Ann. Henri Poincaré 7 (2006), 1085–1098

1424-0637/061085-14, *published online* 2006-08-30
DOI 10.1007/s00023-006-0277-5

Annales Henri Poincaré

Upper Bounds on the Rate of Quantum Ergodicity

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Abstract. We study the semiclassical behaviour of eigenfunctions of quantum systems with ergodic classical limit. By the quantum ergodicity theorem almost all of these eigenfunctions become equidistributed in a weak sense. We give a simple derivation of an upper bound of order $|\ln \hbar|^{-1}$ on the rate of quantum ergodicity if the classical system is ergodic with a certain rate. In addition we obtain a similar bound on transition amplitudes if the classical system is weak mixing. Both results generalise previous ones by Zelditch.

1. Introduction

The quantum ergodicity theorem by Shnirelman, Zelditch and Colin de Verdière, [Šni74, Zel87, CdV85], states that almost all eigenfunctions of a quantum mechanical Hamilton operator become equidistributed in the semiclassical limit if the underlying classical system is ergodic.

Consider as example an Hamiltonian of the form

$$\mathcal{H} = -\hbar^2 \Delta + V \tag{1}$$

on $L^2(\mathbb{R}^d)$ with a smooth potential satisfying $|\partial^\alpha V(x)| \leq C_\alpha (1+|x|^2)^{m/2}$ for some $m \in \mathbb{R}$ and all $\alpha \in \mathbb{N}^d$. Assume that for a fixed energy E the classical energy-shell $\Sigma_E := \{(\xi, x) \in \mathbb{R}^d \times \mathbb{R}^d \,;\, \xi^2 + V(x) = E\}$ is compact, then the spectrum of $\mathcal{H}$ is discrete in a neighbourhood of E, and we will denote by $N(I(E,\hbar))$ the number of eigenvalues in the interval $I(E,\hbar) := [E - \alpha\hbar, E + \alpha\hbar]$, $\alpha > 0$. If now the Hamiltonian flow generated by $H = \xi^2 + V(x)$ is ergodic on Σ_E then the normalized eigenfunctions ψ_n of $\mathcal{H}$ satisfy

$$\lim_{\hbar \to 0} \frac{1}{N(I(E,\hbar))} \sum_{E_n \in I(E,\hbar)} |\langle \psi_n, \mathrm{Op}[a]\psi_n\rangle - \overline{a}_E|^2 = 0 \tag{2}$$

with $\overline{a}_E := \frac{1}{\mathrm{vol}(\Sigma_E)} \int_{\Sigma_E} a \, \mathrm{d}\mu_E$ and where a is a smooth bounded function on phase space and $\mathrm{Op}[a]$ its Weyl quantization (defined below in (4)). This result is the semiclassical version of the quantum ergodicity theorem, which was derived in [HMR87]. It implies that almost all of the expectation values $\langle\psi_n, \mathrm{Op}[a]\psi_n\rangle$ tend to $\overline{a}_E$ in the limit $\hbar \to 0$, so in this sense the eigenfunctions become equidistributed on the energy-shell.

Our aim is to derive an upper bound on the rate by which the left-hand side of (2) approaches zero. For the eigenfunctions of the Laplacian on manifolds of negative curvature such a bound has been derived by Zelditch [Zel94]. The bound we give is of the same order, so we do not get an improvement on the rate, but the advantage of our method is that it is simpler and uses only ergodicity with a certain rate as condition on the classical flow. Therefore it applies to a larger class of systems. The main input in the proof is the result on the semiclassical propagation of observables up to Ehrenfest time, [BGP99, BR02].

We will now describe the classes of Hamiltonians and observables we consider, see, e.g., [DS99] for more details. We say $a(\hbar, x, \xi) \in S^m$ for $m \in \mathbb{R}$ if a is smooth, satisfies

$$|\partial^\gamma_{x,\xi} a(\hbar, x, \xi)| \leq C_\gamma (1 + |x|^2 + |\xi|^2)^{m/2} \tag{3}$$

for all $\gamma \in \mathbb{N}^{2d}$ and $\hbar \in (0, 1/2]$, and has an asymptotic expansion $a(\hbar, x, \xi) \sim \sum_{n\in\mathbb{N}} \hbar^n a_n(x, \xi)$, i.e., $(a - \sum_{n=0}^{N-1} \hbar^n a_n)\hbar^{-N}$ satisfies (3) for all $N \in \mathbb{N}$. Now let M be a smooth manifold, the set of operators $\Psi^m(M)$ is given by local Weyl quantization of these classes, if $a \in S^m$ in some local chart, then $\mathrm{Op}[a]$ is defined as

$$\mathrm{Op}[a]\psi = \frac{1}{(2\pi\hbar)^d} \iint \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\langle x-y,\xi\rangle} a\big(\hbar, \frac{x+y}{2}, \xi\big)\psi(y)\ \mathrm{d}y\mathrm{d}\xi\ . \tag{4}$$

A general operator $A \in \Psi^m(M)$ is then an operator that is locally of the form (4) with some $a \in S^m$. For sake of simplicity we will in the following always assume that M is either $\mathbb{R}^d$ or a compact manifold and in the case $M = \mathbb{R}^d$ (3) and (4) should be valid globally. Then we do not have to worry about estimates at infinity and if operators are properly supported. The function a is called the local symbol of the operator A and the leading term in the asymptotic expansion of a is called the principal symbol

$$\sigma(A) := a_0\ , \tag{5}$$

the principal symbol can be glued together to a function on T^*M, but the full symbol not. The operators in $\Psi^0(M)$ are bounded on $L^2(M)$ (uniformly in $\hbar$) and will form our basic class of observables.

