Chaotic Spectroscopy

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We discuss the spectra of quantized chaotic billiards from the point of view of scattering theory. We show that the spectral and the resonance density functions both fluctuate about a common mean. A semiclassical treatment explains this in terms of classical scattering trajectories and periodic orbits of the Poincaré scattering map. This formalism is used to interpret recent experiments where the spectra of chaotic cavities were measured by microwave scattering.

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A discrete spectrum is a property of a closed system. However, the process of measuring the spectrum of a bounded system consists of coupling the system to an external continuum. Thus, for the purpose of measurement, the closed system is turned into a scattering system. For example, the spectrum of an H atom in a static magnetic field is interrogated by scattering light and measuring resonant absorption [1], and the spectrum of a cavity can be measured by measuring the reflectivity of microwaves coupled to it via a coaxial cable [2]. This simple observation was the motivation for our attempt to study spectra of classically chaotic systems from the point of view of scattering theory. The first results of this endeavor are presented in this Letter, where we discuss in particular the spectra of two-dimensional chaotic billiards. We show that, in the short-wave (semiclassical) limit, a secular function $Z^{sc}(E)$ (the function whose zeros coincide with the spectrum of the closed system) can be constructed using scattering information exclusively. The study of this function gives important relations between the *spectral* number function $N(E)$, which counts the number of eigenenergies up to the energy E, and a corresponding *resonance* number function $N_R(E)$, which counts the number of scattering resonances up to the energy E. We show that the difference between these two functions is an oscillating function with a vanishing mean. This allows us to derive Weyl's formula for the mean spectral density, from a scattering point of view. A further application of the semiclassical approximation allows us to write $Z^{sc}(E)$ in terms of classical trajectories, and, in particular, in terms of periodic orbits of the Poincaré scattering map (PSM) [3]. We then establish a link between the well-known Gutzwiller trace formula [4] and a recent semiclassical result for the resonance density function [5,6]. In doing so we connect the theory of chaotic scattering with the theory of spectral fluctuations in chaotic bound systems. We finally illustrate the theoretical results by some numerical data, and use them to discuss actual experiments.

Consider a two-dimensional billiard defined by a closed curve Σ. The eigenfunctions $\Psi_b(\mathbf{r})$ are solutions of the wave equation, subject to Dirichlet boundary conditions on Σ. To turn this into a scattering problem we remove a small interval σ from Σ, and replace it by an infinite tube or waveguide, which runs along the normal to Σ at σ. We assume that the transverse dimension of the tube, D, is much smaller than the radius of curvature at σ, so that σ is well approximated by a straight line.

The wave function in the waveguide can be written in terms of the normal modes as

$$\Psi_s(x,y)=\sum_{l=1}^{L}\frac{1}{k_l^{1/2}}[A_l(E)e^{-ik_lx}+B_l(E)e^{ik_lx}]\sin\left(\frac{\pi yl}{D}\right)+\sum_{l=1}^{\infty}\frac{1}{k_{l+L}^{1/2}}C_l(E)e^{-|k_{l+L}|x}\sin\left(\frac{\pi y(l+L)}{D}\right), \tag{1}$$

where $L=[kD/\pi]$, x and y denote the longitudinal and transverse directions, respectively, k is the wave number ($E=k^2\hbar^2/2m$), and $k_n=[k^2-(\pi n/D)^2]^{1/2}$ is the longitudinal wave number. Evanescent solutions correspond to modes with $n>L$. At $x\to\infty$, where the measurement takes place, the evanescent term vanishes. The S matrix is defined as the ratio of the incoming to outgoing modes at infinity: $\mathbf{B}(E)=S(E)\mathbf{A}(E)$.

