ANNALES DE L'I. H. P., SECTION A

MONIQUE COMBESCURE
DIDIER ROBERT

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Annales de l'I. H. P., section A, tome 61, nº 4 (1994), p. 443-483
<http://www.numdam.org/item?id=AIHPA_1994__61_4_443_0>

Ann. Inst. Henri Poincaré,

Vol. 61, n° 4, 1994, p. 443-483 *Physique théorique*

Distribution of matrix elements and level spacings for classically chaotic systems

by

Monique COMBESCURE

Laboratoire de Physique Théorique et Hautes Énergies, URA CNRS, Université de Paris-Sud, 91405 Orsay Cedex, France.

and

Didier ROBERT

Département de Mathématiques, URA CNRS 758, Université de Nantes 44072 Nantes Cedex 03, France.

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.

RÉSUMÉ. – Pour des systèmes quantiques obtenus par quantification de systèmes classiques chaotiques, nous établissons quelques résultats rigoureux concernant le comportement semi-classique des éléments matriciels d'observables sur un système orthonormé d'états propres de l'hamiltonien.

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 $X = \mathbb{R}^n$. Our proofs can be easily translated on some

Riemannian compact manifold X (a torus for example, 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 $I_{cl} \subset \mathbb{R}$ be a classical energy interval such that the spectrum of $P(\hbar)$ is purely discrete in I_{cl}. 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 $E_j(\hbar) \in I_{cl}$. Let us denote by $p(x, \xi) \in C^\infty(T^*(X))$ the corresponding classical Hamiltonian and assume that on some energy shell $\Sigma_E := \{(x, \xi) \in T^*(X); p(x, \xi) = E\}$, $E \in I$, 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 $A_{jk}(\hbar) := \langle A(\hbar)\varphi_j, \varphi_k\rangle$ [scalar product in $L^2(X)$].

The matrix elements are important for at least 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 how they appear. 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 ease. We have an orthonormal basis of eigenfunctions: $\{\varphi_j\}_{j\in\mathbb{N}}$, $P\varphi_j = E_j\varphi_j$. Let us consider a small perturbation P_γ of P, $P_\gamma := P + \gamma A$ where A is a bounded operator in $\mathcal{H}$ and $\gamma \in \mathbb{R}$ is 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":

$$E_j^\gamma = E_j + \gamma\varepsilon_1 + \gamma^2\varepsilon_2 + \cdots \tag{1}$$

$$\varphi_j^\gamma = \varphi_j + \gamma\psi_1 + \gamma^2\psi_2 + \cdots \tag{2}$$

Asking that ψ_1 is orthogonal to φ_j, we get:

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

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

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 problem in the configuration space $\mathbb{R}^n$. There is considerable literature discussing the behaviour of the $A_{jk}(\hbar)$ as the Planck constant $\hbar \searrow 0$ and $E_j(\hbar)$, $E_k(\hbar) \to E \in I_{cl}$, in connection with the chaotic properties of the classical dynamics on Σ_E. (*See* references

[23], [24], [31], [30], [10].) In particular, if the classical dynamics is ergodic on Σ_E, then it is claimed that for the diagonal elements we have:

$$\left.\begin{array}{c}\lim\limits_{\hbar\searrow 0} A_{jj}(\hbar) = \langle a\rangle_E \\ \text{(the average of } a \text{ for the Liouville measure on } \Sigma_E)\end{array}\right\} \tag{3}$$

and for the non diagonal elements:

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

Until now these claims have not been completely proven. Following the work of Shnirelman [35], Zelditch [38], Colin de Verdière [5], Helffer-Martinez-Robert [16] 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 in the quantum mechanics case some results obtained by Zelditch [39] in the high energy limit for the Laplace operator.

Our results hold for general smooth Hamiltonians, but let us state in this introduction one of the main applications of this paper, in the particular case of Schrödinger operators: $P(\hbar) = -\hbar^2\Delta + V$.

Let us assume that the potential V is real, C^∞-smooth on $\mathbb{R}^n$ and $E < \liminf\limits_{|x|\to\infty} V(x)$. Then for small $\hbar$, the spectrum of $P(\hbar)$ close to E (say in $[E-\varepsilon_1, E+\varepsilon_1]\,\varepsilon_1 > 0$) is purely discrete. So we have $P(\hbar)\varphi_j = E_j(\hbar)\varphi_j$ where $\{\varphi_j\}$ is an orthonormal basis of Range $\{\Pi_{P(\hbar)}([E-\varepsilon_1, E+\varepsilon_1])\}$ where $\Pi_P(J)$ denotes the spectral projector of the operator P on the interval J.

Let us assume that E is a regular value for V. Then $\Sigma_E := \{(x, \xi) \in \mathbb{R}^n;\ \xi^2 + V(x) = E\}$ is a smooth hypersurface equipped with the Liouville measure and invariant for the Hamiltonian flow generated by Newton's equations: $\Phi^t(x, \xi) := \exp(t[2\xi\,\partial_x - (\partial_x V)\,\partial_\xi])$.

Our basic assumption is that the dynamical system: $(\Sigma_E, d\sigma_E, \Phi^t)$ is mixing (*see* Section 2 for definitions).

Let us consider $\hbar$-dependent energy intervals: $I(\hbar) = [\alpha(\hbar), \beta(\hbar)]$, $\alpha(\hbar) < E < \beta(\hbar)$ with $\lim\limits_{\hbar\to 0}(\beta(\hbar) - \alpha(\hbar)) = 0$, $\beta(\hbar) - \alpha(\hbar) \geq \varepsilon_2\hbar$, for some $\varepsilon_2 > 0$ and denote: $\Lambda(\hbar) = \{j,\ E_j(\hbar) \in I(\hbar)\}$. $S_m\,(m \in \mathbb{N})$ will denote the space of smooth classical observables $a : \mathbb{R}^{2n} \to \mathbb{C}$ such that for $|\alpha| + |\beta| \geq m$ the derivatives $\partial_x^\alpha\,\partial_\xi^\beta\,a(x, \xi)$ are bounded in $\mathbb{R}^{2n}$. Let us introduce the quantum observable $\hat{A}(\hbar) := \mathrm{op}_\hbar^w(a)$ (Weyl quantization of *a, see* Section 2) and the matrix elements $A_{jk}(\hbar) := \langle A(\hbar)\varphi_j, \varphi_k\rangle$. We can now formulate the main application of our results:

THEOREM 1.1. – *Under the above assumptions we have:*

(i) *There exists* $M(\hbar) \subseteq \Lambda(\hbar)$ *such that:*

$$\lim_{\hbar\searrow 0}\frac{\#M(\hbar)}{\#\Lambda(\hbar)} = 1, \qquad \lim_{[\hbar\searrow, 0\, j\in M(\hbar),\, k\in\Lambda(\hbar),\, j\neq k]} A_{jk}(\hbar) = 0,$$

(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:*

$$\lim_{\hbar\searrow 0}\frac{\#\tilde{\Omega}(\hbar)}{\#\Omega(\hbar)} = 1 \quad \text{and} \quad \lim_{\hbar\searrow 0} A_{jk}(\hbar) = 0, \qquad (5)$$
$$\text{uniformly for } (j, k) \in \tilde{\Omega}(\hbar)$$

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

This theorem will be proved in Section 3 as consequence of more general results. Let us remark here that no other assumption on V at infinity is needed, because we know that the bound states ϕ_j are exponentially localized in $\{V(x) \leq E + \varepsilon_1\}$. ([1], [14], [19]).

The results can be extended to non smooth or non bounded observables a as we shall see in Section 3.

Besides the theorem above, the goal of this paper is to formulate different results concerning the semi-classical limit of the matrix elements $A_{jk}(\hbar)$ and the corresponding transition energies defined as:

$$\omega_{jk}(\hbar) := \left(\frac{E_j(\hbar) - E_k(\hbar)}{\hbar}\right)$$

We will also discuss the variance of the statistical distribution of the series $\{A_{jk}(\hbar)\}_{jk}$ according to a definition proposed by Wilkinson [37]. We will give a rigourous proof of the semi-classical $\hbar$-expansion which appeared in [37].

The unifying theme of our paper is the role of different "sum rules" (*see* [24], [10]). The idea is to consider sums such as:

$$S_{\theta, j}(\hbar) = \sum_k |A_{jk}(\hbar)|^2 \, \theta\left(\frac{E_j(\hbar) - E_k(\hbar)}{\hbar}\right) \tag{6}$$

We initially transform this sum using the Parseval relation and try to control the classical limit by direct estimates or by the WKB method. In this way, we get different results, according to the choice of the test functions θ, which will generally 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 [32] (for integrable systems *see* [2]).

The content of this paper is organized as follows.

In Section 2 we recall some well known facts and notations concerning semi-classical spectral analysis.

In Section 3, after displaying some rough but general estimates on non diagonal matrix elements, we state our main results for a large class of quantum Hamiltonians. The two first theorems are extensions to the quantum mechanical case of result obtained earlier by Zelditch in the high energy "regime" for the Laplace operator on compact Riemannian manifolds. In this paper, we want to put emphasis on quantum systems such that the corresponding classical system is ERGODIC or MIXING on a fixed energy shell.

Our third result is a mathematically rigorous formulation of a result by Wilkinson on the variance of the matrix elements which is an extension of the Gutzwiller-Poisson trace formula (we call it the semi-classical variance theorem).

In Section 4 we give detailed proofs of our results concerning estimates of non diagonal matrix elements stated in Sections 1 and 3.

In Section 5 we show how to prove the semi-classical variance theorem using the WKB-construction as it has been done for the Gutzwiller-Poisson formula.

