Geometrical theory of diffraction and spectral statistics

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Abstract.   We investigate the influence of diffraction on the statistics of energy levels in quantum systems with a chaotic classical limit. By applying the geometrical theory of diffraction we show that diffraction on singularities of the potential can lead to modifications in semiclassical approximations for spectral statistics that persist in the semiclassical limit $\hbar \to 0$. This result is obtained by deriving a classical sum rule for trajectories that connect two points in coordinate space.

1. Introduction

Correlations in the spectra of quantum systems with a chaotic classical limit are expected to follow random matrix theory. This is the content of the random matrix hypothesis [1,2], which has found confirmation by numerical investigations in many systems. Theoretical support for this conjecture has been obtained by semiclassical approximations based on periodic orbits [3,4] as well as field theoretical methods [5]. In particular, it has been shown by the semiclassical method that the leading asymptotic behaviour of two-point correlation functions for long-range correlations agrees with results of random matrix theory. This result has been obtained by using mean properties of periodic orbits as expressed by the sum rule of Hannay and Ozorio de Almeida [6]. It is expected that a proof of the random matrix hypothesis would be possible if certain correlations between periodic orbits were known [7].

The semiclassical analysis is based on the trace formula for the density of states [8]. This is a leading order approximation, as $\hbar \to 0$, in terms of the periodic orbits of the corresponding classical system. For most systems this approximation is not exact, and there are corrections in higher order of $\hbar$. A particularly important correction occurs if the potential has discontinuities or singularities which lead to wave diffraction. This is the case in many standard examples of chaotic systems. It leads to additional contributions to the trace formula in terms of so-called creeping orbits or in terms of trajectories that are closed or that connect two points in coordinate space [9–12]. In the present paper we investigate systems in which the diffraction occurs at point-like objects, for example at a delta-like singularity of the potential, at a magnetic flux line in a two-dimensional system, or at a corner in a billiard system. For these systems we examine whether diffractive corrections to the trace formula can have an influence on spectral statistics that persists in the semiclassical limit $\hbar \to 0$. The analysis is done by deriving a classical sum rule for the orbits that arise in the geometrical theory of diffraction. With this input the diffractive corrections to the diagonal approximation for the spectral form factor are calculated, and it is shown that these corrections in general do not vanish as $\hbar \to 0$.

2. Sum rules for transient orbits

Semiclassical approximations for the Green function $G(q_b, q_a, E)$ of a quantum system involve classical trajectories that go from q_a to q_b at energy E. In general, there is an infinite number of these trajectories. Moreover, in a chaotic system the number of trajectories that connect the two points in a time less than T increases exponentially with T. In this section we use the ergodic property of chaotic systems in order to obtain a sum rule for orbits connecting two points in coordinate space. We call these trajectories transient orbits.

Consider a particle with energy E that starts at time $t = 0$ at a point q_a in coordinate space. The classical probability density for the particle to be found at time $t = T$ at a point q_b is given by

$$P(q_b; T, q_a, E) = \frac{\int d^f p_a \, \delta(E - H(q_a, p_a))\delta(q(T) - q_b)}{\int d^f q_b \int d^f p_a \, \delta(E - H(q_a, p_a))\delta(q(T) - q_b)} \tag{1}$$

where the function $q(t)$ denotes the position of the particle with initial position q_a and momentum p_a at $t = 0$, and f is the number of degrees of freedom of the system. The integration in the numerator extends over all initial momenta corresponding to energy E, and the denominator gives the normalization constant. The probability density is only different from zero if there are classical trajectories that connect the points q_a and q_b in time T.

Let us assume that the particle moves in the field of a vector and a scalar potential and that the Hamiltonian is given by

$$H(q, p) = \frac{1}{2m}\left(p - \frac{e}{c}A(q)\right)^2 + V(q). \tag{2}$$

In the following we express the transition probability density for this Hamiltonian in terms of classical trajectories.

The numerator in (1) is evaluated by introducing a local coordinate system in the vicinity of a trajectory where one coordinate is along the trajectory and the others are perpendicular to it,

$$\int d^f p_a \, \delta(E - H(q_a, p_a))\delta(q(T) - q_b) = \sum_\gamma \frac{1}{v_a v_b}\left|\det'\left(\frac{\partial q_b}{\partial p_a}\right)_\gamma\right|^{-1} \delta(T_\gamma - T). \tag{3}$$

The sum is over all trajectories from q_a to q_b at energy E, v_a and v_b are the velocities at q_a and q_b, respectively, T_γ is the time along the trajectory γ, and the prime at the determinant denotes that the matrix of derivatives involves only the coordinates orthogonal to the trajectory.