We will assume that the Hamiltonian $\mathcal{H}$ is a selfadjoint operator in $\mathcal{H} \in \Psi^m(M)$, for some $m > 0$, and denote by Φ^t the Hamiltonian flow on T^*M generated by the principal symbol $H_0 = \sigma(\mathcal{H})$ of $\mathcal{H}$. Let $\Sigma_E := \{(x, \xi) \in T^*M\,;\, H_0(x, \xi) = E\} \subset T^*M$ denote the energy surface and $\mathrm{d}\mu_E$ the Liouville measure on Σ_E. If E is a regular value of H_0 and Σ_E is compact, then the spectrum of $\mathcal{H}$ is discrete in a neighbourhood of E. If furthermore the set of periodic orbits of Φ^t on Σ_E has measure zero, then the number of eigenvalues close to E satisfies the Weyl estimate

$$N(I(E,\hbar)) = \frac{2\alpha}{(2\pi)^d \hbar^{d-1}} \operatorname{vol}(\Sigma_E)(1+o(1)) \;, \tag{6}$$

where $\operatorname{vol}(\Sigma_E) := \int_{\Sigma_E} \mathrm{d}\mu_E$ and $\mathrm{d}\mu_E$ denotes the Liouville measure on Σ_E, see [PR85, Ivr98, DS99].

The autocorrelation function at energy E of a function a on T^*M is defined as

$$C_E[a](t) := \frac{1}{\operatorname{vol}(\Sigma_E)} \int_{\Sigma_E} a \circ \Phi^t a \,\mathrm{d}\mu_E - \left(\overline{a}_E\right)^2 \;, \tag{7}$$

where

$$\overline{a}_E := \frac{1}{\operatorname{vol}(\Sigma_E)} \int_{\Sigma_E} a \,\mathrm{d}\mu_E \;. \tag{8}$$

The flow Φ^t is ergodic on Σ_E if for every $a \in L^2(\Sigma_E, \mathrm{d}\mu_E)$ one has

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T C_E[a](t)\,\mathrm{d}t = 0 \;, \tag{9}$$

see [Wal82]. We will say that Φ^t is ergodic with rate $\gamma > 0$ on Σ_E if for every $a \in C^\infty(\Sigma_E)$ and $f \in \mathcal{S}(\mathbb{R})$ there is a constant C such that

$$\frac{1}{T} \int f\left(\frac{t}{T}\right) C_E[a](t)\;\mathrm{d}t \le C(1+|T|)^{-\gamma} \;. \tag{10}$$

The rate of ergodicity can be related to the more common rate of mixing, the system is called mixing if $\lim_{t\to\infty} C_E[a](t) = 0$, and if $|C_E[a](t)| \le C(1+|t|)^{-\tilde{\gamma}}$, then $\tilde{\gamma}$ is called the rate of mixing. We see from (10) that for $0 < \tilde{\gamma} < 1$ we have at least a rate of ergodicity $\gamma = \tilde{\gamma}$, whereas for $\tilde{\gamma} > 1$ we have at least $\gamma = 1$. So a rate of mixing implies a rate of ergodicity, but the contrary is not true, there are dynamical systems which are not mixing but which can have a large rate of ergodicity due to an oscillatory behaviour of $C_E[a](t)$. Examples are easily found among maps, for instance the Kronecker map.

Our main result is now

Theorem 1. *Assume M is either compact or $M = \mathbb{R}^d$ and let $\mathcal{H} \in \Psi^m(M)$, for some $m > 0$, be selfadjoint with principal symbol H_0. Assume that E is a regular value of H_0, that Σ_E is compact and denote by E_n, ψ_n the eigenfunctions and eigenvalues of $\mathcal{H}$ in the interval $I(E,\hbar) = [E-\alpha\hbar, E+\alpha\hbar]$, $\alpha > 0$. If the Hamiltonian flow Φ^t generated by H_0 is ergodic with rate $\gamma > 0$ on Σ_E, then for any $A \in \Psi^0(M)$ there exists a $C > 0$ such that*

$$\frac{1}{N(I(E,\hbar))} \sum_{E_n \in I(E,\hbar)} |\langle \psi_n, A\psi_n\rangle - \overline{\sigma(A)}_E|^2 \le C \begin{cases} |\ln \hbar|^{-\gamma} & \text{if } 0 < \gamma \le 1 \\ |\ln \hbar|^{-1} & \text{if } \gamma \ge 1 \end{cases} \;, \tag{11}$$

where $\overline{\sigma(A)}_E$ is defined in (8).

This result is an extension of a previous result by Zelditch, [Zel94], who obtained the same logarithmic bound for $\gamma > 1$ for eigenfunctions of the Laplacian on compact manifolds of negative curvature (in order to connect the two setups one has to rescale the Laplacian with $\hbar$). The improvement lies in the weakening of the assumptions to a rate of ergodicity and in a simpler proof, this is possible because we can use the recent results on propagation of observables up to Ehrenfest time [BGP99, BR02]. But Zelditch obtained in [Zel94] as well logarithmic bounds for higher moments of the expectation values, something we do not. A similar result to Theorem 1 has been stated recently by Robert in the review [Rob04].

Further systems where Theorem 1 applies are Schrödinger operators $\mathcal{H} = -\hbar^2\Delta + V$ on the 2-torus with the smooth potentials V constructed by Donnay and Liverani [DL91], for which the classical flow is ergodic and mixing, see [BT03]. These examples have been recently generalized to higher dimensions in [BT05]. The assumptions on M are made for sake of simplicity and because they cover the examples which are mainly studied in the literature, they could be relaxed.

