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A semiclassical sum rule for matrix elements of classically chaotic systems

Michael Wilkinson†

Instituto de Fisica Gleb Wataghin, Universidade Estadual de Campinas, Campinas, 13110, SP, Brazil and Department of Physics, California Institute of Technology, Pasadena, CA 91125, USA

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Abstract. In the semiclassical limit, the sum

$$S(E,\Delta E)=\sum_{nm}|A_{nm}|^2\delta[E-\tfrac{1}{2}(E_n+E_m)]\delta[\Delta E-(E_n-E_m)]$$

of matrix elements of an arbitrary operator $\hat{A}$ can be related to the classical correlation function of the Weyl symbol $A(\boldsymbol{q},\boldsymbol{p})$ of $\hat{A}$:

$$C_A(E,t)=\int \mathrm{d}\alpha\,\delta(E-H(\alpha))A(\alpha)A(\alpha_t).$$

$S(E,\Delta E)$ is proportional to the Fourier transform of $C_A(E,t)$ over t, plus a set of correction terms associated with periodic trajectories in phase space.

If the system has a chaotic classical limit, the matrix elements are independently Gaussian distributed with mean value zero, and $S(E,\Delta E)$ gives the variance of this distribution.

1. Introduction

The semiclassical quantum mechanics of systems which have a chaotic classical limit is still far from being thoroughly understood. This paper describes a new result applicable to these systems, which relates the matrix elements $A_{nm}=\langle n|\hat{A}|m\rangle$ of an arbitrary operator $\hat{A}$ to the correlation function of the Weyl symbol $A(\boldsymbol{q},\boldsymbol{p})$ of $\hat{A}$.

Since there is no known quantisation scheme for classically chaotic systems (and it is unlikely that such a scheme exists), it is not possible to write down analytic expressions for the eigenstates $|n\rangle$ and $|m\rangle$. It is only possible to produce a statistical theory describing the probability distribution of the matrix elements. It is believed that on energy scales of size $\mathrm{O}(\hbar)$, the properties of classically chaotic quantum systems can be modelled by random matrix theory (Pechukas 1983, Berry 1983). These results imply that, provided $|E_n-E_m|\leq \mathrm{O}(\hbar)$, the A_{nm} are independent and Gaussian distributed, with mean value zero when $n\neq m$. To characterise the distribution of the A_{nm} it only remains to calculate the variance of the A_{nm}s.

† Present address: Department of Physics and Applied Physics, John Anderson Building, University of Strathclyde, Glasgow G4 0NG, UK.

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The principal result of this paper is a semiclassical sum rule for the matrix elements: the sum

$$S(E, \Delta E) = \sum_{nm} |A_{nm}|^2 \delta[E - \tfrac{1}{2}(E_n + E_m)]\delta[\Delta E - (E_n - E_m)] \tag{1.1}$$

will be related to the classical correlation function $C_A(E, t)$ of the Weyl symbol $A(\boldsymbol{q}, \boldsymbol{p})$ of $\hat{A}$. In (1.1) the Dirac δ functions are slightly smeared out over a finite range ε: we could write

$$\delta(x) = \frac{1}{(2\pi\varepsilon)^{1/2}} \exp\left(-\frac{x^2}{2\varepsilon^2}\right). \tag{1.2}$$

The sum $S(E, \Delta E)$ is therefore a smooth function of E and ΔE. The values of ε for the first and second δ functions will be written ε_E and $\varepsilon_{\Delta E}$, respectively.

The correlation function $C_A(E, t)$ is defined by

$$C_A(E, t) = \int \mathrm{d}\alpha\, \delta(E - H(\alpha))A(\alpha)A(\alpha_t) \tag{1.3}$$

where α is a point $(\boldsymbol{q}, \boldsymbol{p})$ in phase space and $\alpha_t = (\boldsymbol{q}(t), \boldsymbol{p}(t))$ is the point obtained from α by evolution of Hamilton's equations for time t. If the values of ε_E and $\varepsilon_{\Delta E}$ are sufficiently large, then the relationship between S and C_A is simple: in § 2 it will be shown that

$$S(E, \Delta E) = \frac{1}{(2\pi\hbar)^{d+1}} \int_{-\infty}^{\infty} \mathrm{d}t \exp\left(\frac{\mathrm{i}\Delta E t}{\hbar}\right) C_A(E, t) \tag{1.4}$$

for a system with d degrees of freedom. This result has also been obtained by Feingold and Peres (1986), using a different and less rigorous argument.