The denominator is evaluated by changing the integration over momentum into one over velocity and evaluating it in hyperspherical coordinates. The remaining integral over coordinates gives one, and one obtains

$$\int d^f q_b \int d^f p_a \, \delta(E - H(q_a, p_a))\delta(q(T) - q_b) = \frac{(mv_a)^{f-1}}{v_a}\mathcal{S}^{(f)} \tag{4}$$

where $\mathcal{S}^{(f)} = 2\pi^{f/2}/\Gamma(f/2)$ is the surface area of an f-dimensional hypersphere with unit radius. Altogether the result is

$$P(q_b; T, q_a, E) = \sum_\gamma \frac{1}{v_b(mv_a)^{f-1}\mathcal{S}^{(f)}}\left|\det'\left(\frac{\partial q_b}{\partial p_a}\right)_\gamma\right|^{-1} \delta(T_\gamma - T). \tag{5}$$

In an ergodic system the property that typical trajectories fill out phase space uniformly can be used to describe the probability density for long times T. In order to apply ergodicity we smooth the singular function P over some range of the final coordinate

$$\langle P(q_b; T, q_a, E)\rangle_\varepsilon \equiv \int d^f q_b' \, P(q_b'; T, q_a, E)\delta_\varepsilon(q_b - q_b') \tag{6}$$

where δ_ε is a smoothed delta function whose width is parametrized by ε, and which is normalized to one

$$\int_{V(q)<E} \mathrm{d}^f q \, \delta_\varepsilon(\boldsymbol{q} - \boldsymbol{q}_b) = 1. \tag{7}$$

It is assumed that the width ε is classically small so that the potentials do not change appreciably within this region. The integral in (6) results in the replacement of the second delta function in the numerator of (1) by δ_ε.

In order to describe the properties of the probability density P we employ the property of an ergodic system that the time average of a function along a trajectory is equal to its phase space average for almost all trajectories

$$\lim_{T\to\infty} \frac{1}{T} \int_{T_0}^{T} \mathrm{d}t \, f(\boldsymbol{q}(t), \boldsymbol{p}(t)) = \frac{\int \mathrm{d}^f q \, \mathrm{d}^f p \, \delta(E - H(\boldsymbol{q}, \boldsymbol{p})) f(\boldsymbol{q}, \boldsymbol{p})}{\int \mathrm{d}^f q \, \mathrm{d}^f p \, \delta(E - H(\boldsymbol{q}, \boldsymbol{p}))} \tag{8}$$

and we choose for f the smoothed delta function δ_ε. The phase space average over this function is evaluated similarly as before and yields

$$\frac{\int \mathrm{d}^f q \, \mathrm{d}^f p \, \delta(E - H(\boldsymbol{q}, \boldsymbol{p}))\delta_\varepsilon(\boldsymbol{q} - \boldsymbol{q}_b)}{\int \mathrm{d}^f q \, \mathrm{d}^f p \, \delta(E - H(\boldsymbol{q}, \boldsymbol{p}))} = \frac{(mv_b)^{f-1}\mathcal{S}^{(f)}}{v_b \Sigma(E)} + \mathcal{O}(\varepsilon) \tag{9}$$

where $\Sigma(E)$ is the volume of the energy surface in phase space. After integrating (8) with (9) over the initial momenta and dividing by the normalization constant one obtains the following result for the probability density:

$$\lim_{T\to\infty} \frac{1}{T} \int_{T_0}^{T} \mathrm{d}t \, \langle P(\boldsymbol{q}_b; t, \boldsymbol{q}_a, E) \rangle_\varepsilon = \frac{(mv_b)^{f-1}\mathcal{S}^{(f)}}{v_b \Sigma(E)} + \mathcal{O}(\varepsilon). \tag{10}$$

This property of P has the following interpretation. When the first term on the right-hand side is multiplied by a volume element $\mathrm{d}^f q$ it is the ratio between the volume of the part of the energy surface in phase space corresponding to the element $\mathrm{d}^f q$ around $\boldsymbol{q}_b$ and the volume of the total energy surface. Thus the probability of a particle to be found in a neighbourhood of $\boldsymbol{q}_b$ is equal to the relative volume of the energy surface of this neighbourhood.

Equation (10) gives an expression for the probability density P that is smoothed over an ε-neighbourhood of the final point in an ergodic system. Using (5), it is a sum rule for classical trajectories that start at $\boldsymbol{q}_a$ and visit the ε-neighbourhood of $\boldsymbol{q}_b$. In order to obtain a sum rule for trajectories that hit $\boldsymbol{q}_b$ one has to take the limit $\varepsilon \to 0$. Here one faces the problem that one would like to interchange the two limits $\varepsilon \to 0$ and $T \to \infty$, a problem that occurs also in the derivation of sum rules for periodic orbits [6].

One can argue that the two limits can be interchanged if the classical trajectories do not have conjugate points. Then the terms $[\det'(\partial \boldsymbol{q}_b/\partial \boldsymbol{p}_a)]^{-1}$ decrease exponentially with the transition time T_γ. This means that the contribution of a single trajectory to the probability density is exponentially small for long times. The integral over the probability density $\int_{T_0}^{T} \mathrm{d}t \, P(\boldsymbol{q}_b; t, \boldsymbol{q}_a, E)$ is a discontinuous function of the final coordinate $\boldsymbol{q}_b$, but its variation inside the ε-environment of $\boldsymbol{q}_b$ becomes very small for long times T, and the two limits $\varepsilon \to 0$ and $T \to \infty$ can be interchanged.