For strongly chaotic systems the bound (11) is far from the conjectured optimal one. For eigenfunctions of the Laplace Beltrami operator on compact surfaces of negative curvature, where the corresponding classical system is the geodesic flow, which is Anosov, Rudnick and Sarnak [RS94, Sar03] have conjectured that

$$\left|\langle\psi_n, \rho\psi_n\rangle - \int \rho \,\mathrm{d}\nu_g\right| \leq C_\varepsilon E_n^{-1/4+\varepsilon} \tag{12}$$

holds for all $\varepsilon > 0$. Here ρ is a sufficiently nice function on the surface and $\mathrm{d}\nu_g$ is the Riemannian volume element. Translated in our context that would imply a bound $\hbar^{1-\varepsilon}$ in (11). A very precise prediction for the behaviour of the sum on the left-hand side of (11) has been derived in [EFK$^+$95], for a compact uniformly hyperbolic system with time reversal invariance and no other symmetry it reads

$$\begin{aligned}\frac{1}{N(I(E,\hbar))} \sum_{E_n\in I(E,\hbar)} &|\langle\psi_n, A\psi_n\rangle - \overline{\sigma(A)}_E|^2 \\ &= 2\frac{(2\pi\hbar)^{d-1}}{\operatorname{vol}\Sigma_E}\int_{-\infty}^{\infty} C_E[\sigma(A)](t)\,\mathrm{d}t + o(\hbar^{d-1})\ .\end{aligned} \tag{13}$$

Numerical tests of these predictions have been performed in [EFK$^+$95, AT98, BSS98]. They were confirmed for uniformly hyperbolic systems like manifolds of negative curvature. For non-uniformly hyperbolic systems like Euclidean billiards the findings are less clear and the rate is sometimes slower, at least in the tested energy range. So understanding the rate of quantum ergodicity remains a major open problem. Very recently Luo and Sarnak, see [Sar03], established a result of the form (13) for the discrete spectrum of the Laplacian on the modular surface. But due to the arithmetic nature of the system the right-hand side of (13) differs and an additional factor related to L-functions appears.

The reason for the rather large gap between the estimate (11) and the conjectured one is our poor understanding of the quantum time evolution for large times for the case that the underlying classical system is hyperbolic. In our present techniques the hyperbolicity leads to exponentially growing remainder terms and this reduces us to time scales which are logarithmic in $\hbar$. But for systems which are ergodic but not hyperbolic we can hope to get much stronger results. Examples for such systems can be constructed as maps on the torus and these will be studied in a separate paper.

The method we use to prove Theorem 1 can be used as well to get a bound on the off-diagonal matrix elements. We say that the flow Φ^t is weak mixing with rate $\gamma > 0$ on Σ_E if for all smooth a on Σ_E and $f \in \mathcal{S}(\mathbb{R})$ there is a constant C such that for all $\varepsilon \in \mathbb{R}$

$$\frac{1}{T} \int f\left(\frac{t}{T}\right) C_E[a](t) \mathrm{e}^{\mathrm{i}\varepsilon t} \, \mathrm{d}t \leq C(1 + |T|)^{-\gamma} \, . \tag{14}$$

That the above quantity tends to 0 for $T \to \infty$ is equivalent to weak mixing, see [Wal82], so the above condition quantifies the rate of weak mixing. As for the rate of ergodicity, a rate of mixing implies a similar rate of weak mixing.

Theorem 2. *Under the same conditions as in Theorem 1 we have for $\gamma > 0$*

$$\frac{1}{N(I(E,\hbar))} \sum_{\substack{n,m\,;\, E_n \in I(E,\hbar) \\ |E_n - E_m| \leq \hbar/|\ln \hbar|}}' |\langle \psi_n, A\psi_m \rangle|^2 \leq C \begin{cases} |\ln \hbar|^{-\gamma} & \text{if } 0 < \gamma \leq 1 \\ |\ln \hbar|^{-1} & \text{if } \gamma \geq 1 \end{cases} , \tag{15}$$

and if the flow is weak mixing with a rate $\delta > 0$, then for any $\varepsilon \in \mathbb{R}$

$$\frac{1}{N(I(E,\hbar))} \sum_{\substack{n,m\,;\, E_n \in I(E,\hbar) \\ |E_n - E_m - \hbar\varepsilon| \leq \hbar/|\ln \hbar|}}' |\langle \psi_n, A\psi_m \rangle|^2 \leq C \begin{cases} |\ln \hbar|^{-\delta} & \text{if } 0 < \delta \leq 1 \\ |\ln \hbar|^{-1} & \text{if } \delta \geq 1 \end{cases} , \tag{16}$$

where the prime at the sum indicates that we sum over E_m, E_n with $E_m \neq E_n$.

The behaviour of off-diagonal matrix elements have been studied in [Zel90, Zel96] where it was shown that ergodicity and weak mixing imply that the above sums tend to zero for $\hbar \to 0$. Further results have been derived in [Tat99].

The plan of the paper is as follows. In Section 2 we collect some preliminaries, and in Section 3 we do the proof of Theorems 1 and 2.

2. Preliminaries

The proofs of Theorems 1 and 2 rest on two ingredients, a microlocal version of Weyl's law and a version of Egorov's Theorem which is valid up to Ehrenfest time. In this section we will recall these results and present them in the form we need.