We now make the approximation that one is allowed to neglect the contributions of the evanescent modes even at $x=0$. This is consistent with the semiclassical approximation, as evanescent modes cannot be represented by classical trajectories which impinge on σ with real angles of incidence. This approximation holds for $L\gg 1$ and for energies not too close to the threshold energies, where modes which were previously evanescent become propagating. The S matrix then represents the constraints that the Dirichlet boundary conditions on $\Sigma-\sigma$ impose on the wave function at σ. In order to close the billiard we must also require that $\Psi_s(\mathbf{r})$ vanish on σ. Neglecting the contribution of evanescent modes, this implies $\mathbf{A}(E)=-\mathbf{B}(E)=-S(E)\mathbf{A}(E)$ on σ, which can be fulfilled only if

$$Z^{sc}(E)\equiv\det[I+S(E)]=0. \tag{2}$$

$Z^{sc}(E)$ is therefore the semiclassical secular function, which has zeros at the eigenenergies of the billiard, expressed as a function of the unitary scattering matrix S.

A more rigorous derivation of (2) and a systematic discussion of the role played by the evanescent modes will be presented elsewhere.

Special attention should be given to the vicinity of the threshold energies $E_l=(\pi l\hbar/D)^2/2m$, where the dimension of $S(E)$ increases by 1, and $S(E)$ has a branch point when considered as a function of complex E. To avoid the complications which the threshold introduces, we shall allow the energies to vary only between two successive thresholds. If the area of the billiard, A, is sufficiently large, a large number of eigenenergies ($\sim\frac{1}{2}\pi LA/D^2$) will be found in this interval. This allows a meaningful discussion of the spectral fluctuations. Using the methods developed by Weidenmüller [7] one can then generalize the discussion to the entire real energy axis. This is, however, deferred to a later publication.

$Z^{sc}(E)$ can be written in terms of the eigenphases $\theta_l(E)$ of $S(E)$,

$$Z^{sc}(E)=\exp\left[i\sum_{l=1}^{L}\frac{1}{2}\theta_l(E)\right]2^L\prod_{l=1}^{L}\cos\left[\frac{1}{2}\theta_l(E)\right]. \tag{3}$$

Only the last term can vanish for real values of E. Therefore, the number of eigenenergies in the interval (E_L,E) is given by

$$\begin{aligned}N(E)-N(E_L)\equiv N(E')|_{E_L}^{E}&=-\frac{1}{\pi}\lim_{\epsilon\to 0}\operatorname{Im}\ln\prod_{l=1}^{L}\cos\left[\frac{1}{2}\theta_l(E'+i\epsilon)\right]\Bigg|_{E_L}^{E}\\&=\left[-\frac{1}{\pi}\lim_{\epsilon\to 0}\operatorname{Im}\ln[Z^{sc}(E'+i\epsilon)]+\frac{1}{2\pi}\sum_{l=1}^{L}\theta_l(E')\right]_{E_L}^{E},\end{aligned} \tag{4}$$

where $N(E)$ is the spectral counting function.

To interpret the above result, consider the Wigner time delay [8,9], defined as

$$\tau(E)=\frac{\hbar}{iL}\operatorname{Tr}S^\dagger\frac{\partial S}{\partial E}=\frac{\hbar}{L}\frac{\partial}{\partial E}\sum_{l=1}^{L}\theta_l(E). \tag{5}$$

Near an isolated pole of the S matrix, $\tau(E)$ is a Lorentzian whose area is normalized to $2\pi\hbar/L$ and whose width is the resonance width. This can easily be seen from the pole expansion of S. The function

$$N_R(E)=\frac{L}{2\pi\hbar}\int_{E_L}^{E}dE'\,\tau(E') \tag{6}$$

is therefore the resonance counting function: It increases *smoothly* when a pole (resonance) is traversed [10]. By inserting (5) into (6) and using (4) we then get

$$N(E)-N_R(E)=-\frac{1}{\pi}\lim_{\epsilon\to 0}\operatorname{Im}\ln Z^{sc}(E+i\epsilon). \tag{7}$$

Differentiating (7) with respect to E we get the difference between the level density $d(E)$ and the "resonance density" $d_R(E)=(L/2\pi\hbar)\tau(E)$:

$$\zeta(E)=d(E)-d_R(E)=-\frac{1}{\pi}\lim_{\epsilon\to 0}\operatorname{Im}\frac{\partial}{\partial E}\ln Z^{sc}(E+i\epsilon). \tag{8}$$