This argumentation does not apply, however, if there are caustics of the classical motion inside the ε-neighbourhood. On a caustic the term $[\det'(\partial \boldsymbol{q}_b/\partial \boldsymbol{p}_a)]^{-1}$ is divergent. This divergence is integrable so that the smoothed version of the sum rule (10) is still valid. It might be possible that in the generic situation where the point $\boldsymbol{q}_b$ itself does not lie on a caustic, the two limits can still be interchanged. We point out, however, that for applications in semiclassical approximations quantum mechanics provides a natural smoothing of the probability density, so that only a smoothed version of the sum rule is required.

In cases where the two limits can be interchanged we obtain the following sum rule for trajectories from q_a to q_b at energy E:

$$\lim_{T \to \infty} \frac{1}{T} \sum_{T_\gamma < T} \frac{1}{v_b(mv_a)^{f-1}\mathcal{S}^{(f)}} \left| \det' \left(\frac{\partial q_b}{\partial p_a} \right)_\gamma \right|^{-1} = \frac{(mv_b)^{f-1}\mathcal{S}^{(f)}}{v_b \Sigma(E)} \tag{11}$$

and the differentiated version is

$$\sum_\gamma \frac{1}{v_b(mv_a)^{f-1}\mathcal{S}^{(f)}} \left| \det' \left(\frac{\partial q_b}{\partial p_a} \right)_\gamma \right|^{-1} \delta(T - T_\gamma) \approx \frac{(mv_b)^{f-1}\mathcal{S}^{(f)}}{v_b \Sigma(E)} \qquad T \to \infty \tag{12}$$

where it is implied that the left-hand side has to be smoothed over some small time interval ΔT in order to obtain a smooth function.

In the following we give several variants of the sum rule that can be obtained in an analogous way.

- For chaotic area-preserving maps on a $(2f)$-dimensional unit torus, $(q_{n+1}, p_{n+1}) = h(q_n, p_n)$, the corresponding result is

$$\sum_{(q_n, q_0) = (q_b, q_a)} \left| \det \left(\frac{\partial q_n}{\partial p_0} \right) \right|^{-1} \approx 1 \qquad n \to \infty \tag{13}$$

where the sum extends over all points (q_0, p_0) for which $q_0 = q_a$ and $q_n = q_b$. In the appendix it is shown that this sum rule is exact for cat maps for all $n > 0$.

- For billiard systems the sum rule (12) can be expressed in a geometrical form. In two dimensions the result is

$$\frac{1}{2\pi} \sum_\gamma \frac{1}{|M_{12}|} \delta(L - L_\gamma) \approx \frac{1}{A} \qquad L \to \infty \tag{14}$$

where A is the area of the billiard, L_γ is the geometrical length of a trajectory and $M_{12} = p_a(\partial q_b^\perp / \partial p_a^\perp)$ is an element of the stability matrix, scaled by p_a in order to be energy independent. Equation (14) expresses that a particle is equally likely to be found anywhere in the billiard if it travels a sufficiently long distance L. Consequently, the probability density that it is found at some point q_b is equal to A^{-1}.

- For applications in the next section one requires sum rules for a subset of transient orbits for which the angular orientations of the initial and the final velocities, ϕ_a and ϕ_b, are fixed,

$$\sum_{\phi_a, \phi_b \text{ fixed}} \left| \det' \left(\frac{\partial q_b}{\partial p_a} \right)_\gamma \right|^{-1} \delta(T - T_\gamma) \approx \frac{(mv_a)^{f-1}(mv_b)^{f-1}}{\Sigma(E)} \, d\Omega_a \, d\Omega_b \qquad T \to \infty. \tag{15}$$

Here the sum extends over all transient trajectories for which the initial and final angular directions lie in solid angle elements $d\Omega_a$ and $d\Omega_b$, respectively, around the directions ϕ_a and ϕ_b.

- In integrable systems a similar sum rule can be obtained, if the ergodic average is performed over an invariant torus instead of the energy surface.

$$\sum_{\phi_a \text{ fixed}} \frac{1}{v_b(mv_a)^{f-1}\mathcal{S}^{(f)}} \left| \det' \left(\frac{\partial q_b}{\partial p_a} \right)_\gamma \right|^{-1} \delta(T - T_\gamma)$$

$$\approx \frac{1}{(2\pi)^f \mathcal{S}^{(f)}} \sum_{I(q_b, p_b) = I_a} \left| \det \left(\frac{\partial I(q_b, p_b)}{\partial p_b} \right) \right|^{-1} d\Omega_a \qquad T \to \infty \tag{16}$$

where $\boldsymbol{I}$ are the action variables of the system. This equation has the following interpretation. The left-hand side is a sum over all trajectories for which the initial angular direction lies in a solid angle element $\mathrm{d}\Omega_a$ around the direction ϕ_a. This direction ϕ_a, the energy E and the initial position $\boldsymbol{q}_a$ determine the action variable $\boldsymbol{I}_a = \boldsymbol{I}(\boldsymbol{q}_a, \boldsymbol{p}_a)$ and thus the torus on which the motion occurs. The right-hand side is a summation over all final momenta $\boldsymbol{p}_b$ for which the points $(\boldsymbol{q}_b, \boldsymbol{p}_b)$ lie on this torus.