The estimates collected in this section will be finally applied to compute

$$\operatorname{Tr} \rho\big((E - \mathcal{H})/\hbar\big) B U^*(t) A U(t) \tag{17}$$

for $A, B \in \Psi^0(M)$. This quantity can be localized by splitting $B = \sum_j \operatorname{Op}[b_j]$ with b_j supported (modulo $\hbar^\infty$) in local charts. So whenever we write $\operatorname{Op}[a]$ in the following we will tacitly assume that a covering with local charts is fixed with respect to which $\mathrm{Op}[a]$ is defined as in (4).

For a function $a \in C^\infty(\mathbb{R}^m)$ we will use the notation

$$|a|_k := \sum_{|\alpha|\leq k} \sup_{x\in\mathbb{R}^m} |\partial^\alpha a(x)| \tag{18}$$

for $k \in \mathbb{N}$.

Proposition 1. *Assume that $\mathcal{H} \in \Psi^m(M)$ is selfadjoint and has principal symbol H_0. Assume furthermore that E is a regular value of H_0 and that Σ_E is compact. Let ρ be a smooth function on $\mathbb{R}$ such that the Fourier transform $\hat{\rho}$ has compact support in a small neighbourhood of* 0 *which contains no period of a periodic orbit of Φ^t on Σ_E. Then there is a constant $C > 0$ such that for every* $\mathrm{Op}[b] \in \Psi^0(M)$ *we have*

$$\left| \sum_{E_n} \rho\left(\frac{E - E_n}{\hbar}\right) \langle \psi_n, \mathrm{Op}[b]\psi_n\rangle - \frac{\hat{\rho}(0)}{(2\pi)^d \hbar^{d-1}} \overline{\sigma(b)}_E \right| \leq C\hbar^{2-d} |\rho|_5 |b|_{2d+8} \ . \tag{19}$$

The proposition is a standard result and well known in the literature, except that the way that the error term depends on b is usually not made explicit. Since the main tool in deriving the formula (19) is the method of stationary phase, or variants thereof, it comes as no surprise that the error term can be estimated by a finite number of derivatives of b. An analogous result for high-energy asymptotics on compact manifolds was derived in [Zel94]. For convenience we will sketch the proof of Proposition 1, for details we frequently refer to [DS99].

Proof. We first observe that without loss of generality we can assume that b is supported in a compact neighbourhood of the energy-shell Σ_E. Let $f(E)$ be a smooth function with compact support such that $f(H(x,\xi))$ has compact support and $f(H(x,\xi)) \equiv 1$ on a neighbourhood of Σ_E. By the functional calculus one has then $f(\mathcal{H}) \in \Psi(1)$, see [DS99]. Let $U(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}t\mathcal{H}}$ be the time evolution operator, i.e., the solution to $\mathrm{i}\hbar\partial_t U(t) = \mathcal{H}U(t)$ with initial condition $U(0) = I$. One then constructs an approximation to the operator $U_f(t) = U(t)f(\mathcal{H})$ by solving the initial value problem

$$\big(\mathrm{i}\hbar\partial_t - \mathcal{H}\big)U_f(t) = 0 \ , \quad U_f(0) = f(\mathcal{H}) \tag{20}$$

approximately for small t, i.e., for every $N \in \mathbb{N}$ one can find an $V^{(N)}(t)$ such that

$$\big(\mathrm{i}\hbar\partial_t - \mathcal{H}\big)V^{(N)}(t) = \hbar^{N+1} R_N(t) \ , \quad V^{(N)}(0) = f(\mathcal{H}) \ , \tag{21}$$

with $\|R_N(t)\| \leq C$ for $t \in [-T_0, T_0]$ where T_0 is smaller then the period of the shortest periodic orbit on Σ_E. Then Duhamel's principle gives

$$U_f(t) = V^{(N)}(t) + \mathrm{i}\hbar^N \int_0^t U_f(t - t')R_N(t') \,\mathrm{d}t' \tag{22}$$

and therefore

$$\begin{aligned}|\operatorname{Tr} U_f(t)\operatorname{Op}[b] - \operatorname{Tr} V^{(N)}(t)\operatorname{Op}[b]| &\leq \hbar^N |t| \sup_{t'\in[0,t]} |\operatorname{Tr} U_f(t-t')R_N(t')\operatorname{Op}[b]| \\ &\leq \hbar^N C_N \operatorname{Tr}|\operatorname{Op}[b]|\end{aligned} \tag{23}$$

since $|t|\sup_{t'\in[0,t]}\|U_f(t-t')R_N(t')\| \leq C$ for $t\in[-T_0,T_0]$ and we have used the general relation $|\operatorname{Tr} AB| \leq \|A\|\operatorname{Tr}|B|$ if A is bounded and B of trace class. Since b is of compact support $\operatorname{Op}[b]$ is of trace class and its trace norm can be estimated as

$$\operatorname{Tr}|\operatorname{Op}[b]| \leq C\frac{1}{(2\pi\hbar)^d}\,|b|_{2d+1}\ , \tag{24}$$

see [DS99, Chapter 9]. The kernel of $V^{(N)}(t)$ satisfying (21) is given by

$$V^{(N)}(t,x,y) = \frac{1}{(2\pi\hbar)^d}\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[\varphi(t,x,\xi)-y\xi]}a^{(N)}(t,x,\xi)\ \mathrm{d}\xi \tag{25}$$