In Section 6 we add two results related with our subject. The first is an extension of Helton's result in the quantum mechanical setting, which can help to understand the connection between the level spacings and the non periodical paths. The second is a semi-classical sum-rule which appears frequently in the physics literature and which is rigorously proved here.

In the Appendix (A) we show how to construct families of energy transitions satisfying the assumptions of the theorem (1.1) (ii).

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* [33].

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

$$(\mathrm{op}_\hbar^w\, b)\, \psi(x) = (2\,\pi\,\hbar)^{-n} \int\!\!\int e^{\frac{i}{\hbar}\langle x-y,\,\xi\rangle}\, b\left(\frac{x+y}{2},\, \xi\right) \psi(y)\, dy\, d\xi \quad (7)$$

We shall also use the notations $\mathrm{op}_\hbar^w\, b := b_\hbar^w := B(\hbar)$; 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:

$$p(\hbar,\, x;\, \xi) \asymp \sum_{0 \le j < +\infty} \hbar^j\, p_j(x,\, \xi) \quad (8)$$

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:*

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

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

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

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 [33]) 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.

Examples of Hamiltonians satisfying (H_1) *to* (H_4):

$$(\text{ex. }1)\, P(\hbar) = -\hbar^2 (\nabla - i\,\vec{a}(x))^2 + V(x)$$

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

$$\begin{gathered}
\liminf_{|x| \to +\infty} V(x) > E \\
\exists\, \gamma > 0 \text{ such that } \forall\, \alpha, \quad |\partial_x^\alpha V(x)| \le c_\alpha (V(x) + \gamma) \\
\exists\, M > 0 \text{ such that } |V(x)| \le C (V(y) + \gamma)(1 + |x - y|)^M \qquad (9) \\
|\partial_x^\alpha \vec{a}(x)| \le c_\alpha (V(x) + \gamma)^{1/2}
\end{gathered}$$

$$(\text{ex. }2)\, P(\hbar) = -\hbar^2 \sum \partial_{x_i} g_{ij}(x)\, \partial_{x_j} + V(x)$$

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

$$\begin{gathered}
\exists\, C \text{ a real number } \exists\, \mu(x)\, (x \in \mathbb{R}^n) \\
\text{such that } \frac{\mu(x)}{C} |\xi|^2 \le \left|\sum g_{ij}(x)\, \xi_i\, \xi_j\right| \le C\, \mu(x)\, |\xi|^2 \\
\text{with } \frac{1}{C} \le \mu(x) \le C (V(x) + \gamma) \qquad (10)
\end{gathered}$$

We also give an example of a non local Hamiltonian:

$$(\text{ex. }3)\, P(\hbar) = \sqrt{m^2 - \hbar^2 \Delta} + V(x) \qquad (11)$$

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

In the following the function and operator norms in $L^2(\mathbb{R}^n)$ will be denoted by $\|\cdot\|$.

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

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

This implies that for every closed interval $J_{cl} := [E_-, E_+] \subset I_{cl}$, *and for* $\hbar > 0$ *small enough, the spectrum of* $P(\hbar)$ *in* J_{cl} *is purely discrete* [17]. *In what follows we fix such an interval* J_{cl}.

For a fixed energy level $E \in]E_-, E_+[$, *we assume:*

(H_6) E *is a regular value of* p_0. *That means:* $p_0(x, \xi) = E \Rightarrow \nabla_{(x, \xi)} p_0(x, \xi) \ne 0$. *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 with 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 volume of literature on this subject, but there are few rigorous mathematical results about quantum consequences of classical chaos.

Let us recall some well established results concerning semi-classical asymptotics of bound states, which will be used in this paper:

(R_1) *the Weyl formula with Hörmander estimate* ([21], [17], [22]).

Under the assumptions (H_1) to (H_5), if $\lambda, \mu \in I_{cl}$, $\lambda < \mu$, are regular values for p_0, then we have:

$$\#\{j, E_j(\hbar) \in [\lambda, \mu]\} = (2\pi\hbar)^{-n} \operatorname{Vol}_{\mathbb{R}^{2n}} \{p_0^{-1}[\lambda, \mu]\} + O(\hbar^{1-n}) \quad (12)$$

(R_2) *the Weyl formula with Duistermaat-Guillemin-Ivrii estimate* ([9], [28], [22]).

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:

$$\begin{aligned}\#\{j, E_j \in [\lambda, \mu]\} =& (2\pi\hbar)^{-n} \operatorname{Vol}_{\mathbb{R}^{2n}} \{p_0^{-1}[\lambda, \mu]\} \\ &+ c_1 \hbar^{1-n} + o(\hbar^{1-n})\end{aligned} \quad (13)$$

where c_1 was computed in [28] ($c_1 = 0$ if $p_1 = 0$).

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 $\lim_{\hbar \to 0}(\beta(\hbar) - \alpha(\hbar)) = 0$, $\beta(\hbar) - \alpha(\hbar) \geq \varepsilon_2 \hbar$, for some $\varepsilon_2 > 0$. 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* [16])

$$\lim_{\hbar\searrow 0} \frac{\sum_{j\in\Lambda(h)} A_{jj}(\hbar)}{\#\Lambda(\hbar)} = \int_{\Sigma_E} a\, d\sigma_E \tag{14}$$

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)],

$$\lim_{\hbar\searrow 0} \left(\frac{(2\pi\hbar)^n (\#\Lambda(\hbar))}{\beta(\hbar) - \alpha(\hbar)}\right) = \int_{\Sigma_E} \frac{d\Sigma_E}{|\nabla p_0|} := |\Sigma_E| \tag{15}$$

The above asymptotic result is an easy corollary of [16] (Théorème 1.1, p. 315). For a particular case *see* also [3].

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* $(x, \xi) \in \Sigma_E$:

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

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

THEOREM 2.1 (Ergodic Semi-Classical Theorem) ([35], [5], [38], [16]). – *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:*

$$\lim_{\hbar\searrow 0} \left(\frac{\#M(\hbar)}{\#\Lambda(\hbar)}\right) = 1,$$

and

$$\lim_{[\hbar\searrow 0,\, j\in M(\hbar)]} A_{jj}(\hbar) = \int_{\Sigma_E} a\, d\sigma_E, \tag{16}$$

$$\forall a \in \mathcal{B}_\infty$$

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

3. NEW RESULTS FOR THE NON DIAGONAL MATRIX ELEMENTS

We begin with a crude estimate which nevertheless 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:*

$$|A_{jk}(\hbar)| \leq c_0 \frac{\hbar}{|E_k(\hbar) - E_j(\hbar)|}, \qquad \forall E_j, \quad E_k \in J_{cl}, \quad E_j(\hbar) \neq E_k(\hbar) \tag{17}$$

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

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

But from the $\hbar$-Weyl calculus (*see* for example [33]) we have the well known commutator estimate:

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

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 literature).*

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* $\square(\hbar) \subseteq \Lambda(\hbar) \times \Lambda(\hbar)$ *such that*

$$\lim_{\hbar \searrow 0} \frac{\# \square(\hbar)}{\# \Lambda(\hbar)^2} = 1, \qquad \text{and} \qquad \lim_{[\hbar \searrow 0, (j,k) \in \square(\hbar)]} A_{jk}(\hbar) = 0 \tag{18}$$

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

$$\begin{aligned} \sum_{(j,k) \in \Lambda(\hbar)^2} |A_{jk}(\hbar)|^2 &= \sum_{j \in \Lambda(\hbar)} \langle \Pi_P(I(\hbar)) \cdot A \varphi_j, A \varphi_j \rangle \\ &\leq \sum_{j \in \Lambda(\hbar)} \langle A^2 \varphi_j, \varphi_j \rangle \end{aligned} \tag{19}$$

But we know that $\lim_{\hbar\searrow 0} \#\Lambda(\hbar) = +\infty$ (*see* [28] and (15)). 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 [16] (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:*

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

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

THEOREM 3.5 (Ergodic case). – *We assume that the assumptions* (H_1) *to* (H_8) *are fulfilled. Let us consider an observable* $A = op_\hbar^w(a)$ *with* $a \in S_m$ i.e.

$$\text{for } |\alpha| + |\beta| \geq m, \quad \exists C > 0 \quad \text{such that } |\partial_x^\alpha \partial_\xi^\beta a(x, \xi)| \leq C \tag{20}$$

(i) *For every* $\varepsilon > 0$ *there exists* $T_\varepsilon > 0$ *and* $\hbar_\varepsilon > 0$ *such that:*

$$\begin{gathered} \forall j \in M(\hbar), \quad \forall k \in \Lambda(\hbar), \quad 0 < \hbar \leq \hbar_\varepsilon; \\ |E_j(\hbar) - E_k(\hbar)| \leq \frac{\pi\hbar}{2T_\varepsilon} \quad \Rightarrow \quad |A_{jk}(\hbar)| \leq \varepsilon \end{gathered} \tag{21}$$

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

(α) $\tilde{\Omega}(\hbar) \subseteq \Lambda(\hbar)^2$ *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:*

$$\lim_{\hbar\searrow 0} \frac{\#\tilde{\Omega}(\hbar)}{\#\Omega(\hbar)} = 1 \quad \text{and} \quad \lim_{[\hbar\searrow 0} A_{jk}(\hbar) = 0, \tag{22}$$
$$\text{uniformly for } (j, k) \in \tilde{\Omega}(\hbar)$$

The above statement means: for all $\varepsilon > 0$, *there exists* $\hbar_\varepsilon > 0$, *such that for every* $0 < \hbar < \hbar_\varepsilon$ *and for every* $(j, k) \in \tilde{\Omega}(\hbar)$ *we have* $|A_{jk}(\hbar)| \leq \varepsilon$.