In order to obtain a sum rule for all transient trajectories one has to integrate (16) over all initial directions. In contrast to the chaotic case this is not always possible, since the integral can be divergent due to caustics. In cases where it is possible one has

$$\sum_\gamma \frac{1}{v_b(mv_a)^{f-1}\mathcal{S}^{(f)}} \left| \det' \left(\frac{\partial \boldsymbol{q}_b}{\partial \boldsymbol{p}_a} \right)_\gamma \right|^{-1} \delta(T - T_\gamma)$$

$$\approx \frac{1}{(2\pi)^f \mathcal{S}^{(f)}} \int \mathrm{d}\Omega_a \sum_{\boldsymbol{I}(\boldsymbol{q}_b, \boldsymbol{p}_b) = \boldsymbol{I}_a} \left| \det \left(\frac{\partial \boldsymbol{I}(\boldsymbol{q}_b, \boldsymbol{p}_b)}{\partial \boldsymbol{p}_b} \right) \right|^{-1} \qquad T \to \infty. \quad (17)$$

This sum rule can be verified, for example, for an f-dimensional rectangular billiard with side lengths a_i, $i = 1, \ldots, f$. There the number of transient trajectories with length in an interval $\mathrm{d}L$ around L is given asymptotically for large L by $\mathcal{S}^{(f)}L^{f-1}\,\mathrm{d}L/V$ where $V = \prod_{i=1}^n a_i$ is the volume of the billiard, and $L = v_a T$. The absolute value of the determinant on the left-hand side of (17) is $(L/(mv_a))^{f-1}$, the actions are $I_i = a_i|p_i|/\pi$, and the sum on the right-hand side is $(2\pi)^f/V$. Altogether one obtains on both sides V^{-1}. Incidentally, the sum rule for chaotic billiard systems yields the same result in this case. The reason is that for rectangular billiards the determinant on the right-hand side of (17) is the same for all tori.

The sum rule (12) contains implicit information about the number of transient orbits. Let us assume that due to the exponential sensitivity of trajectories on initial conditions one has $\langle |\det'(\partial \boldsymbol{q}_b/\partial \boldsymbol{p}_a)|^{-1} \rangle \sim c' \exp(-hT)$ where c' and h are constants, and the averaging is performed over trajectories with $T_\gamma \approx T$. With this assumption one obtains the following asymptotic law for the number of transient orbits:

$$\rho(T) = \frac{\mathrm{d}\mathcal{N}(T)}{\mathrm{d}T} \sim c \exp(hT) \qquad T \to \infty \quad (18)$$

where $\mathcal{N}(T)$ is the number of transient trajectories with $T_\gamma < T$, $\rho(T)$ the density of these orbits, and c is a constant that is determined by c'. For Riemannian manifolds with no conjugate points one can show that $\lim_{T\to\infty} T^{-1} \log \mathcal{N}(T) = h$ is the topological entropy of the system [13]. Equation (18) with topological entropy h would imply that the number of transient orbits grows by an order of T stronger than the number of periodic orbits for which $\rho_{po}(T) \sim \exp(hT)/T$. One arrives at a similar conclusion for the number of transient orbits if one considers systems in which a code for these orbits exists [11, 14, 15]. For cat maps the law (18) is proved in the appendix.

3. Influence of diffractive orbits on spectral statistics

Diffraction of quantum wavefunctions on singularities of the potential leads to corrections in semiclassical expansions in terms of classical trajectories. In approximations for the density of states there are additional terms besides periodic orbits. These are expressed in terms of diffractive orbits. We concentrate on cases where the source of diffraction is point-like for which some examples are given below. In these cases the diffractive orbits are trajectories that start from and return to the source of diffraction n times, where n is an arbitrary positive

integer. They are composed of a sequence of arbitrary n transient orbits of the last section for which the initial and the final points of the trajectory are identical and are located at the source of diffraction. Alternatively, they can be considered as closed trajectories that are scattered n times on the source of diffraction.