There are corrections to (1.4) which are rapidly varying functions of Ea and ΔE, and which become important when the δ functions in (1.1) are not sufficiently smeared out. Each of these corrections is associated with a periodic trajectory of the classical motion in phase space. These periodic orbit corrections are calculated in § 3 for periodic trajectories which are isolated (have the energy E as their only parameter), and which are unstable. In many classically chaotic systems (K systems) all the periodic orbits are of this type; the Sinai billiard (Sinai 1970) and the pseudosphere (Balazs and Voros 1986) are examples.

The periodic orbit corrections oscillate more rapidly as a function of E as the return time τ of the orbit increases, so that as ε_E is decreased it is necessary to include longer periodic orbits in the correction terms. Only a finite number of these periodic orbit corrections are meaningful, however, because the semiclassical approximations used are valid in the limit $\hbar \to 0$ with time τ fixed, but break down if we make $\tau \to \infty$ with $\hbar$ fixed. Section 4 discusses how large ε_E and $\varepsilon_{\Delta E}$ must be before the periodic orbit terms can be neglected and how small they can be before the periodic orbit corrections cease to be valid.

The results contained in this paper are closely related to an expression for the density of states, $n(E)$, derived by Gutzwiller (1971, 1980). There are also close connections with the derivation of the Kubo formula (Kubo 1956, Greenwood, 1958). These relationships are discussed in § 5.

It is striking that equation (1.4) implies that the Fourier transform of the correlation function of any $A(\alpha)$ must be everywhere positive. It is desirable to see how this can be proved directly using only the laws of classical mechanics. This is done in the appendix.

2. A sum rule for matrix elements

Using the Fourier integral representation of the S functions on (1.1), we find

$$S(E,\Delta E)=\frac{1}{(2\pi\hbar)^2}\int_{-\infty}^{\infty}\mathrm{d}t\,\exp\left(\frac{\mathrm{i}\Delta Et}{\hbar}\right)\int_{-\infty}^{\infty}\mathrm{d}\Delta t$$
$$\times\exp\left(\frac{\mathrm{i}E\Delta t}{\hbar}\right)\operatorname{Tr}[\hat{A}\hat{U}(t+\tfrac{1}{2}\Delta t)\hat{A}\hat{U}(-t+\tfrac{1}{2}\Delta t)] \tag{2.1}$$

where $\hat{U}(t)$ is the propagator, $\hat{U}(t)=\Sigma_n\,|n\rangle\langle n|\exp(-\mathrm{i}E_nt/\hbar)$. To evaluate $S(E,\Delta E)$ we have to evaluate the trace appearing in (2.1). A particularly transparent way of evaluating the trace in the semiclassical limit ($\hbar\to 0$) is to use a coherent state basis. The trace of an operator can be written

$$\operatorname{Tr}\hat{X}=\frac{1}{(2\pi\hbar)^d}\int\mathrm{d}\alpha\langle\alpha|\hat{X}|\alpha\rangle \tag{2.2}$$

where $|\alpha\rangle$ is a coherent state at the point $\alpha=(q,p)$ in phase space. The advantage of using a coherent state basis is that the operators $\hat{A}$ and $\hat{U}(t)$ act classically on the coherent states $|\alpha\rangle$. In the limit $\hbar\to 0$:

$$\hat{A}|\alpha\rangle=A(\alpha)|\alpha\rangle \tag{2.3}$$

where $A(\alpha)$ is the value of the Weyl symbol of $\hat{A}$ at the point α. For short times t