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* $a(x, \xi) = x$ for $|x| \leq \sqrt{E+1}$]. *We can compare this fact with* (21).

To give further results we introduce a stronger assumption:

(H_9) *The dynamical system* $(\Sigma_E, d\sigma_E, \Phi^t)$ *is mixing, that means:*

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

THEOREM 3.7 (Mixing case). – *Let us assume* (H_1) *to* (H_9) *and let* $A(\hbar)$ *be an observable like in Theorem* 3.5

(i) *There exists* $M(\hbar) \subseteq \Lambda(\hbar)$ $(M(\hbar)$ *is the same as in Theorems* 2.1 *and* 3.5) *such that:*

$$\lim_{\hbar\searrow 0} \frac{\#M(\hbar)}{\#\Lambda(\hbar)} = 1, \qquad \lim_{[\hbar\searrow 0,\, j\in M(\hbar),\, k\in\Lambda(\hbar),\, j\neq k]} A_{jk}(\hbar) = 0,$$

$\forall\, a \in S_m$.

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

$$\lim_{\hbar \searrow 0} \frac{\#\tilde{\Omega}(\hbar)}{\#\Omega(\hbar)} = 1 \qquad \text{and} \qquad \lim_{\hbar \searrow 0} A_{jk}(\hbar) = 0, \tag{23}$$
$$\text{uniformly for} \quad (j, k) \in \tilde{\Omega}(\hbar)$$

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

Let us remark that the observable $A(\hbar)$ is not necessarily bounded. This can be applied, for example, to the position or momentum observables (conductivity).

We shall see that the results can also be extended to non smooth symbols by replacing Weyl quantization by anti-Wick quantization. It is well known that anti-Wick quantization can be defined in the following way: let us introduce the fundamental normalized bound state of the harmonic oscilator:

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

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

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

Then the anti-Wick quantization of a classical observable a is given by:

$$\mathrm{op}_\hbar^{AW}(a)\varphi = (2\pi\hbar)^{-n} \int\int_{\mathbb{R}^{2n}} a(y, \eta) \langle \varphi, \Psi_{\hbar, y, \eta}\rangle \Psi_{\hbar, y, \eta}\, dy\, d\eta$$

we have the three following useful properties (*see* [16]):

(AW1) $a \geq 0 \Rightarrow \mathrm{op}_\hbar^{AW}(a) \geq 0$

(AW2) $\mathrm{op}_\hbar^{AW}(a)$ admits an $\hbar$-Weyl symbol $a_W(\hbar)$ given by:

$$a_W(\hbar, x, \xi) = (\pi\hbar)^{-n} \int\int_{\mathbb{R}^{2n}} a(y, \eta) \times \exp\left(-\frac{1}{\hbar}[(x-y)^2 + (\xi-\eta)^2]\right) dy\, d\eta$$

(AW3) For every $a \in \mathcal{B}_\infty$, $\|\mathrm{op}_\hbar^{AW}(a) - \mathrm{op}_\hbar^{w}(a)\| = O(\hbar)$ as $\hbar \searrow 0$.

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

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

We have the following result:

THEOREM 3.8 (non smooth observables). – *The Theorems* 3.5 *and* 3.7 *can be extended to any quantum observable* $A(\hbar) = \mathrm{op}_{\hbar}^{AW}(a)$ *with any bounded Borel function* a *in the phase space* $\mathbb{R}^{2n}$ *satisfying* (R) *and also for* $A(\hbar) = \mathrm{op}_{\hbar}^{w}(a)$ *with* a *a bounded Borel function satisfying* (R) *and depending only on position variables or only on momentum variables.*

More precisely we have:

(I) *(Ergodic case) Under the conditions* (H_1) *to* (H_8) *for every* $\varepsilon > 0$ *there exists* $T_\varepsilon > 0$ *and* $\hbar_\varepsilon > 0$ *such that:*

$$\begin{gathered}\forall (j,\, k) \in M(\hbar) \times M(\hbar), \quad 0 < \hbar \le \hbar_\varepsilon; \\ |E_j(\hbar) - E_k(\hbar)| \le \frac{\pi\,\hbar}{2\,T_\varepsilon} \quad \Rightarrow \quad |A_{jk}(\hbar)| \le \varepsilon\end{gathered} \tag{24}$$

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

$$\lim_{[\hbar\searrow 0,\,(j,\,k)\in M(\hbar)\times M(\hbar),\,j\ne k]} A_{jk}(\hbar) = 0 \tag{25}$$

(III) *The statements* (ii) *in Theorems* 3.5 *and* 3.7 *hold for the above observable* $A(\hbar)$ *if furthermore we assume that* $\Omega(\hbar) \subseteq M(\hbar) \times M(\hbar)$.

COMPARAISON WITH PREVIOUS RESULTS [39]

In [39], *S. Zelditch proved analogous results in the high energy "regime", for the Laplace-Beltrami operator* Δ *on Riemannian compact manifold* M. *Our results seem more accurate for the following reasons. In the case considered in* [39] *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* ([9], [22]). *In* [39], *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). Nevertheless such a result could also be obtained in the high energy case considered in* [39] *using Duistermaat-Guillemin results* [9]. *Furthermore our proofs show that the number of non-controlled non diagonal matrix elements is independent of the observable* A, *and we get results also for non bounded or non smooth observables.*

Let us remark that the Proposition 1.1 of [39] concerning the so called "coherent non vanishing families" $A_{jk}(\hbar)$ can also be extended in our setting:

$\mathcal{B}_\infty \ni a \rightarrow A_{jk}(\hbar)$ is a Schwartz distribution on the phase space $T^*(\mathbb{R}^n)$. If we replace $A(\hbar)$ by $\tilde{A}(\hbar) := \mathrm{op}_\hbar^{AW}(a)$ then $\mathcal{B}_\infty \ni a \overset{\mu_{jk}}{\rightarrow} \tilde{A}_{jk}(\hbar)$ define complex valued Radon measures $d\mu_{jk}$ on $\mathbb{R}^{2n}$. It is proved in [16] that $d\mu_{jj}$ are positive bounded Radon measures and the non diagonal case follows easily by the parallelogram identity (Section 4). Following [39] 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:*

$$\forall a \in C_0^\infty(\mathbb{R}^{2n}),$$

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

then we have:

(i)

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

with

$$\tau := i^{-1} \frac{\displaystyle\int \{a,\, p_0\}(z)\, d\mu(z)}{\displaystyle\int a(z)\, d\mu(z)}$$

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

$$\forall t \in \mathbb{R}, \quad \forall a \in C_0^\infty(\mathbb{R}^{2n}),$$

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

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* [33]), we get:

$$\left\langle \frac{1}{\hbar} [A(\hbar), P(\hbar)] \varphi_j, \varphi_k \right\rangle = \left(\frac{E_j(\hbar) - E_k(\hbar)}{\hbar} \right) A_{jk}(\hbar)$$
$$= \langle \mathrm{op}_\hbar^w (\{a, p_0\}) \cdot \varphi_j, \varphi_k \rangle + O(\hbar) \quad (26)$$

$$\langle A(\hbar, t) \varphi_j, \varphi_k \rangle = \exp\left(\frac{it}{\hbar} (E_k(\hbar) - E_j(\hbar)) \right) A_{jk}(\hbar)$$
$$= \langle \mathrm{op}_\hbar^w (a(\Phi^t)) \varphi_j, \varphi_k \rangle + O(\hbar) \quad (27)$$

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:

$$\lim_{\hbar \searrow 0} \frac{1}{\# \Omega(\hbar)} \sum_{(j, k) \Omega(\hbar)} |A_{jk}(\hbar)|^2 \geq \kappa \quad (28)$$

But we have:

$$\frac{1}{\# \Lambda(\hbar)} \sum_{(j, k) \in \Lambda(\hbar)^2} |A_{jk}(\hbar)|^2$$
$$= \frac{1}{\# \Lambda(\hbar)} \sum_{j \in \Lambda(\hbar)} \langle \Pi_{P(\hbar)}(I(\hbar)) \cdot A \varphi_j, A \varphi_j \rangle$$
$$\leq \frac{1}{\# \Lambda(\hbar)} \sum_{j \in \Lambda(\hbar)} \langle A^2(\hbar) \varphi_j, \varphi_j \rangle \quad (29)$$

then, using a variant of Theorem 1.3 in [16] (*see* the remark below) we get:

$$\lim_{\hbar \searrow 0} \frac{1}{\# \Lambda(\hbar)} \sum_{(j, k) \in \Lambda(\hbar)^2} |A_{jk}(\hbar)|^2 = \int_{\Sigma_E} |a|^2\, d\sigma_E \quad (30)$$

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

$$K(\#\Lambda(\hbar)) \geq \sum_{(j,\,k)\in\Lambda(\hbar)^2} |A_{jk}(\hbar)|^2 \geq \sum_{(j,\,k)\in\Omega(\hbar)} |A_{jk}(\hbar)|^2 \geq \kappa(\#\Omega(\hbar)) \tag{31}$$

and (ii) of the proposition follows. ■

Our third main result in this paper is a mathematically rigorous version of Wilkinson's result concerning the variance of the statistical distribution of the matrix elements $A_{jk}(\hbar)$ [37].