Within the geometrical theory of diffraction (GTD) the contribution of all diffractive orbits with n scattering events to the density of states is given by [9–11]

$$d^{(n)}(E) = \frac{1}{\pi n} \left(\frac{\hbar^2}{2m} \right)^n \frac{\mathrm{d}}{\mathrm{d}E} \mathrm{Im} \left[\sum_{\gamma_1} \cdots \sum_{\gamma_n} \mathcal{G}_{\gamma_1}(E) \mathcal{D}(\phi_{a,\gamma_2}, \phi_{b,\gamma_1}) \mathcal{G}_{\gamma_2}(E) \mathcal{D}(\phi_{a,\gamma_3}, \phi_{b,\gamma_2}) \right.$$
$$\left. \cdots \mathcal{G}_{\gamma_n}(E) \mathcal{D}(\phi_{a,\gamma_1}, \phi_{b,\gamma_n}) \right] \tag{19}$$

where

$$\mathcal{G}_{\gamma_i}(E) = \frac{1}{\mathrm{i}\hbar(2\pi\,\mathrm{i}\hbar)^{(f-1)/2}} \sqrt{\frac{1}{v_a v_b} \left| \det' \left(\frac{\partial \boldsymbol{q}_b}{\partial \boldsymbol{p}_a} \right)_{\gamma_i} \right|^{-1}} \exp \left\{ \frac{\mathrm{i}}{\hbar} S_{\gamma_i}(E) - \mathrm{i}\frac{\pi}{2} \nu_{\gamma_i} \right\}. \tag{20}$$

Expression (20) is the semiclassical contribution of a transient orbit γ_i to the Green function; S_{γ_i} is its action and ν_{γ_i} the number of conjugate points along it. Furthermore, v_a and v_b are the initial and final velocities. They are identical since the initial and final point of the trajectory are identical, and we write them in the following without subscript.

A diffractive orbit is composed of n transient orbits, and it is labelled by a set of n indices $\gamma_1, \ldots, \gamma_n$. It is customary to consider cyclic permutations of these indices to correspond to the same diffractive orbit. The contribution of a diffractive orbit to the density of states in (19) can be interpreted in the following way. In the GTD approximation the diffraction is treated as a local process that occurs at the source of diffraction. The diffraction coefficient $\mathcal{D}(\phi_{a,\gamma_{i+1}}, \phi_{b,\gamma_i})$ contains the amplitude and phase for the scattering from the incoming direction of the transient orbits γ_i into the outgoing direction of the transient orbit γ_{i+1}. In some sense, the diffractive trajectories can be considered as generalized periodic orbits which are closed in momentum space by the scattering at the singularity of the potential.

Some examples for the diffraction coefficients are as follows.

• Diffraction on a corner with angle θ in a two-dimensional billiard system [16, 17]:

$$\mathcal{D}(\phi_a, \phi_b) = \frac{2}{N} \sin \frac{\pi}{N} \left[\left(\cos \frac{\pi}{N} - \cos \frac{\phi_a + \phi_b}{N} \right)^{-1} - \left(\cos \frac{\pi}{N} - \cos \frac{\phi_a - \phi_b}{N} \right)^{-1} \right] \tag{21}$$

where $N = \theta/\pi$, and ϕ_a and ϕ_b are the angles of the outgoing and incoming trajectory, measured with respect to one side of the corner such that $\phi_a, \phi_b \in [0, \theta]$.

• Diffraction on a flux line in a two-dimensional system [18]:

$$\mathcal{D}(\phi_a, \phi_b) = \frac{2 \sin(\alpha\pi)}{\cos \left(\frac{\phi_a - \phi_b}{2} \right)} \exp \left\{ \mathrm{i} \frac{\phi_a - \phi_b}{2} \right\} \tag{22}$$

where α is the flux parameter and ϕ_a and ϕ_b are the directions of the outgoing and incoming trajectory.

• Diffraction on a delta-like singularity of the potential in two dimensions [19, 20]:

$$\mathcal{D} = \frac{2\pi}{\mathrm{i}\frac{\pi}{2} - \gamma - \log(\frac{ka}{2})} \tag{23}$$

where $k = \sqrt{2mE}/\hbar$ and a is a parameter characterizing the strength of the potential, and γ is Euler's constant.

- Diffraction on a delta-like singularity of the potential in three dimensions [19, 20]:

$$\mathcal{D} = \frac{4\pi a}{1 + ika}. \tag{24}$$

In the first two examples the diffraction coefficient is energy independent but it depends on the incoming and outgoing directions of the trajectories. There are directions in which the diffraction coefficient diverges. There the GTD approximation breaks down and has to be replaced by a uniform approximation [21, 18]. In the last two cases, the diffraction coefficient has no angular dependence, but depends on energy. It corresponds to pure s-wave scattering, and the GTD approximation is valid for all angular directions.