$$\langle\alpha|\hat{U}(t)|\alpha\rangle=\exp\left(\frac{-\mathrm{i}H(\alpha)t}{\hbar}\right)\langle\alpha|\alpha_t\rangle=\exp\left(\frac{-\mathrm{i}H(\alpha)t}{\hbar}\right)f_\alpha(t/\hbar^{1/2}) \tag{2.4}$$

where α_t is the point reached by classical evolution from α for time t and f_α is a function which describes the overlap between the coherent states $|\alpha\rangle$ and $|\alpha_t\rangle$. This overlap has value unity at $t=0$, so $f_\alpha(0)=1$, and decays to zero in a time of $\mathrm{O}(\hbar^{1/2})$, since the coherent states have Wigner functions which decay over a range of $\mathrm{O}(\hbar^{1/2})$. For long times, $\langle\alpha|\hat{U}(t)|\alpha\rangle$ is small unless α lies very close to a periodic orbit in phase space, since $\hat{U}(t)|\alpha\rangle$ is close to $|\alpha_t\rangle$.

Now we use these results to evaluate (2.1). Using (2.2), (2.3), we find, in the limit $\hbar\to 0$:

$$S(E,\Delta E)=\frac{1}{(2\pi\hbar)^{d+2}}\int_{-\infty}^{\infty}\mathrm{d}t$$
$$\times\exp\left(\frac{\mathrm{i}\Delta Et}{\hbar}\right)\int_{-\infty}^{\infty}\mathrm{d}\Delta t\,\exp\left(\frac{\mathrm{i}E\Delta t}{\hbar}\right)\int\mathrm{d}\alpha\,A(\alpha)A(\alpha_{t+\Delta t/2})\langle\alpha|\hat{U}(\Delta t)|\alpha\rangle. \tag{2.5}$$

The integral

$$F(E,t)=\frac{1}{(2\pi\hbar)^{d+1}}\int_{-\infty}^{\infty}\mathrm{d}\Delta t\,\exp\left(\frac{\mathrm{i}E\Delta t}{\hbar}\right)\int\mathrm{d}\alpha\,A(\alpha)A(\alpha_{t+\Delta t/2})\langle\alpha|\hat{U}(\Delta t)|\alpha\rangle \tag{2.6}$$

has a contribution $F_0(E,t)$ from $\Delta t=0$, plus a set of contributions $F_j(E,t)$ from the jth periodic orbits. The periodic orbit contributions will be discussed in § 3. The direct term $F_0(E,t)$ can be evaluated using (2.4):

$$F_0(E,t)=\frac{1}{(2\pi\hbar)^{d+1}}\int\mathrm{d}\alpha\,A(\alpha)A(\alpha_t)\int_{-\infty}^{\infty}\mathrm{d}\Delta t\,\exp\left(\frac{\mathrm{i}[E-H(\alpha)]t}{\hbar}\right)f_\alpha(\Delta t/\hbar^{1/2}). \tag{2.7}$$

Now

$$I(E)=\int_{-\infty}^{\infty}\mathrm{d}\Delta t\,\exp\left(\frac{\mathrm{i}[E-H(\alpha)]t}{\hbar}\right)f_\alpha(\Delta t/\hbar^{1/2})$$
$$=(2\pi\hbar)^{1/2}\tilde{f}_\alpha((E-H(\alpha))/\hbar^{1/2}) \tag{2.8}$$

where $\tilde{f}_\alpha$ is the Fourier transform of f_α. In the limit $\hbar\to 0$, we can write this

$$I(E)=2\pi\hbar\delta(E-H(\alpha))\frac{1}{(2\pi)^{1/2}}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\tilde{f}_\alpha(\omega)$$
$$=2\pi\hbar\delta(E-H(\alpha)) \tag{2.9}$$

since $f_\alpha(0)=1$. We now have

$$F_0(E,t)=\frac{1}{(2\pi\hbar)^d}C_A(E,t) \tag{2.10}$$

where $C_A(E,t)$ was defined in (1.3). Ignoring the periodic orbit corrections, we have

$$S_0(E,\Delta E)=\frac{1}{(2\pi\hbar)^{d+1}}\int_{-\infty}^{\infty}\mathrm{d}t\,\exp\left(\frac{\mathrm{i}\Delta Et}{\hbar}\right)C_A(E,t)$$
$$C_A(E,t)=\int\mathrm{d}\alpha\,\delta(E-H(\alpha))A(\alpha)A(\alpha_t). \tag{2.11}$$