In physics literature (*see* for example [37], [27]) 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 [37] proposed the following definition for the variance:

$$\begin{aligned} S_{(f,\,g)}(\hbar,\, E,\, \Delta E) &= \sum_{[E_j(\hbar),\, E_k(\hbar)\in J_{cl}]} |A_{jk}(\hbar)|^2 f_\hbar\left(E - \frac{1}{2}(E_j(\hbar) + E_k(\hbar))\right) \\ &\quad \times g_\hbar(\Delta E - (E_j(\hbar) - E_k(\hbar))) \end{aligned} \tag{32}$$

where E is inside the interval $J_{cl} \subset I_{cl}$ and $f_\hbar,\, g_\hbar$ are Gaussian regularizations 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 compactly supported Fourier transform: $\hat{f}(v) = \int_{\mathbb{R}} e^{-iuv} f(u)\,du$. Then we define $f_\hbar(u) := \frac{1}{\hbar} f\left(\frac{u}{\hbar}\right)$.

THEOREM 3.10. – *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. Then under assumptions* (H_1) *to* (H_6) *we have the following asymptotic expansion,* $\mathrm{mod}(O(\hbar^\infty))$, *as* $\hbar \searrow 0$:

$$S_{(f,\,g)}(\hbar,\, E,\, \Delta E) \asymp \hbar^{-n-1} \cdot \left(\sum_{j\geq 0} \Gamma_j\left(E,\, \frac{\Delta E}{\hbar}\right) \hbar^j\right) \tag{33}$$

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

$$\Gamma_0(E,\, \tau) = \hat{f}(0) \int \hat{g}(t)\, e^{it\tau}\, C_a(E,\, t)\, dt \tag{34}$$

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 analog of Gutzwiller trace formula* [13] *by taking* Supp $(\hat{f})$ *compact but arbitrarily 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) *satisfies*

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

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 $\hat{f} \longrightarrow \gamma_j(\hbar;\ \hat{f},\ \hat{g},\ E,\ \Delta E)$ *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 [12], [25].) *But it seems difficult to get rigorous results for* Supp $(\hat{f})$ *non compact even very fast decreasing!*

4. PROOF OF THE MAIN RESULTS: THEOREMS 3.5, 3.7, 3.8, 1.1

Let $a \in \mathcal{B}_\infty$ be such that $\langle a \rangle_E = 0$ (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:

$$\sum_{E_k \in J_{cl}} |A_{jk}(\hbar)|^2 = \|\Pi_{P(\hbar)}(J_{cl})\, A(\hbar)\, \varphi_j\|^2 \leq \|A(\hbar)\varphi_j\|^2 \qquad (35)$$

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

$$A_{\theta_T}(\hbar) = \int_{\mathbb{R}} \theta_T(t)\, A(\hbar, t)\, dt,$$

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 [33]) with a $\hbar$-Weyl principal symbol $a(t; x, \xi) = a(\Phi^t(x, \xi))$. In particular we have:

$$\begin{gathered}\|A(\hbar, t) - \mathrm{op}_\hbar^w(a(t))\| = O(\hbar) \quad \text{as } \hbar \searrow 0 \\ \text{uniformly for } t \text{ in every bounded interval}\end{gathered} \tag{36}$$

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

$$\langle A_{\theta_T}(\hbar)\varphi_i, \varphi_k\rangle = 2\pi\,\hat{\theta}_T(\omega_{jk}(\hbar))\,A_{jk}(\hbar) \tag{37}$$

We shall use the elementary inequality: $\frac{\sin(u)}{u} \geq \frac{2}{\pi}$ for $0 \leq u \leq \frac{\pi}{2}$. ($\star$)

Hence we get from (28)

$$\sum_{E_k \in J_{cl}} 4\pi^2 \left(\frac{\sin(T\omega_{jk})}{T\omega_{jk}}\right)^2 |A_{jk}(\hbar)|^2 \leq \langle A_{\theta_T}^* A_{\theta_T}\varphi_j, \varphi_j\rangle \tag{38}$$

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

$$\left| \langle A_{\theta_T}^* A_{\theta_T}\varphi_j, \varphi_j\rangle - \int_{\Sigma_E} \left|\frac{1}{2T}\int_{-T}^{T} a(\Phi^t(z))\,dt\right|^2 d\sigma_E(z) \right| \leq 8\varepsilon^2 \tag{39}$$

Now, using that $\langle a\rangle_E = 0$ 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 [39] by estimating the variances (we always assume $\langle a\rangle_E = 0$):

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

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

$$\mathcal{V}_{\Omega(\hbar)}(A) \leq \frac{\pi^2}{4(\#\Omega(\hbar))} \sum_{\omega_{jk}(\hbar)T<\pi/2,\, E_j\in I(\hbar),\, E_k\in J_{cl}} |A_{jk}(\hbar)|^2 \left|\frac{\sin(\omega_{jk}T)}{\omega_{jk}T}\right|^2 \tag{40}$$

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

Using (39), (35) with $A = A_{\theta_T}$ we can see easily that it exists $c > 0$ such that for $\hbar$ small enough we have:

$$\mathcal{V}_{\Omega(\hbar)}(\mathcal{A}) \leq \frac{c}{\#\Lambda(\hbar)} \cdot \sum_{j \in \Lambda(\hbar)} \langle A_{\theta_T}^* \cdot A_{\theta_T} \varphi_j, \varphi_j \rangle + O(\hbar) \tag{41}$$

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

The proof of the second part of Theorem 3.5 follows from (41) by the same argument used in the first part (*see* 39) and using the Lemma 3.4. To prove that we can choose $\tilde{\Omega}(\hbar)$ independently of $A(\hbar)$ we use the construction of [16], p. 321 (*see* also [5]). ■

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 [10] and in Prosen-Robnik [30].

LEMMA 4.1. – *Let $J_{m, cl} := [\alpha_m, \beta_m]$, $m = 1, 2$, 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 $E_j(\hbar) \in J_{2, cl}$, we have:*

$$\sum_{E_k(\hbar) \in J_{1, cl}} |A_{jk}(\hbar)|^2 \exp(-it\,\omega_{jk}(\hbar)) = \langle \varphi_j, A(t, \hbar)\, \chi(P(\hbar))\, A(\hbar)\, \varphi_j \rangle + O(\hbar) \tag{42}$$

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

Proof of the Lemma. – Using Parseval equality, for $E_j(\hbar) \in J_{2, cl}$ we have:

$$\sum_{E_k(\hbar) \in J_{1, cl}} |A_{jk}(\hbar)|^2 \exp(-it\,\omega_{jk}(\hbar)) = \langle \varphi_j, A(t, \hbar)\, \Pi_{P(\hbar)}(J_{1, cl})\, A(\hbar)\, \varphi_j \rangle \tag{43}$$

But we have from localization properties of χ:

$$\begin{aligned} &\langle \varphi_j, A(t, \hbar)\, \Pi_{P(\hbar)}(J_{1, cl})\, A(\hbar)\, \varphi_j \rangle \\ &\quad = \langle \varphi_j, A(t, \hbar)\, \chi(P(\hbar))\, A(\hbar)\, \varphi_j \rangle \\ &\qquad + \langle \varphi_j, A(t, \hbar)\, \Pi_{P(\hbar)}(J)\, [A(\hbar), \chi(P(\hbar))]\, \varphi_j \rangle \end{aligned} \tag{44}$$

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 $\theta_T(t) = \frac{1}{T}\theta\left(\frac{t}{T}\right)$. Here we choose $\hat{\theta}(\lambda) = \left(\frac{\sin\lambda}{\lambda}\right)^2$

So from (42) we have:

$$\sum_{E_k \in J_{cl}} |A_{jk}(\hbar)|^2\, \hat{\theta}_T(\omega_{jk}(\hbar) - \tau) = \int_{\mathbb{R}} e^{it\alpha}\, \theta_T(t)\, \langle \varphi_j,\, A(t,\hbar)\,\chi(P(\hbar))\,A(\hbar)\,\varphi_j\rangle\, dt + O(\hbar) \tag{45}$$

with $O(\hbar)$ uniform in $T > 0$, $\tau \in \mathbb{R}$ and $E_j(\hbar) \in \Lambda(\hbar)$.

The calculus on $\hbar$-admissible operators [33] 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 for some $\hbar_{\varepsilon,T} > 0$:

$$\begin{gathered} |\langle \varphi_j,\, A(t,\hbar)\,\chi(P(\hbar))\,A(\hbar)\,\varphi_j\rangle - C_a(E,t)| < \frac{\varepsilon}{2}, \\ \forall \hbar \in]0, \hbar_{\varepsilon,T}], \quad \forall t \in [-T^2, T^2] \quad \text{and} \quad j \in M(\hbar) \end{gathered} \tag{46}$$

Then we use (45), splitting the integral according $|t| < T^2$ and $|t| > T^2$ and using (46), we get, for some $\gamma > 0$, independent of $\hbar$, ε, T, τ:

$$|A_{jk}(\hbar)|^2\, \hat{\theta}_T(\omega_{jk}(\hbar) - \tau) \leq \int_{\mathbb{R}} |\theta(u)\cdot C_a(E, Tu)|\, du + \frac{\varepsilon}{2} + \gamma \int_{|u| \geq T} |\theta(u)|\, du \tag{47}$$

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

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

hence there exists $T_\varepsilon > 0$ such that:

$$\begin{gathered} |A_{jk}(\hbar)|^2\, \hat{\theta}_{T_\varepsilon}(\omega_{jk}(\hbar) - \tau) \leq \varepsilon, \qquad \forall \hbar \in]0, \hbar_\varepsilon[\ (\hbar_\varepsilon := \hbar_{\varepsilon, T_\varepsilon}); \\ \forall (j,k) \in M(\hbar) \times \Lambda(\hbar), \quad \forall \alpha \in \mathbb{R} \end{gathered} \tag{48}$$