In the following we consider the influence of diffractive orbits on semiclassical approximations for the spectral form factor which is defined by

$$K(\tau) = \int_{-\infty}^{\infty} \frac{d\eta}{\bar{d}(E)} \left\langle d_{\text{osc}}\left(E + \frac{\eta}{2}\right) d_{\text{osc}}\left(E - \frac{\eta}{2}\right)\right\rangle_E \exp(2\pi i\eta\tau\bar{d}(E)) \tag{25}$$

where $\langle \ldots \rangle_E$ denotes an average over an energy interval that is small in comparison with E but contains many energy levels. If the oscillatory part of the density of states is semiclassically approximated by classical trajectories in the form

$$d_{\text{osc}}(E) \approx \sum_\gamma A_\gamma \exp\left(\frac{i}{\hbar} S_\gamma(E)\right) \tag{26}$$

then the spectral form factor is expressed by a double sum over trajectories. We consider here only the diagonal approximation to this double sum that describes the form factor for small values of τ. In leading semiclassical order

$$K_d(\tau) = \frac{2\pi\hbar}{\bar{d}(E)} \sum_\gamma g_\gamma |\bar{A}_\gamma|^2 \delta(T - T_\gamma) \tag{27}$$

where $T = 2\pi\hbar\bar{d}(E)\tau$ and g_γ is the number of terms in the sum for which the actions $S_\gamma(E)$ are identical. $\bar{A}_\gamma$ is the average over all g_γ amplitudes of the orbits which have the same action as the orbit γ in case that these amplitudes are different.

Let us first consider the case of single-diffractive orbits $n = 1$. Then

$$A_\gamma = \frac{T_\gamma \mathcal{D}(\phi_{a,\gamma}, \phi_{b,\gamma})}{4\pi m v (2\pi\hbar)^{(f-1)/2}} \sqrt{\left| \det'\left(\frac{\partial q_b}{\partial p_a}\right)_\gamma \right|^{-1}} \tag{28}$$

and one obtains for the contribution of diffractive orbits with one scattering event to the diagonal approximation of the form factor

$$K_d^{(1)}(\tau) = \frac{2\pi\hbar(2/\beta)}{\bar{d}(E)} \sum_\gamma \frac{T_\gamma^2 |\mathcal{D}(\phi_{a,\gamma}, \phi_{b,\gamma})|^2}{(4\pi m v)^2 (2\pi\hbar)^{f-1}} \left| \det'\left(\frac{\partial q_b}{\partial p_a}\right)_\gamma \right|^{-1} \delta(T - T_\gamma). \tag{29}$$

The degeneracy of the actions is in this case $g = 2/\beta$ (except for an exponentially small fraction of the orbits for large T) where β is an integer denoting the symmetry class of the system. $\beta = 1$ for systems in which the only symmetry is an anti-unitary symmetry and $\beta = 2$ for systems without any symmetry. Applying the sum rule (15) and the leading asymptotic approximation for the mean density of states $\bar{d}(E) \sim \Sigma(E)/(2\pi\hbar)^f$ one obtains

$$d^2 K_d^{(1)}(\tau) = \frac{1}{8\beta\pi^2} \left(\frac{m v}{2\pi\hbar}\right)^{2f-4} |\mathcal{D}(\phi_a, \phi_b)|^2 \tau^2 \, d\Omega_a \, d\Omega_b \tag{30}$$

for the partial contribution to $K_d^{(1)}(\tau)$ from diffractive orbits with fixed initial and final directions.

For the examples given above this result has the following implications. For the corner diffraction and diffraction on a flux line the prefactor of τ^2 is independent of $\hbar$. It implies that diffraction has an influence on statistical properties of energy levels in the semiclassical limit $\hbar \to 0$. Although the contributions of diffractive orbits to the density of states are by an order $\sqrt{\hbar}$ smaller than those of periodic orbits, they still give a finite contribution to the diagonal approximation of the spectral form factor as $\hbar \to 0$. The complete contribution to $K_d^{(1)}$ that is obtained by integrating over all angular directions ϕ_a and ϕ_b requires the use of uniform approximations, since the GTD approximation yields a divergent result. However, since all contributions to $K_d^{(1)}$ are positive there is a non-vanishing contribution of order τ^2 to the diagonal approximation of the form factor in the semiclassical limit. For the examples of diffraction on delta singularities the diffraction is isotropic and the integration over the angular directions can be performed as below. Here the prefactor of τ^2 is energy dependent, and there is a significant difference between the two- and three-dimensional result. In two dimensions the prefactor vanishes in the semiclassical limit, although very slowly like $(\log \hbar)^{-2}$, whereas in three dimensions the prefactor approaches a constant.

The contributions of diffractive orbits with n scattering events to $K_d(\tau)$ are obtained in a similar way. They are composed of n transient orbits and it is sufficient to consider only cases in which all these n orbits are different, since the relative number of the other cases is exponentially suppressed for large times T. The degeneracy of the actions of diffractive orbits is then $g = (2/\beta)^n n!$. The index γ in (26) is now a multiple index $\gamma = (\gamma_1, \ldots, \gamma_n)$ and

$$\bar{A}_\gamma = \frac{T_\gamma}{2\pi\hbar n} \left(\frac{\hbar}{2mv(2\pi\hbar)^{(f-1)/2}} \right)^n \overline{\mathcal{D}}^{(n)}(\phi_{a,\gamma_1}, \phi_{b,\gamma_1}, \ldots, \phi_{a,\gamma_n}, \phi_{b,\gamma_n})$$