In §§ 3 and 4 it will be shown that the periodic orbit corrections are rapidly oscillating functions of E with period $O(\hbar)$, so that this approximation is adequate provided that the smearing parameter $\varepsilon_E > O(\hbar)$.

3. Periodic orbit corrections

In this section the corrections $F_j(E,t)$ to (2.6) from the jth periodic orbit will be evaluated. Time-reversed traversals of periodic orbits must be included, as well as multiple repetitions, since the integral over Δt in equation (2.8) extends from $-\infty$ to $+\infty$.

The function $F_j(E,t)$ is the contribution to

$$F(E,t)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}\Delta t\,\exp\left(\frac{\mathrm{i}E\Delta t}{\hbar}\right)\mathrm{Tr}[\hat{A}\hat{U}(t+\tfrac{1}{2}\Delta t)\hat{A}\hat{U}(-t+\tfrac{1}{2}\Delta t)] \tag{3.1}$$

from the jth periodic orbit. When calculating these periodic orbit terms a coordinate space representation will be used to calculate the trace, since the equation for the propagator is better known in this representation. The details of the calculation depend on the nature of the periodic orbits and the calculation will only be carried through for isolated unstable periodic orbits in a system with two degrees of freedom.

In the coordinate representation, the semiclassical approximation to the propagator $\hat{U}(t)$ (Gutzwiller 1967) is

$$\langle\boldsymbol{x}|\hat{U}(t)|\boldsymbol{x}'\rangle=K(\boldsymbol{x},\boldsymbol{x}';t)=(2\pi\mathrm{i}\hbar)^{-d/2}\left[\det\left(\frac{\partial^2\sigma}{\partial\boldsymbol{x}\,\partial\boldsymbol{x}'}\right)\right]^{1/2}$$
$$\times\exp\left(\frac{\mathrm{i}}{\hbar}\sigma(\boldsymbol{x},\boldsymbol{x}';t)-\frac{\mathrm{i}\gamma\pi}{2}\right) \tag{3.2}$$

where $\sigma(\boldsymbol{x},\boldsymbol{x}';t)$ is the action to go from $\boldsymbol{x}$ to $\boldsymbol{x}'$ in time t and γ is the number of focal points between $\boldsymbol{x}$ and $\boldsymbol{x}'$, where $\det(\partial^2\sigma/\partial\boldsymbol{x}\,\partial\boldsymbol{x}')$ diverges. It is convenient to simplify equation (3.2) by using a coordinate system in which x measures distance along the classical path, and y measures distance in a perpendicular direction. The dependence of σ on y, y' can be approximated by a quadratic form, and the matrix $\partial^2\sigma/\partial \boldsymbol{x}\, \partial \boldsymbol{x}'$ is diagonal, so that

$$K(\boldsymbol{x}, \boldsymbol{x}'; t) = (2\pi \mathrm{i}\hbar)(vv')^{-1/2}\left(-\frac{\partial E}{\partial t}\right)^{1/2} s_{12}^{-1/2} \exp\left(\frac{\mathrm{i}\sigma(x, x', t)}{\hbar} - \frac{\mathrm{i}\gamma\pi}{2}\right)$$
$$\times \exp\left(\frac{\mathrm{i}}{2\hbar}[s_{11}y^2 + 2s_{12}yy' + s_{22}y'^2]\right) \tag{3.3}$$

for a system with two degrees of freedom. In equation (3.3), $v = \mathrm{d}x/\mathrm{d}t$, $v' = \mathrm{d}x'/\mathrm{d}t$, and we have used