where $\varphi(t,x,\xi)$ is a solution to the Hamilton Jacobi equation

$$\partial_t\varphi(t,x,\xi) + H(x,\varphi_x'(t,x,\xi)) = 0 \tag{26}$$

with initial condition $\varphi(0,x,\xi)=x\xi$, and $a^{(N)}(t,x,\xi)\in C^\infty([-T_0,T_0],S^1)$ is the solution of a corresponding transport equation with initial condition $a^{(N)}(0,x,\xi) = f(H(x,\xi)) + O(\hbar)$ given by the symbol of $f(\mathcal{H})$. See [DS99, Chapter 10] for the proof and more details. If $\tilde{b} = \mathrm{e}^{\mathrm{i}\hbar\partial_x\partial_\xi}b$ denotes the left symbol of $\operatorname{Op}[b]$ (the case $t=0$ in [DS99, Equation (7.5)]) then we get from (25)

$$\begin{aligned}&\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Et}\operatorname{Tr}\left[V^{(N)}(t)\operatorname{Op}[b]\right]\hat{\rho}(t)\ \mathrm{d}t \\ &\qquad = \frac{1}{(2\pi\hbar)^d}\iiint \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[\varphi(t,x,\xi)-x\xi+Et]}\hat{\rho}(t)a^{(N)}(t,x,\xi)\tilde{b}(x,\xi)\ \mathrm{d}x\mathrm{d}\xi\mathrm{d}t\ .\end{aligned} \tag{27}$$

The main contributions to this integral come from the points where the phase is stationary, the stationary phase condition reads

$$\partial_t\varphi(t,x,\xi)+E=0\ ,\quad \partial_x\varphi(t,x,\xi)-\xi=0 \quad\text{and}\quad \partial_\xi\varphi(t,x,\xi)-x=0\ . \tag{28}$$

In view of (26) the first equation means that $H(x,\xi)=E$ and the second and third imply that $\Phi^t(x,\xi)=(x,\xi)$, i.e., (x,ξ) has to lie on a periodic orbit with period t. Since by assumption the support of $\hat{\rho}$ does not contain any period of a periodic orbit, the only stationary points left are at $t=0$, and consist of the whole energy shell Σ_E. Because E is assumed to be a non-degenerate energy level we can choose new coordinates (E',z) in a neighbourhood of Σ_E such that $H(E',z)=E'$, and when we use furthermore that $\varphi(t,x,\xi) = x\xi - tH(x,\xi) + r(t,x,\xi)$ with $r(t,x,\xi)=O(t^2)$, which follows from (26), then the above integral becomes

$$\frac{1}{(2\pi\hbar)^d}\iiint \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[(E-E')t+r(t,E',z)]}\hat{\rho}(t)a^{(N)}(t,E',z)\tilde{b}(E',z)J(E',z)\ \mathrm{d}E'\mathrm{d}t\mathrm{d}z\ , \tag{29}$$

where $J(E', z)$ denotes the Jacobian of the change of coordinates. We can now apply the stationary phase theorem with remainder estimate, see, e.g., [DS99, Chapter 5], to the t, E' integrals and get

$$\begin{aligned}\frac{1}{2\pi\hbar}\iint \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[(E-E')t+r(t,E',z)]}\hat\rho(t)a^{(N)}(t,E',z)\tilde b(E',z)J(E',z)\ \mathrm{d}E'\mathrm{d}t\\ = \hat\rho(0)a^{(N)}(0,E,z)\tilde b(E,z)J(E,z)+O(\hbar|\rho|_5|\tilde b|_5)\ ,\end{aligned} \tag{30}$$

where the implied constant does only depend on a and φ. With the initial condition $a^{(N)}(0,E,z) = 1 + (\hbar^\infty)$ and $|\partial^\alpha b - \partial^\alpha \tilde b| \le C|b|_{|\alpha|+2d+3}$ we then finally obtain

$$\begin{aligned}\left|\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Et}\,\mathrm{Tr}(V^{(N)}(t)\,\mathrm{Op}[b])\hat\rho(t)\ \mathrm{d}t - \frac{\hat\rho(0)}{(2\pi\hbar)^{d-1}}\int_{\Sigma_E}\sigma(b)\ \mathrm{d}\mu_E\right|\\ \le C\hbar^{d-2}|\rho|_5|b|_{2d+8}\ .\end{aligned} \tag{31}$$

On the other hand side, by the spectral resolution of $U(t)$ we have

$$\int \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Et}\,\mathrm{Tr}(U_f(t)\,\mathrm{Op}[b])\hat\rho(t)\ \mathrm{d}t = 2\pi\sum_{E_n}\rho\left(\frac{E-E_n}{\hbar}\right)\langle\psi_n,\mathrm{Op}[b]\psi_n\rangle \tag{32}$$

and so finally we get

$$\begin{aligned}&\sum_{E_n}\rho\left(\frac{E-E_n}{\hbar}\right)\langle\psi_n,\mathrm{Op}[b]\psi_n\rangle\\ &\quad= \frac{\hat\rho(0)}{(2\pi)^d\hbar^{d-1}}\overline{\sigma(b)}_E + O(\hbar^{d-2}|\rho|_5|b|_{2d+8}) + O(\hbar^{d-N}|\rho|_0|b|_{2d+1})\end{aligned} \tag{33}$$

where the implied constants do only depend on a, φ and f. □

We want to use this proposition with $\mathrm{Op}[b] = \mathrm{Op}[a]U^*(t)\,\mathrm{Op}[a]U(t)$ where $\mathrm{Op}[a] \in \Psi^0$. In order to do so we will use the Theorem of Egorov with remainder estimate from [BGP99] and [BR02, Proposition 2.7].