$$\times \prod_{i=1}^n \sqrt{\left| \det' \left(\frac{\partial \boldsymbol{q}_b}{\partial \boldsymbol{p}_a} \right)_{\gamma_i} \right|^{-1}} \tag{31}$$

where $T_\gamma = \sum_{i=1}^n T_{\gamma_i}$, and

$$\overline{\mathcal{D}}^{(n)}(\phi_{a,\gamma_1}, \phi_{b,\gamma_1}, \ldots, \phi_{a,\gamma_n}, \phi_{b,\gamma_n}) = \left\langle \prod_{i=1}^n \mathcal{D}(\phi_{a,\gamma_{i+1}}, \phi_{b,\gamma_i}) \right\rangle \tag{32}$$

is the average over all $n!$ permutations of the γ_i. For simplicity of notation we abbreviate the argument of $\overline{\mathcal{D}}^{(n)}$ by an index γ. Using the relation

$$\delta(T - T_\gamma) = \int_0^\infty dT_1 \ldots dT_n \left[\prod_{i=1}^n \delta(T_i - T_{\gamma_i}) \right] \delta\left(T - \sum_{i=1}^n T_i \right) \tag{33}$$

one can write the contribution of n-fold diffractive orbits to the diagonal approximation of the form factor in the form

$$K_d^{(n)}(\tau) = \frac{T^2 (2/\beta)^n n!}{2\pi\hbar n^2 \bar{d}(E)} \int_0^\infty dT_1 \ldots dT_n \, \delta\left(T - \sum_{i=1}^n T_i \right)$$

$$\times \sum_\gamma |\overline{\mathcal{D}}_\gamma^{(n)}|^2 \prod_{i=1}^n \left[\frac{1}{(4\pi mv_a)^2(2\pi\hbar)^{f-3}} \left| \det' \left(\frac{\partial \boldsymbol{q}_b}{\partial \boldsymbol{p}_a} \right)_{\gamma_i} \right|^{-1} \delta(T_i - T_{\gamma_i}) \right]. \tag{34}$$

After using sum rule (15) n times one is left with the integrals over the T_i which yield

$$\int_0^\infty dT_1 \ldots dT_n \, \delta\left(T - \sum_{i=1}^n T_i \right) = \frac{T^{n-1}}{(n-1)!} \tag{35}$$

which can be shown by induction, and the final result is

$$d^{2n} K_d^{(n)}(\tau) = \frac{\tau^{n+1}}{n} \left(\frac{1}{8\beta\pi^2} \left(\frac{mv}{2\pi\hbar} \right)^{2f-4} \right)^n |\overline{\mathcal{D}}^{(n)}(\phi_{a,1}, \ldots, \phi_{b,n})|^2 \, d\Omega_{a,1} \ldots d\Omega_{b,n}. \tag{36}$$

The interpretation is similar as before. The n-fold diffractive orbits contribute to $K_d(\tau)$ in order τ^{n+1}. For corner diffraction and diffraction on a flux line the prefactor of τ^{n+1} is independent of $\hbar$ and persists in the semiclassical limit. The remarkable point is that the order in $\hbar$ of the contributions of these orbits to the density of states can be arbitrarily large, their amplitude is by an order $\hbar^{n/2}$ smaller than those of periodic orbits, but they still give a finite contribution to the form factor in the semiclassical limit! For the diffraction on delta singularities of the potential, the prefactor of τ^{n+1} again vanishes slowly in the two-dimensional case and approaches a constant in three dimensions as $\hbar \to 0$.

For the isotropic case where the diffraction coefficient is angular independent, the integration over the angular directions can be performed, and the contributions of all diffractive orbits can be summed. Also adding the contribution of periodic orbits, the complete expression for the diagonal form factor is

$$K_d(\tau) = \frac{2}{\beta}\tau + \sum_{n=1}^{\infty} \frac{\tau^{n+1}}{n} \mathcal{C}^n = \frac{2}{\beta}\tau - \tau \log(1 - \mathcal{C}\tau) \qquad \tau < \mathcal{C}^{-1} \tag{37}$$

where

$$\mathcal{C} = \frac{|\mathcal{D}|^2 [\mathcal{S}^{(f)}]^2}{8\beta\pi^2} \left(\frac{mv}{2\pi\hbar} \right)^{2f-4}. \tag{38}$$

For an s-wave scatterer in a three-dimensional billiard system the constant approaches the value $\mathcal{C} = 8$ in the limit $\hbar \to 0$.

The results for the contributions of diffractive orbits to the spectral form factor can also be applied to a rectangular billiard with an s-wave scatterer, since the same sum rule applies in this case. The form factor for this system has been studied in [22].

4. Conclusions

The main result of this paper is that diffraction can have an influence on spectral statistics in the semiclassical limit. The semiclassical treatment of diffraction leads to corrections to the diagonal approximation for the spectral form factor $K(\tau)$ that do not vanish in the semiclassical limit $\hbar \to 0$. This is in contrast, for example, to corrections due to bouncing ball orbits in the stadium billiard, which vanish if the semiclassical limit is performed while keeping the argument of $K(\tau)$ fixed.