$$\frac{\partial^2\sigma}{\partial x\, \partial x'} = \left(\frac{\partial p}{\partial x'}\right)_{x,t} = -\left(\frac{\partial p}{\partial t}\right)_{x,x'}\left(\frac{\partial t}{\partial x'}\right)_{p,x} = -\left(\frac{\partial H}{\partial p}\right)^{-1}\frac{\partial E}{\partial t}\left(\frac{\partial t}{\partial x'}\right) = -(vv')^{-1}\frac{\partial E}{\partial t}. \tag{3.4}$$

Now (3.3) is used to evaluate $F_j(E, t)$. It is convenient to choose the x coordinate so that $v = v' =$ constant. Integrating over the internal coordinate labels using the stationary phase approximation gives

$$F_j(E, t) = \frac{-\mathrm{i}}{(2\pi\hbar)^2}\int_0^{\tau_j} A_j(T)A_j(\tau + \tfrac{1}{2}\tau_j + t)s_{12}^{1/2} \exp\left(\frac{\mathrm{i}}{2\hbar}[s_{11}y^2 + 2s_{12}yy' + s_{22}y'^2]\right)$$
$$\times \int_{-\infty}^{\infty} \mathrm{d}\Delta t\left(\frac{-\partial E}{\partial t}\right) \exp\left(\frac{\mathrm{i}\sigma(x, x, \Delta t) + E\Delta t}{\hbar} - \frac{\mathrm{i}\gamma_j\pi}{2}\right) \tag{3.5}$$

where $A_j(\tau)$ is the value of $A(\boldsymbol{q}, \boldsymbol{p})$ after moving for time τ around the jth periodic orbit and τ_j is the period of the orbit. Integrating over Δt the stationary phase approximation gives

$$F_j(E, t) = \frac{1}{(2\pi \mathrm{i}\hbar)^{3/2}}\int_0^{\tau_j} \mathrm{d}\tau\, A_j(\tau)A_j(\tau + \tfrac{1}{2}\tau_j + t)a_j \exp\left(\frac{\mathrm{i}S_j(E)}{\hbar} - \frac{\mathrm{i}\gamma\pi}{2}\right) \tag{3.6}$$

where $S_j(E)$ is the reduced action for the jth orbit

$$S_j(E) = \oint \boldsymbol{p}\cdot \mathrm{d}\boldsymbol{q} \tag{3.7}$$

and

$$a_j = s_{12}^{1/2}\int_{-\infty}^{\infty} \mathrm{d}y \exp\left(\frac{\mathrm{i}}{2\hbar}(s_{11} + s_{22} + 2s_{12})y^2\right). \tag{3.8}$$

The coefficients of the quadratic form can be related to those of the monodromy matrix M of the periodic trajectory, defined by

$$\begin{pmatrix} x' \\ p' \end{pmatrix} = \tilde{M}_j(E, \tau)\begin{pmatrix} x \\ p \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}\begin{pmatrix} x \\ p \end{pmatrix}. \tag{3.9}$$

Using $p = \partial S/\partial x$, $p' = -\partial S/\partial x'$, we find

$$\begin{pmatrix} s_{11} & s_{12} \\ s_{12} & s_{22} \end{pmatrix} = \frac{1}{m_{12}}\begin{pmatrix} m_{22} & -1 \\ -1 & m_{11} \end{pmatrix}. \tag{3.10}$$

Hence equation (3.7) becomes

$$a_j = (2\pi \mathrm{i}\hbar)^{1/2}\{\det[\tilde{M}_j(E,\tau) - \tilde{1}]\}^{-1/2} \tag{3.11}$$

which is independent of τ.