Theorem 3 ([BR02])**.** *Assume that $\mathcal{H} \in \Psi^m(M)$ is selfadjoint, let $U(t) := \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}t\mathcal{H}}$ and assume that Σ_E is compact. Then there exists a constant $\Gamma_1 > 0$ such that for every $\mathrm{Op}[a] \in \Psi^0(M)$ with support in a neighbourhood of Σ_E there is a $C > 0$ with*

$$\|U^*(t)\,\mathrm{Op}[a]U(t) - \mathrm{Op}[a\circ\Phi^t]\| \le C\hbar\mathrm{e}^{\Gamma_1|t|} \tag{34}$$

Proof. The case $M = \mathbb{R}^d$ is [BR02, Proposition 2.7]. For compact M one could use a partition of unity and the results from [BR02] in local coordinates. But to keep track of Φ^t and $U(t)$ in different charts for large t gets cumbersome, so we sketch a proof close to the one in [BR02] but using the global calculus of Safarov, [Saf97].

Let us equip M with a Riemannian metric g, let r_g be the injectivity radius of (M, g) and let $d(x, y)$ be the metric distance on M induced by g. For two points $x, y \in M$ with $d(x, y) < r_g$ let $\gamma_{xy}(s)$, $s \in [0, 1]$ be the unique geodesic joining x and y and set $z(x, y) := \gamma_{xy}(\frac{1}{2})$ and for $\xi \in T^*_{z(x,y)}M$, $\varphi(x, y, \xi) := -\dot\gamma_{xy}(\frac{1}{2})\xi$. Then for a function $a \in C_0^\infty(T^*M)$ the operator $\mathrm{Op}_g[a]$ is defined to be the operator with kernel

$$K(x,y) = \rho(x,y)\frac{1}{(2\pi\hbar)^d}\int_{T_{z(x,y)}M} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\varphi(x,y,\xi)} a(z(x,y),\xi)\,\mathrm{d}\xi \tag{35}$$

where $\rho(x,y)$ is a smooth cutoff function with $\rho(x,y) = 1$ for $d(x,y) \leq \delta$ and $\rho(x,y) = 0$ for $d(x,y) \geq r_g - \delta$ for some $\delta > 0$. If $M = \mathbb{R}^d$ and g is the Euclidean metric then this quantization reduces to Weyl quantization (modulo $O(\hbar^\infty)$ due to the cutoff function). The class of operators obtained by this quantization is the same as the standard one for the usual symbol classes, and we have for a $\mathrm{Op}[a] \in \Psi^0(M)$ that

$$\|\mathrm{Op}_g[a] - \mathrm{Op}[a]\| \leq C|a|_K\hbar\ , \tag{36}$$

for some $K \in \mathbb{N}$. We collect now some facts we need about the global calculus. For $a, b \in C_0^\infty(T^*M)$ there is an $a\#b$ such that $\mathrm{Op}_g[a]\,\mathrm{Op}_g[b] = \mathrm{Op}_g[a\#b]$ and

$$a\#b = ab + \frac{\mathrm{i}\hbar}{2}\{a,b\} + \hbar^2 R_2(a,b) \tag{37}$$

where the remainder satisfies $|R_2(a,b)|_{C^k} \leq C_k|a|_{C^{k+K}}|b|_{C^{k+K}}$, for some $K \in \mathbb{N}$. This remainder estimate is not explicitly contained in [Saf97], but is follows directly from the structure of the product formula. We will use furthermore the two estimates for $a \in C_0^\infty(T^*M)$

$$\|\mathrm{Op}_g[a]\| \leq C|a|_{C^L}\ ,\quad |a\circ\Phi^t|_{C^k} \leq C_k\mathrm{e}^{k\Gamma'|t|}\ , \tag{38}$$

for some constants $L \in \mathbb{N}$, $\Gamma' > 0$. The first one is the Calderon Vallaincourt Theorem and the second one is Lemma 2.2 in [BR02]. The calculus just sketched is actually the semiclassical version of the one in [Saf97], but the results can be proved the same way.

Since we are working in the neighbourhood of an compact energy shell Σ_E we can localize $\mathcal{H}$ and assume that $\mathcal{H} = \mathrm{Op}_g[H]$, where H has compact support in a neighbourhood of Σ_E. Now let us consider

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}&U(t)\,\mathrm{Op}_g[a\circ\Phi^t]U^*(t)\\ &= U(t)\Big(\mathrm{Op}_g[\{H, a\circ\Phi^t\}] - \frac{\mathrm{i}}{\hbar}\big[\mathrm{Op}_g[H], \mathrm{Op}_g[a\circ\Phi^t]\big]\Big)U^*(t)\\ &= -\hbar U(t)\,\mathrm{Op}_g[R_2^-(H, a\circ\Phi^t)]U^*(t)\end{aligned} \tag{39}$$

where we have used (37) and defined $R_2^-(a,b) := R_2(a,b) - R_2(b,a)$. Integrating this equation leads to

$$\begin{aligned}U^*(t)\,\mathrm{Op}_g[a]U(t) - &\mathrm{Op}_g[a\circ\Phi^t]\\ &= \hbar\int_0^t U(t-t')\,\mathrm{Op}_g[R_2^-(H, a\circ\Phi^{t'})]U^*(t-t')\,\mathrm{d}t'\end{aligned} \tag{40}$$

and with the estimates (38) this gives

$$\begin{aligned} \|U^*(t)\,\mathrm{Op}_g[a]U(t) - \mathrm{Op}_g[a\circ\Phi^t]\| &\leq \hbar\int_0^t \|\mathrm{Op}_g[R_2^-(H, a\circ\Phi^{t'})]\|\,\mathrm{d}t' \\ &\leq C\hbar\mathrm{e}^{\Gamma|t|} \end{aligned} \tag{41}$$

for some constants $\Gamma, C > 0$. Using (36) we obtain then (34). □

From this we get

Corollary 1. *Under the assumption in Theorem 3 there exists a constant $\Gamma > 0$ such that for every $\mathrm{Op}[a] \in \Psi^0(M)$ with support in a neighbourhood of Σ_E there is a $C > 0$ with*

$$\|\mathrm{Op}[a]^* U^*(t)\,\mathrm{Op}[a]U(t) - \mathrm{Op}[a^* a\circ\Phi^t]\| \leq C\hbar\mathrm{e}^{\Gamma|t|} \tag{42}$$