Although the corrections to the form factor do not agree with those expected from random matrix theory, the present results do not show that diffraction leads to a deviation from random matrix statistics, since off-diagonal contributions to the form factor have been neglected. They show, however, that a semiclassical proof of the random matrix hypothesis cannot be based on periodic orbits alone if diffraction occurs. Consider, for example, chaotic billiard systems with flux lines. These systems are considered to be standard examples in which spectral correlations are expected to follow the statistics of the Gaussian unitary ensemble (GUE). The diagonal approximation for the form factor in terms of periodic orbits already yields the correct linear GUE form factor up to the Heisenberg time $\tau = 1$ [3]. Moreover, it can be shown that in certain ensemble averages the off-diagonal contributions of periodic orbits vanish [23]. The present results show, however, that diffraction on the flux line leads to additional semiclassical contributions to the diagonal form factor in all higher orders of τ. If the spectral statistics

indeed follow random matrix theory, then these additional contributions have to be cancelled by off-diagonal terms involving diffractive orbits. Such a cancellation would require specific correlations between classical trajectories that start from and return to one point in coordinate space, or between these trajectories and periodic orbits, analogous to the action correlations of periodic orbits [7].

For another example let us assume that the spectral correlations in a particular three-dimensional chaotic system are described correctly by random matrix theory in the semiclassical limit. Then it is generally expected that this property is not changed, if an s-wave scatterer is added to the system. As is shown in the present paper, however, the diagonal approximation for $K(\tau)$ is modified also in this case. This would imply a deviation from random matrix results, if this is not corrected by the off-diagonal terms. Nevertheless, it shows that a single s-wave scatterer *can* lead to deviations from random matrix statistics.

The analysis in this article is based on the geometrical theory of diffraction. For corner diffraction or diffraction on a flux line this is not sufficient for calculating the complete diagonal approximation of the form factor. It would require the application of uniform approximations. Since the semiclassical weight of diffractive orbits is larger in the uniform regime, one can expect an even stronger total influence of diffraction on the spectral form factor in these cases. The main remaining question is, whether deviations from random matrix statistics can be observed in these systems.

Acknowledgments

Appendix. Cat maps

In this appendix we give a simple example for the sum rule for transient orbits. Cat maps are linear, area-preserving, hyperbolic maps on the unit 2-torus

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = M \begin{pmatrix} q_n \\ p_n \end{pmatrix} \qquad \mathrm{mod}\ 1 \tag{39}$$

where $\det M = 1$ due to area preservation, $|\operatorname{Tr} M| > 2$ due to hyperbolicity, and the elements M_{ij} of the matrix M are integers for continuity.

The sum rule (13) has the form

$$\sum_{(q_n, q_0) = (q_b, q_a)} \frac{1}{|(M^n)_{12}|} = 1 \tag{40}$$

where the sum extends over all points (q_0, p_0) for which $q_0 = q_a$ and $q_n = q_b$. The matrix element $(M^n)_{12}$ is the same for all points and can be taken in front of the sum. The number of points over which the sum extends is given by the number of solutions of the equation

$$q_b = (M^n)_{11} q_a + (M^n)_{12} p_a \qquad \mathrm{mod}\ 1. \tag{41}$$

Since p_a varies in the interval $[0, 1)$ there are exactly $|(M^n)_{12}|$ solutions of this equation. This shows that the sum rule (40) is exact for all $n > 0$.

Let $|\operatorname{Tr} M| = 2\cosh(\lambda)$ where $\lambda > 0$ is the Lyapunov exponent of the map, and $\sigma = \operatorname{sign}(\operatorname{Tr} M)$. Then

$$M^n = \frac{1}{u_1 s_2 - u_2 s_1} \begin{pmatrix} u_1 & s_1 \\ u_2 & s_2 \end{pmatrix} \begin{pmatrix} \sigma^n e^{n\lambda} & 0 \\ 0 & \sigma^n e^{-n\lambda} \end{pmatrix} \begin{pmatrix} s_2 & -s_1 \\ -u_2 & u_1 \end{pmatrix} \tag{42}$$

where (u_1, u_2) and (s_1, s_2) are the components of the unstable and stable eigenvectors of M, respectively. One obtains $(M^n)_{12} = -\sigma^n u_1 s_1 (e^{n\lambda} + e^{-n\lambda})/(u_1 s_2 - u_2 s_1)$ and it follows that the number of points contributing to the sum rule is given by

$$\rho(n) \sim \frac{|u_1 s_1|}{|u_1 s_2 - u_2 s_1|} e^{n\lambda} \qquad n \to \infty. \tag{43}$$

This is of the form (18) and it shows, moreover, that the constant c in (18) is not universal. For cat maps it is determined by the directions of the eigenvectors of M.

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