For unstable orbits in two dimensions, we have found

$$F_j(E,t) = \frac{1}{2\pi\hbar\mathrm{i}} \exp\left(\frac{\mathrm{i}S_j(E)}{\hbar} - \frac{\mathrm{i}\gamma_j\pi}{2}\right)\{\det[\tilde{M}_j(E) - \tilde{1}]\}^{-1/2} \int_0^{\tau_j} \mathrm{d}\tau\, A_j(\tau)A_j(\tau + \tfrac{1}{2}\tau_j + t) \tag{3.12}$$

where $S_j(E)$ is the action and $\tilde{M}(E)$ the monodromy matrix for the jth orbit. The correlation function along the orbit,

$$c_j(E,t) = \int_0^{\tau_j} \mathrm{d}\tau\, A_i(\tau)A_i(\tau + \tfrac{1}{2}\tau_j + t) \tag{3.13}$$

is a periodic function of t:

$$c_j(E,t) = \sum_M \alpha_{mj}(E) \exp\left(\frac{-2\pi \mathrm{i} t}{\tau_j}\right). \tag{3.14}$$

The contribution to $S(E, \Delta E)$ from the jth periodic orbit therefore consists of a set of δ functions of ΔE, with amplitudes that are oscillatory functions of E. Pairing the contributions from the jth orbit and its time-reversed partner, this contribution to $S(E, \Delta E)$ is

$$S_j(E,\Delta E) = \frac{1}{2\pi\hbar} 2\sin[S_j(E)/\hbar - \tfrac{1}{2}\gamma_j\pi]\{\det[\tilde{M}_j(E) - \tilde{1}]\}^{-1/2} \sum_m \alpha_{mj}(E)\delta\left(\Delta E - \frac{2\pi m\hbar}{\tau_j}\right) \tag{3.15}$$

for an unstable isolated orbit of a two-dimensional system.

4. Limitations on the energy resolution

The two δ functions appearing in the definition of $S(E, \Delta E)$ are not true Dirac δ functions, but are smeared slightly over a range ε (cf (1.2)). This is equivalent to introducing convergence factors into the integrals in (1.3):

$$\begin{aligned} S(E,\Delta E) = {} & \frac{1}{(2\pi\hbar)^2} \int_{-\infty}^{\infty} \mathrm{d}t \exp\left(\frac{\mathrm{i}\Delta E t}{\hbar}\right) \exp\left(\frac{-\varepsilon_{\Delta E}^2 t^2}{2\hbar^2}\right) \\ & \times \int_{-\infty}^{\infty} \mathrm{d}\Delta t \exp\left(\frac{\mathrm{i}E\Delta t}{\hbar}\right) \exp\left(\frac{-\varepsilon_E^2 \Delta t^2}{2\hbar^2}\right) \mathrm{Tr}[\hat{A}\hat{U}(t + \tfrac{1}{2}\Delta t)\hat{A}\hat{U}(-t + \tfrac{1}{2}\Delta t)]. \end{aligned} \tag{4.1}$$

If $\varepsilon_E \gg h/\tau_1$, where τ_1 is the period of the shortest periodic orbit, then none of the periodic orbits make a contribution to (4.1) and the approximation $S_0(E, \Delta E)$ given by (2.10) is adequate.

If ε_E and $\varepsilon_{\Delta E}$ are not greater than h/τ_1, then the periodic orbit corrections discussed in § 3 must be included. For a given value of ε_E, only periodic orbits with a period up to h/ε_E are required. Only a finite number of the periodic orbit corrections are meaningful for any given value of $\hbar$. The reason for this is that the semiclassical approximations used are valid in the limit $\hbar \to 0$ with time τ fixed, whereas to evaluate

(4.1) in the limit ε_E, $\varepsilon_{\Delta E} \to 0$ we need to calculate the propagators $\hat{U}(\tau)$ in the limit $\tau \to \infty$ with $\hbar$ fixed.