The estimates (48) being uniform in τ we can take $\tau = \omega_{jk}(\hbar)$ so we get

$$|A_{jk}(\hbar)|^2 \le \varepsilon, \qquad \forall \hbar \in]0,\, \hbar_\varepsilon[, \quad \forall (j,\, k) \in M(\hbar) \times \Lambda(\hbar) \tag{49}$$

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 notation, we have:

$$\mathcal{V}_{\Omega(\hbar)}(A) \le \frac{\pi^2}{4}\, \frac{1}{\#\Omega(\hbar)} \sum_{\omega_{jk}(\hbar)\, T<\pi/2,\, E_j \in I(\hbar),\, E_k \in J_{cl}} \times |A_{jk}(\hbar)|^2 \left| \frac{\sin((\omega_{jk}-\tau)\, T)}{(\omega_{jk}-\tau)\, T} \right|^2 \tag{50}$$

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

Then we get, using again the Lemma 4.1:

$$\mathcal{V}_{\Omega(\hbar)}(A) \le c \cdot \frac{1}{\#\Lambda(\hbar)} \sum_{j \in \Lambda(\hbar)} \int_{\mathbb{R}} e^{it\tau}\, \theta_T(t) \times \langle \varphi_j,\, A(t,\, \hbar))\, \chi(P(\hbar)) A(\hbar)\, \varphi_j \rangle\, dt + O(\hbar) \tag{51}$$

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

From (51) the second part of the Theorem 3.7 is obtained using the same arguments as in the first part. ■

Smooth Unbounded Observables. – First of all we have to give a rigorous meaning to the matrix elements $A_{jk}(\hbar)$ for $A(\hbar) := \mathrm{op}_\hbar^w(a)$ not necessarily bounded. The answer follows easily from the lemma:

LEMMA 4.2. – *Let us assume the hypotheses* (H_1) *to* (H_5) *for the Hamiltonian* $P(\hbar)$. *Let* $\chi_0 \in C_0^\infty(I_{cl})$ *and* $a \in S_m$, $m \in \mathbb{N}$. *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 $\chi \in C_0^\infty(I_{cl})$ such that $\chi \equiv 1$ on the support of χ_0. We recall the following result concerning the functional calculus (*see* [17], [6]).

$$\chi(P(\hbar)) = \mathrm{op}_\hbar^w(p_\chi) + \hbar\, \mathrm{op}_\hbar^w(r_\chi(\hbar)) \tag{52}$$

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

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

where C is independent of $\hbar$ and (x, ξ).

For every $\varphi \in \mathcal{S}(\mathbb{R}^n)$ we have:

$$\begin{aligned} A(\hbar)\chi_0(P(\hbar))\varphi &= A(\hbar)\chi(P(\hbar))\chi_0(P(\hbar))\varphi \\ &= A(\hbar)\operatorname{op}_\hbar^w(p_\chi)\,\chi_0(P(\hbar))\,\varphi \\ &\quad + \hbar A(\hbar)\operatorname{op}_\hbar^w(r_\chi(\hbar))\chi_0(P(\hbar))\,\varphi \end{aligned} \tag{53}$$

Let us introduce a commutator:

$$A(\hbar)\operatorname{op}_\hbar^w(r_\chi(\hbar)) = \operatorname{op}_\hbar^w(r_\chi(\hbar)A(\hbar)) + [A(\hbar), \operatorname{op}_\hbar^w(r_\chi(\hbar))] \tag{54}$$

Now, using the rule on the symbolic calculus for Weyl quantization (*see* [33], [6]), we get:

$$\hbar^{-1}[A(\hbar), \operatorname{op}_\hbar^w(r_\chi(\hbar))] = \operatorname{op}^w(\hbar\, b(\hbar)) \tag{55}$$

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

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

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

$$\|A(\hbar)\chi_0(P(\hbar))\varphi\| \le C_1\|\varphi\| + C_2\hbar\,\|A(\hbar)\chi_0(P(\hbar))\varphi\| \tag{56}$$

Then we get the result under the condition $C_2\hbar \le \frac{1}{2}$ on $\hbar$.

We can now extend the result for $m \ge 2$ by an induction argument. Indeed, if $a \in S_m$ then the symbol $b(\hbar)$ defined in (55) belongs to $[S_{m-1}]$. So the induction is clear. ■

The extension of Theorems 3.5 and 3.7 follows easily. From (55) we have:

$$\chi_0(P(\hbar)) \cdot A(\hbar) \cdot \chi_0(P(\hbar)) = \operatorname{op}_\hbar^w(p_{\chi_0})A(\hbar) \cdot \chi_0(P(\hbar)) + O(\hbar)$$

Using the composition rule for $\hbar$-dependent pseudodifferential operators we get:

$$\operatorname{op}_\hbar^w(p_{\chi_0})A(\hbar) \cdot \chi_0(P(\hbar)) = \operatorname{op}_\hbar^w(p_{\chi_0}^2 \cdot a) + O(\hbar)$$

Hence we have:

$$\langle \varphi_j,\, A(\hbar)\,\varphi_k\rangle = \langle \varphi_j,\, \mathrm{op}_\hbar^w\,(p_{\chi_0}^2 \cdot a)\,\varphi_k\rangle + O(\hbar)$$

with $p_{\chi_0}^2 \cdot a \in \mathcal{B}_\infty$. ■

Non Smooth Observables. – Let us consider first the extension of Theorem 3.7 (i). Knowing that the $d\mu_{jk}$ are Radon measures, it is not difficult to see that the conclusions of Theorem 3.7 (i) hold for $A(\hbar) = \mathrm{op}_\hbar^{AW}(a)$ with a continuous and bounded on $\mathbb{R}^{2n}$. It is sufficient to consider only real valued observables. We have the elementary identity:

$$\langle A\,\varphi_j,\, \varphi_k\rangle = \frac{1}{4}\left(\langle A\,(\varphi_j + \varphi_k),\, \varphi_j + \varphi_k\rangle - \langle A\,(\varphi_j - \varphi_k),\, \varphi_j - \varphi_k\rangle\right) \quad (57)$$

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

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

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

$$\left\{\int a\,\mathrm{d}\mu_{jk} \to 0\right\} \quad \Leftrightarrow \quad \left\{\int a\,\mathrm{d}\nu_{jk}^{\pm} \to 2\,\langle a\rangle_E\right\} \quad (58)$$

If a is a real bounded Borel observable then for any $\varepsilon > 0$ we can find $a_1,\, a_2 \in \mathcal{B}_\infty$ such that:

$$a_1 \le a \le a_2, \qquad \text{and} \qquad \int (a_2 - a_1)\, d\sigma_E \le \varepsilon \quad (59)$$

So we have:

$$\int a_1\, d\nu_{jk}^{\pm} \le \int a d\nu_{jk}^{\pm} \le \int a_2\, d\nu_{jk}^{\pm} \quad (60)$$

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

$$\int a_i\, d\nu_{jk}^{\pm} \to 2 \int a_i\, d\sigma_E \quad \text{as } \hbar \searrow 0, \qquad (j,\, k) \in M(\hbar) \times M(\hbar) \quad (61)$$

Hence from [(59), (60), (61)] we get:

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

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.

The other statements are easily proved in the same way. ■

Proof of Theorem 1.1. – Let us recall that here $P(\hbar) = -\hbar^2 \Delta + V(x)$ where V is a smooth electric potential such that $\liminf_{|x| \to +\infty} V(x) > E$. To prove the theorem we shall compare $P(\hbar)$ with $\tilde{P}(\hbar) := -\hbar^2 \Delta + \tilde{V}(x)$ such that P and $\tilde{P}$ have the same symbol in a neighborhood of $\{x, V(x) \leq E\}$ and $\tilde{P}(\hbar)$ satisfies the assumptions (H_1) to (H_4) (*see* Example I). Let us define:

$$\Omega_\eta = \{x \in \mathbb{R}^n, V(x) < E + \eta\}$$
$$X_\eta \in C_0^\infty(\Omega_\eta), \; X_\eta(x) = 1 \quad \text{for} \quad x \in \Omega_{\eta/2}$$
$$\tilde{V}(x) = X_\eta(x) V(x) + (1 - X_\eta(x))(E + \eta)$$

To compare the matrix elements associated with $P(\hbar)$ and $\tilde{P}(\hbar)$, we shall use the semi-classical exponential decay for the bound states of these Hamiltonians proved in [19], [1].

Firstly note that we can shift the energy interval $I(\hbar) = [\alpha(\hbar), \beta(\hbar)]$ by some $O(\hbar^2)$ such that there exists $\delta(\hbar)$ not exponentially small in $\hbar$, and $(I(\hbar) + [-2\delta(\hbar), 2\delta(\hbar)]) \setminus I(\hbar)$ does not meet the spectra of $P(\hbar)$ and $\tilde{P}(\hbar)$.

Let us denote by (E_j, φ_j) the spectral data for $P(\hbar)$ and by $\mathcal{E}$ the subspace spanned by $\{\varphi_j, E_j \in I(\hbar)\}$. The analog spectral data for $\tilde{P}(\hbar)$ are overlined by a tilde.

