambda(\hbar)} = 0$. *Then, for every* $\tau \in \mathbb{R}$ *and every* $\delta > 0$ *we have for* $\hbar \searrow 0$*:*

$$\#\Omega(\tau, \delta, \hbar) = (2\pi\hbar)^{-2n} \delta\hbar\lambda(\hbar)|\Sigma_E|^2 + o(\hbar^{1-2n}\lambda(\hbar)) \tag{78}$$

Now we come to the main goal of this section. Let us choose a large enough integer N_0 and two real numbers C_1, C_2 such that $\frac{C_1}{C_2} > 4$. Let us introduce, for $N \geq N_0$:

$$\Omega_N(\hbar) := \{(j,k); E_j(\hbar), E_k(\hbar) \in I(\hbar), \ \frac{C_2}{N} \leq |\omega_{jk}(\hbar) - \tau| \leq \frac{C_1}{N}\}$$

Then, using the Lemma (A2) with $\delta = \frac{C_i}{N}$, we get that there exists $C_3 > 0$ such that for every $N \geq N_0$ there exists $\hbar_N$ such that for all $\hbar \in]0, \hbar_N]$ we have:

$$\#\Omega_N(\hbar) \geq \frac{C_3}{N} \hbar^{1-2n} \lambda(\hbar) \tag{79}$$

Now, choose a decreasing sequence $\tilde{\hbar}_N > 0$, such that $\lim_{N\to\infty} \tilde{\hbar}_N = 0$ and

$$\tilde{\hbar}_N \leq \min\left\{\hbar_N, N^{\frac{1}{1-n}}\right\}$$

¿From (79), for all $\hbar \in]0, \tilde{\hbar}_N]$ we have

$$\#\Omega_N(\hbar) \geq C_3 \hbar^{-n} \lambda(\hbar) \tag{80}$$

Let us define:

$$\Omega(\hbar) := \Omega_N(\hbar) \ \text{ if } \tilde{\hbar}_{N+1} < \hbar \leq \tilde{\hbar}_N$$

Clearly $\Omega(\hbar)$ satisfies the assumptions (α) and (β). To check the assumption (γ) we remark that from Theorem (A1) we get easily the asymptotic formula:

$$\lim_{\hbar \searrow 0} \frac{\#\Lambda(\hbar)}{\hbar^{-n}\lambda(\hbar)} = (2\pi)^{-n} |\Sigma_E| \tag{81}$$

∎

B Smooth unbounded observables

We want here to give a rigorous meaning to the matrix elements $A_{jk}(\hbar)$ for $A(\hbar) := op_\hbar^w(a)$ not necessarry bounded. The answer follows easily from the following lemma:

Lemma B.1 *Let us assume the hypotheses* (H_1) *to* (H_5) *for the Hamiltonian* $P(\hbar)$. *Let* $\chi_0 \in C_0^\infty(I_{c\ell})$ *and* $a \in C^\infty(\mathbb{R}^{2n})$ *satisfying the following condition:*

$$[S(m)] \ \exists C > 0, \ \exists m \in \mathbb{N} \text{ such that for} |\alpha| + |\beta| \geq m \text{ we have } |\partial_x^\alpha \partial_\xi^\beta a(x,\xi)| \leq C \tag{82}$$

Then there exists $\hbar_0 > 0$ *small enough such that for every* $\hbar \in]0, \hbar_0]$, *the operator* $A(\hbar)\chi_0(P(\hbar))$ *is bounded on* $L^2(\mathbb{R}^n)$.