The semiclassical ($\hbar \to 0$) approximation to the propagator is valid up to a break time τ^*, which tends to infinity as $\hbar \to 0$ (Hepp 1974, Hagedorn 1980). If the system is chaotic, with exponentially diverging trajectories, then it is plausible that

$$\tau^* \sim \frac{1}{\gamma} \ln(S_0/\hbar) \tag{4.2}$$

where γ is the Lyapounov exponent and S_0 is some characteristic classical action of the system. Equation (4.2) can be justified by considering the motion of a wavepacket: the wavepacket has a finite size $\Delta x \sim O(\hbar^{1/2})$, and because of the exponential divergence of classical trajectories Δx increases exponentially. The semiclassical equations describing the motion of the wavepacket assume that it is so small that a quadratic approximation for the action is sufficient. When the wavepacket has spread a size comparable with the size of the system, this is no longer valid and the semiclassical approximation breaks down. Periodic orbit corrections for which the period is longer than τ^* are meaningless, so that ε_E should satisfy

$$\varepsilon_E \gg \hbar/\tau^* = \hbar\gamma/\ln(S_0/\hbar). \tag{4.3}$$

Similarly, the results must also be interpreted with care if $\varepsilon_{\Delta E} \lesssim \hbar/\tau^*$. Recall that the periodic orbit corrections to $F_j(E, t)$ involve calculating matrix elements of the form

$$I = \langle\alpha|\hat{A}\hat{U}(t+\tfrac{1}{2}\Delta t)\hat{A}\hat{U}(-t+\tfrac{1}{2}\Delta t)|\alpha\rangle \tag{4.4}$$

where α lies on a periodic orbit. Using the rule (2.3), this becomes

$$I = \langle\alpha|\hat{U}(\Delta t)|\alpha\rangle A(\alpha)A(\alpha_{t+\Delta t/2}) \tag{4.5}$$

since

$$|\alpha'\rangle = \hat{U}(-t+\tfrac{1}{2}\Delta t)\hat{A}\hat{U}(t+\tfrac{1}{2}\Delta t)|\alpha\rangle = A(\alpha_{t+\Delta t/2})\hat{U}(\Delta t)|\alpha\rangle. \tag{4.6}$$

Equation (4.6) assumes that both Δt and t are smaller than the break time, τ^*. If $t \gg \tau^*$, and the classical motion is chaotic, it is plausible to assume that the propagator $\hat{U}(t+\tfrac{1}{2}\Delta t)$ spreads the coherent state $|\alpha\rangle$ uniformly over phase space (on scales of size $O(\hbar^{1/2})$), so that in this limit (4.6) should be replaced by

$$|\alpha'\rangle = \langle A\rangle\hat{U}(\Delta t)|\alpha\rangle \tag{4.7}$$

where $\langle A\rangle$ is the average of $A(\alpha)$ over the classically allowed regions of phase space. For times $t \approx \tau^*$, it is necessary to interpolate between (4.6) and (4.7). Not enough is known at present about calculating propagators in the limit $t \to \infty$ to know how to do this. From these arguments, it is plausible that the function $c_j(E, t)$ appearing in the periodic orbit corrections (3.13) should be replaced by

$$c_j(E, t) = \int_0^{\tau_j} d\tau[A_j(\tau)A_j(\tau+\tfrac{1}{2}\tau_j+t) - \langle A\rangle^2]f_j(t/\tau^*) + \langle A\rangle^2 \tag{4.8}$$

where $f_j(x)$ has value unity at $x=0$ and decays smoothly to zero as $x \to \pm\infty$. The effect of this change is to smear the δ functions appearing in (3.15) over a width

$$\Delta E^* = h/\tau^*. \tag{4.9}$$

To summarise the results of this section: the periodic orbit corrections are not required if $\varepsilon_E \gg \hbar/\tau_1$, and meaningless if $\varepsilon_E \ll \hbar/\tau^*$, where the break time τ^* is given by (4.2). The delta functions appearing in (3.15) are not true delta functions, but are smeared out over a range $E = \hbar/\tau^*$. The exact form of the smearing function cannot be determined from known results on the long time propagator.