Let d_V be the Agmon distance to the well: $U = \{x \in \mathbb{R}^n, V(x) \leq E\}$ and $d(x) := \min\{d_V(x), d_{\tilde{V}}(x)\}$. We have:

$$\forall \varepsilon > 0, \quad \exists C_\varepsilon$$
$$\text{such that} \quad |\varphi_j(x)| + |\tilde{\varphi}_j(x)| \leq C_\varepsilon \exp\left(\frac{\varepsilon - d(x)}{\hbar}\right) \tag{62}$$

Furthermore it results from [19] that the spaces $\mathcal{E}$ and $\tilde{\mathcal{E}}$ are exponentially closed. It entails that we have:

$$\varphi_j = \sum_k a_{jk} \tilde{\varphi}_k + O(\exp(-\sigma/\hbar)), \qquad (\text{for some } \sigma > 0) \tag{63}$$

where the matrix $\{a_{jk}\}$ satisfies

$$\sum_k a_{km} \bar{a}_{kl} = \delta_{ml} + O(\exp(-\sigma/\hbar)) \tag{64}$$

Moreover for $\hbar$ small enough there exists a bijection $b : \tilde{\Lambda}(\hbar) \to \Lambda(\hbar)$, exponentially closed to the identity.

Let $A(\hbar) = \mathrm{op}_\hbar^w(a)\,(a \in \mathcal{B}_\infty)$ be an observable and let us denote: $A_{jk}(\hbar) = \langle A\varphi_j, \varphi_k\rangle$, $\tilde{A}_{jk}(\hbar) = \langle A\tilde{\varphi}_j, \tilde{\varphi}_k\rangle$. From (64) we get easily:

$$\lim_{\hbar \searrow 0} \left(\frac{\sum_{j \in \Lambda(\hbar)} A_{jj}(\hbar) - \tilde{A}_{jj}(\hbar)}{\#\Lambda(\hbar)} \right) = 0 \tag{65}$$

Let us introduce $\chi \in C_0^\infty(]E - \eta, E + \eta[)$, $\chi \equiv 1$ close to E, and $\tilde{\chi} \in C_0^\infty(]E - 2\eta, E + 2\eta[)$, such that $\tilde{\chi} \equiv 1$ on supp (χ). Now, Theorem 1.1 can be deduced easily by revisiting the proof of Theorem 3.5 and 3.7 and using the following:

LEMMA 4.3. – *With the above notations, we have:*

$$\chi(P(\hbar)) = \chi(\tilde{P}(\hbar)) + O(\hbar^\infty) \tag{66}$$

and for every $T > 0$ *we have:*

$$\exp\left\{-\frac{it}{\hbar} P(\hbar)\,\chi(P(\hbar))\right\}$$

$$= \exp\left\{-\frac{it}{\hbar} \tilde{P}(\hbar)\,\tilde{\chi}(\tilde{P}(\hbar))\right\} + O(\hbar^\infty) \tag{67}$$

uniformly for $|t| \leq T$.

Proof. – Using the usual construction for the functional calculus [33] we get:

$$X(x)\,\chi(P(\hbar)) = X(x)\,\chi(\tilde{P}(\hbar)) + O(\hbar^\infty)$$

But we have:

$$(1 - X(x))\,\chi(P(\hbar))\,u = \sum \chi(E_j)\,\langle u, \varphi_j\rangle\,(1 - X(x))\,\varphi_j$$

Using the exponential decay for the eigenfunctions we have:

$$(1 - X(x))\,\chi(P(\hbar)) = (1 - X(x))\,\chi(\tilde{P}(\hbar)) = O(\hbar^\infty)$$

So we get the first equality.

The second estimate is deduced from the first by the Duhamel principle (time dependent perturbation). ■

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 phenomenom called the levels repulsion [4]. Let us introduce the following assumption on the autocorrelation function:

(H_9^*) $\Gamma_E := \int_{\mathbf{R}} |C_a(E, t)| dt < +\infty.$

Then using the function $\theta(t) = \mathrm{e}^{-\omega|t|}$, $\omega > 0$, we get, as above, that:

$$\forall \varepsilon > 0, \quad \forall \omega > 0, \quad \exists \hbar_{\varepsilon, \omega} > 0,$$

such that

$$|A_{jk}(\hbar)|^2 \frac{\omega}{\omega^2 + \omega_{jk}^2} \leq \pi \int_{\mathbf{R}} C_a(E, t)\, dt + \varepsilon,$$
$$\forall \hbar \in]0, \hbar_{\varepsilon, \omega}[, \quad \forall j \in M(\hbar), \quad \forall k \in \Lambda(\hbar) \tag{68}$$

From (68) we get easily:

PROPOSITION 4.4. – *Under the conditions of* (68), *for every* $K > \pi \Gamma_E - \varepsilon$, *we have:*

$$\{|A_{jk}(\hbar)|^2 \geq K\omega\}$$
$$\Rightarrow \quad \left\{|E_j(\hbar) - E_k(\hbar)|^2 \geq \left(\frac{K - \pi\Gamma_E - \varepsilon}{(\pi\Gamma_E + \varepsilon)}\right)(\hbar\omega)^2\right\} \tag{69}$$

REMARK 4.5. – *The assumption* (H_9^*) *is not completely absurd. In* [29], [34] *the authors consider dynamical systems such that the Fourier transform 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 (PROOF OF THEOREM 3.10)

Let us assume that $\mathrm{Supp}(\hat{f}) \subseteq]-T_0, T_0[$ with $T_0 > 0$ is small enough, and $\mathrm{Supp}(\hat{g})$ is compact. We assume the $P(\hbar)$ satisfies (H_1) to (H_5). The variance considered by Wilkinson [37] is defined by:

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

In fact, Wilkinson considers the case where $\hat{f}$, $\hat{g}$ are Gaussians which seems difficult to treat mathematically. If Supp $(\hat{f})$ is compact but not small, *see* Remark 3.12.

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_{cl} by a smooth one.

LEMMA 5.1. – *Let* $\varepsilon_0 > 0$ *be such that* $[E - \varepsilon_0, E + \varepsilon_0] \subset J_{cl}$ *and* $\chi \in C_0^\infty(J_{cl})$, $\chi = 1$ *on* $[E - \varepsilon_0, E + \varepsilon_0]$, $0 \leq \chi \leq 1$. *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:*

$$S_{(f,\,g)}(\hbar, E, \Delta E) := \sum_{j,\,k} |A_{\chi,\,jk}(\hbar)|^2 \times f_\hbar\left(E - \frac{1}{2}(E_j + E_k)\right) g_\hbar(\Delta E - (E_j + E_k)) + O(\hbar^\infty) \quad (70)$$

Proof. – We have:

$$\begin{aligned} &S_{(f,\,g)}(\hbar, E, \Delta E) - \sum_{j,\,k} |A_{\chi,\,jk}(\hbar)|^2 \\ &\quad \times f_\hbar\left(E - \frac{1}{2}(E_j + E_k)\right) g_\hbar(\Delta E - (E_j + E_k)) \\ &= \sum_{j,\,k} (1 - \chi(E_j)^2\,\chi(E_k)^2)\,|A_{jk}(\hbar)|^2 \\ &\quad \times f_\hbar\left(E - \frac{1}{2}(E_j + E_k)\right) g_\hbar(\Delta E - (E_j + E_k)) \end{aligned} \quad (71)$$

We split the r.h.s of the last equality into two terms according $|E_k - E_j| > \varepsilon_0$ or $|E_k - E_j| \leq \varepsilon_0$. 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 $|E_k - E_j| \leq \varepsilon_0$ we have:

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

But $f \in \mathcal{S}(\mathbb{R})$ (the Schwartz space) so we see that the contribution of $|E_k - E_j| \leq \varepsilon_0$ is $O(\hbar^\infty)$ and (71) gives the lemma. ■

We continue to denote by $S_{(f,\,g)}(\hbar,\, E,\, \Delta E)$ the approximation of the variance mod $(O(\hbar^{\infty}))$ given by the above lemma.

By inverse Fourier transform, we get:

$$f_\hbar\left(E - \frac{1}{2}(E_j + E_k)\right) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \hat{f}(\Delta t)\exp\left(i\frac{\Delta t}{\hbar}\left(E - \frac{1}{2}(E_j + E_k)\right)\right) d\Delta t \qquad (72)$$

$$g_\hbar(\Delta E - (E_j - E_k)) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} \hat{g}(t)\exp\left(i\frac{t}{\hbar}(\Delta E - (E_j - E_k))\right) dt \qquad (73)$$

Now by plugging (72) and (73) in (71), and using Parseval relation for the orthonormal system $\{\varphi_j\}$, we get after computations:

$$S_{(f,\,g)}(\hbar,\, E,\, \Delta E) = \frac{1}{(2\pi\hbar)^2}\,\mathrm{tr}\left\{\int\!\!\int \hat{g}(t)\exp\left(\frac{i}{\hbar}t\,\Delta E\right) A_\chi(\hbar)\hat{f}(\Delta t) \times \exp\left(\frac{-i\,\Delta t}{\hbar}(P(\hbar) - E)\right) \times A_\chi\left(\hbar,\, \frac{\Delta t}{2} - t\right)(\hbar)\, dt\, d\Delta t\right\} \qquad (74)$$

To achieve the proof of the Theorem 3.10 we use the W.K.B. method along the same lines as in [17], [33], [28] 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 $A_\chi\left(\hbar,\, \frac{\Delta t}{2} - t\right)$ are $\hbar$-admissible operators with weight 1 (*see* [33]). Secondly if $\tilde{\chi} \in C_0^\infty(J_{cl})$ is an other cut-off such that $\tilde{\chi} = 1$ on Supp (χ) then we have:

$$\chi(P(\hbar))\exp\left(\frac{i\tau}{\hbar}P(\hbar)\right) = \chi(P(\hbar))\exp\left(\frac{i\tau}{\hbar}\tilde{\chi}(P(\hbar))\cdot P(\hbar)\right)$$

So nothing is changed if we replace in the exponent $P(\hbar)$ by $\tilde{\chi}(P(\hbar))\cdot P(\hbar)$ 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:

$$\begin{aligned} \partial_\tau \phi(\tau, x, \eta) + p_0(x, \partial_x \phi(\tau, x, \eta)) = 0 \\ \phi(0, x, \eta) = x \cdot \eta \end{aligned} \tag{75}$$

and the transport equations (*see* [33]).