Proof: We first prove the result for $m = 1$. Let us consider $\chi \in C_0^\infty(I_{c\ell})$ such that $\chi \equiv 1$ on the support of χ_0. We recall the following result concerning the functional calculus (see [28, 32]).

$$\chi(P(\hbar)) = op_\hbar^w(p_\chi) + \hbar op_\hbar^w(r_\chi(\hbar)) \tag{83}$$

where $p_\chi(x,\xi) := \chi(p_0(x,\xi))$ is a smooth compactly supported symbol, and :

$$|\partial_x^\alpha \partial_\xi^\beta r_\chi(\hbar, x, \xi)| \leq C$$

where C is independent of $\hbar$ and (x,ξ).
For every $\varphi \in \mathcal{S}(\mathbb{R}^n)$ we have:

$$\begin{gathered} A(\hbar)\chi_0(P(\hbar))\varphi = A(\hbar)\chi(P(\hbar))\chi_0(P(\hbar))\varphi = \\ A(\hbar)op_\hbar^w(p_\chi)\chi_0(P(\hbar))\varphi + \hbar A(\hbar)op_\hbar^w(r_\chi(\hbar))\chi_0(P(\hbar))\varphi \end{gathered} \tag{84}$$

Let introduce a commutator:

$$A(\hbar)op_\hbar^w(r_\chi(\hbar)) = op_\hbar^w(r_\chi(\hbar))A(\hbar) + [A(\hbar), op_\hbar^w(r_\chi(\hbar))] \tag{85}$$

Now, using the rule on the symbolic calculus for Weyl quantization (see [6, 32]), we get:

$$\hbar^{-1}[A(\hbar), op_\hbar^w(r_\chi(\hbar))] = op_\hbar^w(b(\hbar)) \tag{86}$$

(let us remark that the "first term" in the $\hbar$-expansion of $b(\hbar)$ is the Poisson bracket $\{a, r_\chi(\hbar)\}$)
We have:

$$|\partial_x^\alpha \partial_\xi^\beta b(\hbar, x, \xi)| \leq C$$

hence, using the Calderon-Vaillancourt theorem, we get for some constants C_1, C_2 independent of $\hbar$ and φ:

$$\|A(\hbar)\chi_0(P(\hbar))\varphi\| \leq C_1\|\varphi\| + C_2\hbar\|A(\hbar)\chi_0(P(\hbar))\varphi\| \tag{87}$$

Then we get the result under the condition $C_2\hbar \leq \frac{1}{2}$ on $\hbar$.
We can extend now the result for $m \geq 2$ by an induction argument. Indeed, if a satisfies $[S(m)]$ then the symbol $b(\hbar)$ defined in (86) satisfies $[S(m-1)]$. So the induction is clear.

C Non smooth observables

It is convenient here to use the anti-Wick quantization which can be defined in the following way: let us intoduce the fondamental normalized bound state of the harmonic oscillator:

$$\Psi_\hbar(x) := (\pi\hbar)^{-n/4} \mathrm{e}^{-x^2/2\hbar}$$

The coherent states centered at the point $(y,\eta) \in \mathbb{R}^{2n}$ is defined by:

$$\Psi_{\hbar,y,\eta}(x) := \left(\exp\frac{i}{\hbar}(\eta.x - y.P).\Psi_\hbar\right)(x)$$

where we denote : $P := \frac{\hbar}{i}\nabla_x$ Then the anti-Wick quantization of a classical observable a is given by:

$$op_\hbar^{AW}(a)\varphi = (2\pi\hbar)^{-n}\int\int_{\mathbb{R}^{2n}} a(y,\eta)\langle\varphi,\Psi_{\hbar,y,\eta}\rangle\Psi_{\hbar,y,\eta}dyd\eta$$

we have the three following useful properties (see [5]):
(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 $a \in \mathcal{B}_\infty$, $\|op_\hbar^{AW}(a) - op_\hbar^{w}(a)\| = O(\hbar)$ as $\hbar \searrow 0$.

To state results we need a mild smoothness assumption: we say that a Borel function a on $\mathbb{R}^{2n}$ satisfies the condition (S) if the following property holds:

$$\forall\varepsilon>0, \exists a_1;\ a_2,\ \text{continuous on}\mathbb{R}^{2n}\ \text{such that :}a_1 \leq a \leq a_2,\ \text{and}\ \int(a_2-a_1)d\sigma_E \leq \varepsilon$$

Let us remark that if a is the caracteristic function of an open set U then the condition (S) means that the boundary of U is $d\sigma_E$-negligible.