Proof. Using the triangle inequality and Egorov's Theorem we get

$$\begin{aligned} &\|\mathrm{Op}[a]^* U^*(t)\,\mathrm{Op}[a]U(t) - \mathrm{Op}[a^* a\circ\Phi^t]\| \\ &\qquad \leq \|\mathrm{Op}[a]^* U^*(t)\,\mathrm{Op}[a]U(t) - \mathrm{Op}[a]^*\,\mathrm{Op}[a\circ\Phi^t]\| \\ &\qquad\quad + \|\mathrm{Op}[a]^*\,\mathrm{Op}[a\circ\Phi^t] - \mathrm{Op}[a^* a\circ\Phi^t]\| \\ &\qquad \leq C\hbar\|\mathrm{Op}[a]\|\mathrm{e}^{\Gamma_1|t|} + \|\mathrm{Op}[a]^*\,\mathrm{Op}[a\circ\Phi^t] - \mathrm{Op}[a^* a\circ\Phi^t]\| \end{aligned} \tag{43}$$

and since $\mathrm{Op}[a]$ is bounded we only have to estimate the second term. By the product formula for pseudo-differential operators and the Calderon Vallaincourt Theorem there exists a $k \in \mathbb{N}$ such that

$$\|\mathrm{Op}[a]\,\mathrm{Op}[b] - \mathrm{Op}[ab]\| \leq C\hbar|a|_k|b|_k \tag{44}$$

where C does not depend on a and b. We use this estimate with $b = a\circ\Phi^t$ and that for some $\Gamma_k > 0$

$$|a\circ\Phi^t|_k \leq C\mathrm{e}^{\Gamma_k|t|}\ , \tag{45}$$

see [BR02, Lemma 2.4]. This proves the corollary with $\Gamma = \max\{\Gamma_1, \Gamma_k\}$. □

Using Corollary 1 together with Proposition 1 we obtain

Corollary 2. *There exists $C > 0$, $\Gamma > 0$ and $k \in \mathbb{N}$ such that for every selfadjoint* $\mathrm{Op}[a] \in \Psi^0(M)$

$$\begin{aligned} &\sum_{E_n, E_m} \rho\left(\frac{E - E_n}{\hbar}\right)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}t(E_n - E_m)}\left|\langle\psi_n, \mathrm{Op}[a]\psi_m\rangle - \overline{\sigma(a)}_E\right|^2 \\ &\qquad = \frac{\hat\rho(0)}{(2\pi)^d\hbar^{d-1}}\,C_E[\sigma(a)](t) + O(\hbar^{2-d}|\rho|_5|a|_k\mathrm{e}^{\Gamma|t|})\ . \end{aligned} \tag{46}$$

This kind of relationship between transition amplitudes and the autocorrelation function is well known, the only new piece is that we have an explicit estimate on the time dependence of the remainder term. In fact if we multiply with a function $f(t)$ of compact support and integrate over t we obtain

$$\sum_{E_n,E_m} \rho\bigg(\frac{E-E_n}{\hbar}\bigg)\hat{f}\bigg(\frac{E_m-E_n}{\hbar}\bigg)\big|\langle\psi_n, \mathrm{Op}[a]\psi_m\rangle - \overline{\sigma(a)}_E\big|^2 = \frac{\hat{\rho}(0)}{(2\pi)^d\hbar^{d-1}}\int C_E[\sigma(a)](t)\, f(t)\, \mathrm{d}t + O(\hbar^{2-d}) \;, \tag{47}$$

which was derived in [FP86, Wil87] and proved in [CR94].

3. Proofs of Theorems 1 and 2

The proof of Theorem 1 will rely on the fact that by Corollary 2 we can let the support of f in (47) become larger with $\hbar$.

Proof of Theorem 1. We will assume in the following that $\overline{a}_E = 0$, this can always be achieved by subtracting $\overline{a}_E$ from a. Choose ρ such that $\rho \geq 0$, $\rho(\frac{E-E'}{\hbar}) \geq 1$ for $E' \in I(E,\hbar)$. Choose furthermore f such that $\hat{f} \in C^\infty([-1,1])$ and $f \geq 0$ and $f(0) = 1$ and set $f_T(\tau) := f(T\tau)$ so that $\widehat{f_T}(t) = \hat{f}(t/T)/T$. Then we have

$$\sum_{E_n\in I(E,\hbar)} |\langle\psi_n, \mathrm{Op}[a]\psi_n\rangle|^2 \leq \sum_{E_n,E_m} \rho\bigg(\frac{E-E_n}{\hbar}\bigg) f_T\bigg(\frac{E_m-E_n}{\hbar}\bigg)|\langle\psi_n, \mathrm{Op}[a]\psi_m\rangle|^2 \;, \tag{48}$$

and with Corollary 2 we get

$$\sum_{E_n,E_m} \rho\bigg(\frac{E-E_n}{\hbar}\bigg) f_T\bigg(\frac{E_m-E_n}{\hbar}\bigg)|\langle\psi_n, \mathrm{Op}[a]\psi_m\rangle|^2 = \frac{\hat{\rho}(0)}{(2\pi)^d\hbar^{d-1}}\int C_E[\sigma(a)](t)\widehat{f_T}(t)\, \mathrm{d}t + O\bigg(\hbar^{2-d}|\rho|_5|a|_k \int \mathrm{e}^{\Gamma|t|}\widehat{f_T}(t)\, \mathrm{d}t\bigg) \;. \tag{49}$$