We would like to evaluate the energy average of this quantity. The function $Z^{sc}(E)$ has zeros on the real E axis, at the positions of the billiard eigenvalues, and poles below the real axis, at the poles of $S(E)$. It therefore has neither poles nor zeros above the real axis. So, an integral of (8) along any contour in the upper half E plane vanishes. $S(E+i\epsilon)$ decays exponentially as $\epsilon\to+\infty$, and so, for large enough ϵ,

$$\left|\frac{\partial}{\partial E}\ln Z^{sc}(E+i\epsilon)\right|\to\left|\frac{\partial}{\partial E}\operatorname{Tr}S\right|\sim\exp(-\eta\epsilon), \tag{9}$$

for some $\eta>0$. This implies that smoothing (8) with a Lorentzian of width ϵ vanishes as $\exp(-\eta\epsilon)$. In other words,

$$\langle d(E)\rangle-\langle d_R(E)\rangle\to 0. \tag{10}$$

We see that the spectral and resonance densities possess a common mean, and the right-hand side of (8) measures the fluctuations in the difference between the two functions. It should be emphasized that $d(E)$ is a genuine spectral density, while $d_R(E)$ is a smoothed density function. Because of this, $N(E)$ is a genuine staircase function, while $N_R(E)$ is a smoothed staircase.

To illustrate these results we have calculated the two number functions for the billiard shape shown in the inset of Fig. 1. The results are shown as a function of the wave number k and not of E for the sake of convenience. The transformation to functions of E is straightforward. We show $N(k)$, $N_R(k)$, and $\tau(k)$ for $L=6$, where the resonances overlap. The two functions wind around each other, as implied by (10). We should emphasize that in the present calculation the spectrum calculated from the zeros of $Z^{sc}(k)$ and the *exact* spectrum differ by less than 10^{-4} times the mean level spacing. This astonishingly good fit may be due to the special features of our model, and in particular the smooth matching between the billiard and the waveguide.

The mean value of the Wigner time delay $\tau(E)$ has been shown [11] to approach the value γ^{-1} in the semiclassical ($\hbar\to 0$, $L\to\infty$) limit, where γ is the classical escape rate from the chaotic scatterer. Simple geometrical considerations give us $\gamma\approx Dv/\pi A$, where A is the area of the billiard, v is the velocity, and D is the size of the opening. Recalling that

$$L=\left[\frac{kD}{\pi}\right]\approx\frac{kD}{\pi}=\frac{mvD}{\pi\hbar}, \tag{11}$$

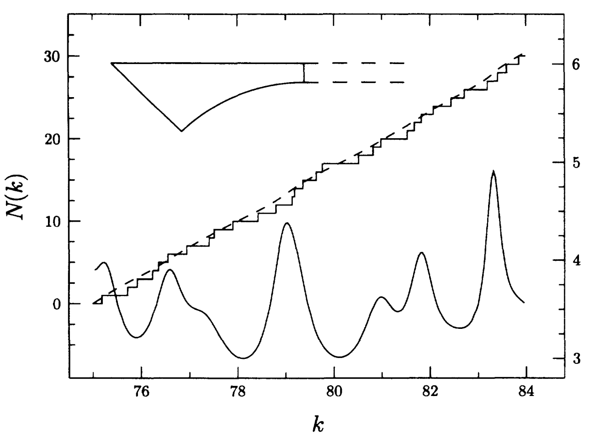

FIG. 1. The time delay (solid curve), spectral number function $N(k)$ (staircase), and the resonance number function $N_R(k)$ (dashed line) for the case of six open channels ($L=6$), as functions of the wave number. Inset: The geometry of the closed billiard and the scattering system. The waveguide connecting to the billiard is also drawn, in dashed lines.

and substituting in (10), we get

$$\langle d(E)\rangle = \langle d_R(E)\rangle = (L/2\pi\hbar)\langle \tau(E)\rangle = mA/2\pi\hbar^2, \qquad (12)$$

which is just the leading term in Weyl's formula for the average level density of a planar billiard in the semiclassical limit. This result also gives a quantum meaning to the classical escape rate γ, namely, $\hbar\gamma$ is proportional to the mean level spacing.