In this way wet get, for $|\tau|$ small enough, accurate approximations $U_{\text{app}}(\tau, \hbar)$ for $U(\tau, \hbar)$ such that:

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

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

$$U_{\text{app}}(\tau, \hbar)(x, y) = (2\pi\hbar)^{-n} \int\int \exp\left(\frac{i}{\hbar}(\phi(\tau, x, \eta) - x \cdot \eta\right) \times (\sum_{j \geq 0} \hbar^j\, u_j(\tau, x, \eta))\, d\eta \tag{76}$$

Hence using the computation rules on $\hbar$-admissible operators [33], finally, the proof of the Theorem 3.10 is achieved by applying the stationary phase theorem to integrals like:

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

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

$$\begin{aligned} & S_0(\hbar, E, \Delta E) \\ & = (2\pi\hbar)^{-n} \int\int\int \hat{g}(t) \exp\left(\frac{i}{\hbar}\,t\,\Delta E\right) \chi^4(p_0(x, \partial_x \phi(\tau; x, \eta))) \\ & \quad \times a(x, \partial_x \phi(\tau; x, \eta))\, a(\Phi^{\tau/2-t}(x, \partial_x \phi(\tau; x, \eta))) \\ & \quad \times \hat{f}(\tau) \exp\left(\frac{i}{\hbar}(\phi(\tau; x, \eta) - x \cdot \eta + \tau E)\right) d\tau\, dx\, d\eta\, dt \end{aligned} \tag{77}$$

Supp $(\hat{f})$ being small enough, the stationary points in the integral (77) in the variables (τ, x, η) are defined by the equations:

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

So, the computation of the first term in the stationary phase theorem [33] gives:

$$\begin{aligned} S_0(\hbar, E, \Delta E) &= (2\pi\hbar)^{-n-1}\hat{f}(0)\int_{\mathbb{R}}\left(\int_{\Sigma_E} a(x, \eta)\, a(\Phi^t(x, \eta))\, d\sigma_E\right) \\ &\times \hat{g}(t)\exp\left(\frac{it}{\hbar}\Delta E\right) dt + \sum_{j\geq 1}\hbar^{-n-1+j} c_j\left(E, \frac{\Delta E}{\hbar}\right) \end{aligned} \tag{78}$$

REMARK 5.2. – *As for Theorems* 3.5 *and* 3.7, *if* $P(\hbar) = -\hbar^2\Delta + V$, *Theorem* 3.10 *is valid without any polynomial control on* V *at infinity.*

6. OTHER RELATED RESULTS

A. Level spacing and non periodical trajectories

Here, we shall prove a quantum mechanical analog of a simple and beautiful result due to Helton [20] (*see* also [13]) for elliptic operators on compact manifolds.

THEOREM 6.1. – *Under the assumptions* (H_1) *to* (H_5) *for* $P(\hbar)$, *assume furthermore that there exists on* Σ_E *a non periodical trajectory for the flow* Φ^t. *Then for every* $c > 0$, $0 < \delta < 1$ *and every* $\hbar_0 > 0$ *the set:*

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

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

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 $\chi \in C_0^\infty(]-c, c[)$ such that $\int \chi^2(\lambda)\, d\lambda = 1$. Following Helton [20] we consider the operator:

$$A_{E,f}(\hbar) = \int \hat{f}(t)\, U(-t, \hbar)\, A_E(\hbar)\, U(t, \hbar)\, dt \tag{79}$$

with

$$A_E(\hbar) = \frac{1}{\hbar^{1-\delta}}\chi\left(\frac{P(\hbar) - E}{\hbar^{1-\delta}}\right)\operatorname{op}_\hbar^w(a)\,\chi\left(\frac{P(\hbar) - E}{\hbar^{1-\delta}}\right), \quad a \in C_0^\infty(\mathbb{R}^{2n}).$$

By inverse Fourier transform, we have also:

$$A_{E,f}(\hbar) = \frac{2\pi}{\hbar^{1-\delta}} \sum_{j,k} f(\omega_{jk}(\hbar)) \times \chi\left(\frac{E_j(\hbar) - E}{\hbar^{1-\delta}}\right) \chi\left(\frac{E_k(\hbar) - E}{\hbar^{1-\delta}}\right) \Pi_k A(\hbar) \Pi_j \quad (80)$$

where Π_k is the projection on the state φ_k. From (79), (80) we have:

$$\int \hat{f}(t) U(-t, \hbar) A_E(\hbar) U(t, \hbar) dt = 0, \qquad \forall a \in \mathcal{B}_\infty \quad (81)$$

From (81) we should 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 ([33]) and functional calculus with parameters for pseudodifferential operators ([6]). We test (81) by computing the trace of the product by any operator $\mathrm{op}_\hbar^w(b)$, $b \in \mathcal{B}_\infty$. We get easily:

$$\lim_{\hbar \searrow 0} (2\pi\hbar)^n \cdot \mathrm{Tr}(A_{E,f}(\hbar) \cdot \mathrm{op}_\hbar^w(b)) = \lim_{\hbar \searrow 0} \int\int \hat{f}(t) a(\Phi^t(z)) \frac{1}{\hbar^{1-\delta}} \chi^2\left(\frac{p(z) - E}{\hbar^{1-\delta}}\right) b(z)\, dz\, dt \quad (82)$$

So we get

$$\int \hat{f}(t) a(\Phi^t(z))\, dt = 0, \qquad \forall z \in \Sigma_E \quad (83)$$

Now, choose $z_0 \in \Sigma_E$ such that $t \to \Phi^t(z_0)$ is not periodic, we should like to deduce from (83) that $\hat{f} \equiv 0$. Using the same arguments as in [18] (p. 866-867) we can easily get 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 form $]-T, T[\times D_{\rho_T}(z_0)$ onto an open neighborhood $\mathcal{N}_T$ of the curve: $\{\Phi^t(z_0), -T < t < T\}$; where $D_{\rho_T}(z_0)$ is the euclidean ball with center z_0 and radius ρ_T in the orthogonal plane to the curve at time 0.*

Furthermore, for every g in $C_0^\infty(]-T, T[)$ we can construct some $a \in C_0^\infty(\mathbb{R}^{2n})$ such that: $g(t) = a(\Phi^t(z_0)) + h(t)$, $\forall t \in \mathbb{R}$ with:

(i) $\mathrm{Supp}(h) \cap\,]-T, T[= \emptyset$,

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

So, with the above notations, using the above lemma and (83) we get:

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

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

REMARK 6.3. – *Using very recent results obtained by S. Dozias* [8] *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 exists* $\gamma_0, \gamma_1, C \in \mathbb{R}$; $\varepsilon > 0$ *such that:*

$$\begin{aligned}&\text{spectrum}\,[P(\hbar)] \cap [E - c\,\hbar^{1-\delta},\, E + c\,\hbar^{1-\delta}] \\ &\quad \subseteq \bigcup_{k\in\mathbb{Z}} [\gamma_0 + \gamma_1\, k\,\hbar - C\,\hbar^{1+\varepsilon},\, \gamma_0 + \gamma_1\, k\,\hbar + C\,\hbar^{1+\varepsilon}]\end{aligned} \tag{84}$$

Clearly (84) *entails that* $\mathcal{T}_{E,\delta}$ *is not dense in* $\mathbb{R}$.

B. Sum rules and classical limits

We want to reexamine the literature on this subject, and make the connection to the technique used in part 4 of this paper.

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

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

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:

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

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

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

$$\begin{aligned}&\hat{\mathcal{R}}_{A,B;j,\hbar}(t) = \langle \varphi_j,\, A(t,\,\hbar)\,\chi(P(\hbar))\,B(\hbar)\,\varphi_j\rangle + O(\hbar^\infty),\\ &\text{for } \mathrm{E_j}(\hbar) \in \tilde{\mathrm{J}}_{\mathrm{cl}},\end{aligned} \tag{85}$$

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

Proof. – We denote $J_{cl} = [\alpha,\, \beta]$ and $\tilde{J}_{cl} = [\lambda,\, \mu]$ 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 $\chi_N \in C_0^\infty\left(\left]\lambda - \frac{\varepsilon}{2^{N-1}},\, \mu + \frac{\varepsilon}{2^{N-1}}\right[\right)$, $\chi_N \equiv 1$ on $\left[\lambda - \frac{\varepsilon}{2^N},\, \mu + \frac{\varepsilon}{2^N}\right]$.