5. Discussion

The matrix elements of classically chaotic quantum systems are independently Gaussian distributed, and the off-diagonal elements have mean value zero. The variance of this distribution is given by

$$\langle |A_{nm}|^2 \rangle = \frac{S(E, \Delta E)}{[n(E)]^2} \tag{5.1}$$

where $n(E)$ is the (smoothed) density of states and $S(E, \Delta E)$ is the sum calculated in this paper.

This result should find applications in any situation where perturbation theory is applied to a classically chaotic system; see, for example, papers by Pechukas (1983) and Berry and Wilkinson (1984). The results may have important implications for the theory used by Pechukas (1983) to justify the application of random matrix theory to classically chaotic systems on energy scales smaller than $O(\hbar)$. Pechukas introduces the function $S(E, \Delta E)$, and argues that this function is a smooth function of ΔE on length scales smaller than size $O(\hbar)$. The results of this paper, in particular (3.16) and (4.7), show that $S(E, \Delta E)$ has structure on length scales $\Delta E^* \sim O(-\hbar/\ln \hbar)$. This suggests that it may be possible to find deviations from random matrix theory predictions on length scales smaller than $O(\hbar)$.

The results presented in this paper are closely related to a formula due to Gutzwiller (1971, 1980), which expresses the density of states $n(E)$ in terms of an average term $n_0(E)$, plus an infinite series of periodic orbit corrections $n_j(E)$. If we set $\hat{A} = \hat{1}$ (the identity operator), then the function $F(E, t)$ is independent of t and is just the density of states:

$$\hat{A} = \hat{1} \Rightarrow F(E, t) = n(E). \tag{5.2}$$

Then, setting $A(\alpha) = 1$, (2.10) and (3.12) yield the average term $n_0(E)$ and the periodic orbit corrections $n_j(E)$ of Gutzwiller's series.

There are also connections with the Kubo formula. Expressed in terms of the matrix elements of (for example) the current operator $\hat{j}$, the Kubo formula for the DC conductivity is a sum of the form (1.1) with $\Delta E = 0$, i.e. $\sigma \propto S(E, 0)$ (Greenwood 1958). It is well known that the Kubo formula can also be expressed as a time integral over the correlation function $\langle j(t) j(0) \rangle$ (Kubo 1956)). The results of §§ 2 and 3 of this paper give a semiclassical calculation of this integral over the correlation function.

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Appendix

Equation (1.4) implies that, for any Hamiltonian system, the Fourier transform of the correlation function of any phase function $A(\alpha)$ is nowhere negative. This appendix shows how this result can be proved using only the laws of classical mechanics.

The classical mechanics of a Hamiltonian system can be represented by the Liouville operator $\hat{L}(t)$, which maps a phase space function $A(\alpha)$ to $A(\alpha_t)$:

$$A_t(\alpha) = A(\alpha_t) = \int d\alpha' \, L(\alpha, \alpha'; t) A(\alpha') \tag{A1}$$

or more formally

$$|A_t\rangle = \hat{L}(t)|A\rangle. \tag{A2}$$

The Liouville operator is a unitary operator, and if the system is chaotic it has a continuous spectrum. Only the notation is different if $\hat{L}$ has a discrete or mixed spectrum. Thus we can write

$$\hat{L}(t) = \int d\chi |\chi\rangle \exp(i\omega(\chi)t)\langle\chi| \tag{A3}$$

(Arnold and Avez 1968). Defining

$$\langle A|\beta\rangle = \int d\alpha \, A^*(\alpha)B(\alpha) \tag{A4}$$

we find

$$C_A(t) = \int d\alpha \, A(\alpha_t)A(\alpha) = \langle A|\hat{L}(t)|A\rangle = \int d\chi \exp(i\omega(\chi)t)|\langle A|\chi\rangle|^2. \tag{A5}$$

The Fourier transform of $c_A(t)$ is

$$\tilde{C}(\omega') = \int d\chi \, \delta(\omega(\chi) - \omega')|\langle\chi|A\rangle|^2 \tag{A6}$$

which is nowhere negative. Note that the result follows from the fact that, like quantum evolution, classical evolution can be represented by a unitary operator.

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