Now we have

$$\bigg|\int \mathrm{e}^{\Gamma|t|}\widehat{f_T}(t)\, \mathrm{d}t\bigg| \leq |\hat{f}|_0 \frac{1}{\Gamma T}\mathrm{e}^{\Gamma T} \tag{50}$$

and with (10) we obtain

$$\bigg|\int C_E[\sigma(a)](t)\widehat{f_T}(t)\, \mathrm{d}t\bigg| \leq \begin{cases} C\frac{1}{T} & \text{for } \gamma \geq 1 \\ C\frac{1}{T^\gamma} & \text{for } 0 < \gamma \leq 1 \end{cases} \;, \tag{51}$$

for large T, since $\overline{a}_E = 0$ by assumption. If we choose

$$T = \frac{1}{\Gamma}\,|\ln(\hbar)| \tag{52}$$

then $\hbar e^{\Gamma T} = 1$, and therefore we get

$$\sum_{E_n,E_m} \rho\left(\frac{E-E_n}{\hbar}\right) f_T\left(\frac{E_m-E_n}{\hbar}\right) |\langle\psi_n, \mathrm{Op}[a]\psi_m\rangle|^2 \leq C\hbar^{d-1}\begin{cases}|\ln\hbar|^{-\gamma} & \text{if } 0<\gamma\leq 1\\ |\ln\hbar|^{-1} & \text{if } \gamma\geq 1\end{cases} . \tag{53}$$

Combining this inequality with the estimate (48) and the asymptotic for the number of eigenvalues in $I(E,\hbar)$, (6), finally gives

$$\frac{1}{N(I(E,\hbar))}\sum_{E_n\in I(E,\hbar)} |\langle\psi_n, \mathrm{Op}[a]\psi_n\rangle|^2 \leq C\begin{cases}|\ln\hbar|^{-\gamma} & \text{if } 0<\gamma\leq 1\\ |\ln\hbar|^{-1} & \text{if } \gamma\geq 1\end{cases} \tag{54}$$

and the proof is complete. □

Theorem 2 is proved along the same lines.

Proof of Theorem 2. The proof is based on relation (53), notice that the only assumption on ρ and f which entered the derivation are that $\hat{f}$ has compact support and $\hat{\rho}$ is supported in $(-T_0, T_0)$. We choose now ρ as before and f such that

$$f \geq \chi_{[-\Gamma,\Gamma]} \tag{55}$$

where $\chi_{[-\Gamma,\Gamma]}$ is the characteristic function of the interval $[-\Gamma,\Gamma]$. Then we get using (53)

$$\frac{1}{N(I(E,\hbar))}\sum_{\substack{n,m\,:\,E_n\in I(E,\hbar)\\ |E_n-E_m|\leq\hbar/|\ln\hbar|}} |\langle\psi_n\, \mathrm{Op}[a]\psi_m\rangle|^2 \leq C\begin{cases}|\ln\hbar|^{-\gamma} & \text{if } 0<\gamma\leq 1\\ |\ln\hbar|^{-1} & \text{if } \gamma\geq 1\end{cases} \tag{56}$$

if $\overline{a}_E = 0$. Together with (54) this gives

$$\frac{1}{N(I(E,\hbar))}\sum_{\substack{n,m\,:\,E_n\in I(E,\hbar)\\ |E_n-E_m|\leq\hbar/|\ln\hbar|}}{}' |\langle\psi_n\, \mathrm{Op}[a]\psi_m\rangle|^2 \leq C\begin{cases}|\ln\hbar|^{-\gamma} & \text{if } 0<\gamma\leq 1\\ |\ln\hbar|^{-1} & \text{if } \gamma\geq 1\end{cases} \tag{57}$$

and since $\langle\psi_m, \overline{a}_E\psi_n\rangle = 0$ if $E_m \neq E_n$, this estimate is true for all $\mathrm{Op}[a] \in \Psi^0(M)$.

With the same choices of ρ and f and by shifting f_T,

$$f_T^{(\varepsilon)}(\tau) := f_T(\tau-\varepsilon) , \tag{58}$$

we get from (49) and (50)

$$\sum_{E_n,E_m} \rho\left(\frac{E-E_n}{\hbar}\right) f_T\left(\frac{E_m-E_n-\hbar\varepsilon}{\hbar}\right) |\langle\psi_n, \mathrm{Op}[a]\psi_m\rangle|^2 = \frac{\hat{\rho}(0)}{(2\pi)^d\hbar^{d-1}} \int C_E[\sigma(a)](t)\widehat{f_T}(t)e^{i\varepsilon t}\, dt + O\left(\hbar^{2-d}|\rho|_5|a|_k|\hat{f}|_0 e^{\Gamma T}\right) . \tag{59}$$

And with the choice (52) and the rate of weak mixing (14) the second relation in Theorem 2 follows. □

Acknowledgments. This work has been supported by the European Commission under the Research Training Network (Mathematical Aspects of Quantum Chaos) n^o HPRN-CT-2000-00103 of the IHP Programme and by the EPSRC under Grant GR/T28058/01.

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Communicated by Jens Marklof
Submitted: March 16, 2005
Accepted: February 2, 2006