Proposition C.1 *The theorems (3.5) and (3.7) (i) can be extended to any quantum observable $A(\hbar) = op_\hbar^{AW}(a)$ with any bounded Borel function a satisfying (S) on the phase space $\mathbb{R}^{2n}$ and for $A(\hbar) = op_\hbar^{w}(a)$ with a a bounded Borel function satisfying (S) and depending only on position variables or only on momentum variables.*
More precisely we have:
(I) Under the conditions (H_1) to (H_8) for every $\varepsilon > 0$ there exists $T_\varepsilon > 0$ and $\hbar_\varepsilon > 0$ such that:

$$\forall(j,k)\in M(\hbar)\times M(\hbar),\ 0<\hbar\leq\hbar_\varepsilon;\ |E_j(\hbar)-E_k(\hbar)| \leq \frac{\pi\hbar}{2T_\varepsilon} \Rightarrow |A_{jk}(\hbar)| \leq \varepsilon \tag{88}$$

(II) Let us assume (H_1) to (H_9). Then we have:

$$\lim_{[\hbar\searrow 0\ (j,k)\in M(\hbar)\times M(\hbar),\ j\neq k]} A_{jk}(\hbar) = 0 \tag{89}$$

(for the moment we are not able to extend part (ii) of the theorems for discontinuous classical observables!)

Proof: Let us consider, for example, Theorem (3.7) (i). Using the property (AW3), the conclusions of Theorem (3.7) (i), (ii) hold for $A(\hbar) = op_\hbar^{AW}(a)$ with a continuous and bounded on $\mathbb{R}^{2n}$.
It is sufficient to consider only real valued observables. We have the elementary identity:

$$\begin{aligned}\langle A\varphi_j,\varphi_k\rangle &= \\ \frac{1}{4}(\langle A(\varphi_j+\varphi_k),\varphi_j+\varphi_k\rangle &- \langle A(\varphi_j-\varphi_k),\varphi_j-\varphi_k\rangle)\end{aligned} \tag{90}$$

which gives an explicit decomposition of the measures $d\mu_{jk}$ into its positive and negative part:

$$\int a d\nu_{jk}^{\pm} := \langle op_{\hbar}^{AW}(a)(\varphi_j \pm \varphi_k), \varphi_j \pm \varphi_k \rangle$$

Hence we have clearly, under the condition $(j,k) \in M(\hbar) \times M(\hbar)$ and $\hbar \searrow 0$:

$$\{\int a d\mu_{jk} \to 0\} \Leftrightarrow \{\int a d\nu_{jk}^{\pm} \to 2 < a >_E\} \tag{91}$$

a satisfies (S), so for any $\varepsilon > 0$ we can find $a_1, a_2 \in \mathcal{B}_\infty$ such that:

$$a_1 \leq a \leq a_2, \text{ and } \int (a_2 - a_1) d\sigma_E \leq \varepsilon \tag{92}$$

So we have:

$$\int a_1 d\nu_{jk}^{\pm} \leq \int a d\nu_{jk}^{\pm} \leq \int a_2 d\nu_{jk}^{\pm} \tag{93}$$

But we know that for $i = 1, 2$:

$$\int a_i d\nu_{jk}^{\pm} \to 2 \int a_i d\sigma_E \ \text{ as } \hbar \searrow 0,\ (j,k) \in M(\hbar) \times M(\hbar) \tag{94}$$

Hence from (92, 93, 94) we get:

$$\int a d\nu_{jk}^{\pm} \to 2 \int a d\sigma_E \ \text{ as } \hbar \searrow 0,\ (j,k) \in M(\hbar) \times M(\hbar)$$

For $a(x,\xi) = f(x)$ or $a(x,\xi) = g(\xi)$, with the Weyl quantization, we use the same positivity arguments by approximating below and above f and g by smooth functions. ∎

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