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

$$\begin{aligned}&\langle \varphi_j,\, A(t)\,\Pi_P(J_{cl})\,B\,\varphi_j\rangle\\ &\quad = \langle \varphi_j,\, A(t)\,\chi_0(P)\,B\,\varphi_j\rangle + \langle \varphi_j,\, A(t)\,\Pi_P(J_{cl})\,[B,\, \chi_0(P)]\,\varphi_j\rangle\end{aligned} \tag{86}$$

the last term in (86) is $O(\hbar)$. To improve this estimate we apply (86) to it remarking that B is replaced by $[A,\, \chi_0(P)]$. So we get:

$$\begin{aligned}&\langle \varphi_j,\, A(t)\,\Pi_P(J_{cl})\,[B,\, \chi_0(P)]\,\varphi_j\rangle\\ &\quad = \langle \varphi_j,\, A(t)\,\chi_1(P)\,[B,\, \chi_0(P)]\,\varphi_j\rangle\\ &\qquad + \langle \varphi_j,\, A(t)\,\Pi_P(J_{cl})\,[[B,\, \chi_0(P)],\, \chi_1]\,\varphi_j\rangle\end{aligned} \tag{87}$$

Using standard rules for the $\hbar$ admissible calculus [33] 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 (87) is $O(\hbar^2)$. Clearly, the procedure can be iterated and at the step N we get:

$$\langle \varphi_j, A(t)\, \Pi_P(J_{cl})\, B\, \varphi_j \rangle = \langle \varphi_j, A(t)\, \chi_0(P)\, B\, \varphi_j \rangle + O(\hbar^N) \tag{88}$$

■

Let us introduce the classical correlation:

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

By applying [16] 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:*

$$\frac{d^l}{dt^l} \hat{\mathcal{R}}_{A,B;j,\hbar}(t) = \frac{d^l}{dt^l} C_{a,b}(E, t) + o(\hbar), \tag{89}$$

as $\hbar \searrow 0$ for $j \in M(\hbar)$ and uniformly in $t \in [-T, T]$

Proof. – We have only to check the uniformity in $t \in [-T, T]$. It is sufficient to consider the case $l = 0$. 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* $C_b(\mathbb{R}^m)$ *(bounded and continuous functions on* $\mathbb{R}^m$ *with the supremum norm). Then we have:*

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

uniformly in $t \in [-T, T]$

REMARK 6.7. – *The semi-classical sum rules* ([10], [30]) *concerning*

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

are obvious consequences of (89) *by computing* $\frac{d^l}{dt^l} C_{a,a}(E, t)$ *at* $t = 0$. *For example we have:*

$$\frac{d}{dt} C_{a,b}(E, t) = \int_{\Sigma_E} \bar{b}(z)\, \{a, p_0\}\, (\Phi^t(z))\, d\sigma_E(z) \tag{90}$$

$$\frac{d^2}{dt^2} C_{a,b}(E, t) = -\int_{\Sigma} \overline{\{b, p_0\}}(z) \cdot \{a, p_0\}(\Phi^t(z))\, d\sigma_E(z) \tag{91}$$

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

REMARK 6.8. – *In* [31] *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:*

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

where PV *is the Cauchy principal value.*

By considering the cases r *even and* r *odd we easily get that, for* $\omega \neq 0$, $\int_{-\infty}^{+\infty} t^r \cdot \sin(\omega t)\, dt = 0$.

If the classical system is mixing in the classical limit, applying the Theorem 6.5, *we have:*

$$\lim_{[\hbar \searrow 0,\, j \in M(\hbar)]} Q_j(t, \hbar) = \int_{\Sigma_E} (a(\Phi^t(z))\, b(z) - b(\Phi^t(z))\, a(z))\, d\sigma_E(z) := \Gamma_{a,b}(t, E), \tag{92}$$

$\Gamma_{a,b}(\cdot, E)$ *is an odd function. If furthermore we have exponential decay for the correlations as in* [29], [34] *then the Fourier transform of* $\Gamma_{a,b}(\cdot, E)$ *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* $\Gamma_{a,b}(\cdot, E) \equiv 0$. *So, as claimed in* [31], *if* $\Gamma_{a,b}(t, E) \neq 0$ *for some time* t, *this shows that for every large times, quantum and classical evolution are very different.*

A APPENDIX

Families of energies transition with a classical limit

The aim of this section is to construct examples of non diagonal matrix elements satisfying assumptions (α), (β), (γ) 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:

$$I(\hbar) = [\alpha(\hbar), \beta(\hbar)], \qquad \text{with} \quad \alpha(\hbar) < E < \beta(\hbar)$$

$$\lambda(\hbar) = \beta(\hbar) - \alpha(\hbar) \lim_{\hbar \searrow 0} \lambda(\hbar) = 0 \quad \text{and} \quad \lambda(\hbar) \geq \varepsilon_2 \hbar,$$

$$\text{for some} \quad \varepsilon_2 > 0$$

$$\Lambda(\hbar) = \{j, E_j(\hbar) \in I(\hbar)\}; \ \omega_{jk}(\hbar) = \left(\frac{E_k(\hbar) - E_j(\hbar)}{\hbar}\right)$$

$$|\Sigma_E| = \int_{\Sigma_E} \frac{d\Sigma_E}{|\nabla p_0|}$$

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

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

Our main tool will be the following result stated in [16]:

THEOREM A.1 (see *also* [28]). – *There exists* $\gamma > 0$, *depending only on the fixed energy* E *and* p *such that:*

$$\forall \varepsilon > 0, \quad \exists \eta_\varepsilon > 0, \quad \exists C_\varepsilon > 0,$$

$$\text{such that for all interval} \quad I \subseteq]E - \eta, E + \eta[, \qquad \forall \hbar \in]0, 1], \tag{93}$$

we have

$$|\#\{j;\ E_j(\hbar) \in I\} - (2\pi\hbar)^{-n} \operatorname{Vol}_{\mathbb{R}^{2n}} p_0^{-1}(I)| \leq \gamma\varepsilon\hbar^{1-n} + C_\varepsilon \hbar^{2-n}$$

We first prove the following lemma:

LEMMA A.2. – *For every* $\delta > 0$ *there exists* $\hbar_\delta > 0$ *such that:*

$$\frac{1}{2}(2\pi\hbar)^{-2n}\delta\hbar\lambda(\hbar)|\Sigma_E|^2 \leq \#\Omega(\tau, \delta, \hbar) \leq \frac{3}{2}(2\pi\hbar)^{-2n}\delta\hbar\lambda(\hbar)|\Sigma_E|^2 \tag{94}$$

under the conditions:

$$0 \le \hbar \le \hbar_\delta, \qquad \left(|\tau| + \frac{\delta}{2}\right) \hbar \le \frac{4}{5} \lambda(\hbar)$$

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

$$\#\Omega(\tau, \delta, \hbar) \ge \# \Bigg\{ (j, k);\ E_j(\hbar) \in I(\hbar)$$

$$\cap \left[\alpha(\hbar) - \left(\tau - \frac{\delta}{2}\right)\hbar,\ \beta(\hbar) - \left(\tau + \frac{\delta}{2}\right)\hbar\right],\ |\omega_{jk}(\hbar) - \tau| \le \frac{\delta}{2}\Bigg\} \tag{95}$$

In what follows γ is a "generic constant" independant of $\hbar$ and ε.

Using Theorem A.1 we have the following estimate:

$$\#\left\{k;\ |\omega_{jk}(\hbar) - \tau| \le \frac{\delta}{2}\right\}$$
$$\ge (2\pi\hbar)^{-n}(\delta\hbar|\Sigma_E| - \gamma\delta\hbar\lambda(\hbar) - \gamma\varepsilon\hbar) \tag{96}$$

under the conditions:

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

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

$$\mathrm{Vol}_{\mathbb{R}^{2n}}\left(p_0^{-1}\left[E_j(\hbar) + \left(\tau - \frac{\delta}{2}\right)\hbar,\ E_j(\hbar) + \left(\tau + \frac{\delta}{2}\right)\hbar\right]\right.$$
$$\ge \delta\hbar\,|\Sigma_E| - \gamma\,\delta\,\hbar\,\lambda(\hbar)$$

In the same way we have also:

$$\#\left\{j;\ E_j(\hbar) \in \left[\alpha(\hbar),\ \beta(\hbar) - \left(\tau + \frac{\delta}{2}\right)\hbar\right]\right\}$$
$$\ge (2\pi\hbar)^{-n}\left(\lambda(\hbar)\,|\Sigma_E| - \left(\tau + \frac{\delta}{2}\right)\hbar|\Sigma_E| - \gamma\lambda(\hbar)^2\right) \tag{97}$$

Now putting together (96) and (97) and choosing $\varepsilon = \frac{\delta}{\Gamma}$ with Γ large enough, we get the lower bound:

$$\# \Omega(\tau, \delta, \hbar) \geq \frac{1}{2} (2\pi\hbar)^{-2n} \delta\hbar\lambda(\hbar) |\Sigma_E|^2 \tag{98}$$

under the conditions of the lemma. ■

By using the same technique as above (with a more accurate 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* $\hbar \searrow 0$:

$$\# \Omega(\tau, \delta, \hbar) = (2\pi\hbar)^{-2n} \delta\hbar\lambda(\hbar) |\Sigma_E|^2 + o(\hbar^{1-2n}\lambda(\hbar)) \tag{99}$$

Now we come to the main goal of this section which is to prove the existence of non diagonal matrix elements satisfying the assumptions of Theorem 3.7. 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 $N \geq N_0$:

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

Then, using the Lemma A.2 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:

$$\# \Omega_N(\hbar) \geq \frac{C_3}{N} \hbar^{1-2n} \lambda(\hbar) \tag{100}$$

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

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

From (100), for all $\hbar \in]0, \tilde{\hbar}_N]$ we have

$$\# \Omega_N(\hbar) \geq C_3 \hbar^{-n} \lambda(\hbar) \tag{101}$$

Let us define:

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

Clearly $\Omega(\hbar)$ satisfies the assumptions (α) and (β). To check the assumption (γ) we remark that from Theorem A.1 we get easily the asymptotic formula:

$$\lim_{\hbar \searrow 0} \frac{(2\pi\,\hbar)^n \# \Lambda(\hbar)}{\lambda(\hbar)} = |\Sigma_E| \tag{102}$$

■

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(Manuscript received February 8, 1994;
Revised version received July 27, 1994.)