Relation (12) was derived in the $L\gg 1$ limit. However, in the low L limit it holds approximately, with an error of up to a factor of $1+1/L$. Equation (12) emphasizes an interesting relation between the resonance width, which is of the order of $\hbar\gamma$, and the mean resonance separation, which is $\sim(2\pi/L)\hbar\gamma$. One can see that resonances overlap for sufficiently high L, while they remain (mostly) isolated for low L values. Thus, Ericson fluctuations [12] are expected only in the semiclassical domain ($L\gg 1$) even when the underlying classical scattering is chaotic [13].

Our main purpose in this work is to discuss the spectral fluctuations in the semiclassical regime. This is achieved by substituting (2) in (8), which yields

$$\zeta^{sc}(E) = \frac{1}{i}\frac{\partial}{\partial E}\ln\det[S(E)+I] = \frac{1}{i}\frac{\partial}{\partial E}\operatorname{Tr}\ln[S(E)+I]$$
$$= \frac{1}{i}\frac{\partial}{\partial E}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\operatorname{Tr}S^n. \qquad (13)$$

Semiclassically, it is possible to express $\operatorname{Tr}S^n$ in terms of periodic orbits of the Poincaré scattering map, as was shown in detail in [14,15]. Thus,

$$\frac{(-1)^n}{n}\operatorname{Tr}S^n \approx \sum_{\substack{\text{p.p.o.}(s),r\\ rn_s=n}} \frac{1}{|\det(I-M_s^r)|^{1/2}} e^{ir(\Phi_s+n_s\pi)}, \qquad (14)$$

where the sum is over primitive periodic orbits (p.p.o.) of the PSM and repetitions r. n_s is the period, $\hbar\Phi_s$ is the action, and M_s is the stability matrix of the primitive orbit s. The Maslov indices associated with orbit s have here been incorporated into Φ_s.

An orbit of the PSM is constructed by following a particle trajectory in the billiard, starting on the window σ at position y and transverse momentum p_y, until it again reaches σ, at position y' and transverse momentum p_y'. The particle is then reinjected into the cavity by reversing the sign of the longitudinal momentum p_x, while keeping the position y and transverse momentum p_y constant. Note that this corresponds to a specular reflection of the particle at σ. The PSM is then the mapping $(y,p_y)\mapsto(y',p_y')$. A periodic orbit of period n of the PSM therefore corresponds to a periodic orbit of the *closed billiard,* which hits the window σ n times. The phase associated with the periodic orbit of the billiard is just Φ_s, plus an additional Maslov phase of π for each reflection of the particle from σ. Using this fact and incorporating (14) into (13) we get the following expression:

$$\zeta^{sc}(E) \approx \sum_{\text{p.o.}\in\sigma}\frac{\hbar^{-1}t_s}{|\det(I-M_s)|^{1/2}}e^{i\Phi_s}, \qquad (15)$$

where the action Φ_s is now the action of the periodic orbit s of the billiard, and the orbit time is $t_s=\hbar\,\partial\Phi_s/\partial E$.

The summation in (15) is now over all periodic orbits *of the closed billiard* which hit σ *at least once.* This expression is highly reminiscent of the Gutzwiller trace formula [16] for the level density of a billiard in the semiclassical limit. It is in fact a Gutzwiller sum over a *subset* of the periodic orbits of the billiard. However, in a chaotic billiard almost all orbits which are long enough eventually reach σ, and in fact the topological entropy of this subset is equal to the topological entropy of the full-billiard periodic-orbit set. Therefore, this sum is beset by the same convergence problems which plague the Gutzwiller sum. It was shown in [5] (see also [17]) that the resonance density function can be expressed as a sum over all *trapped* periodic orbits of the scattering system. These are just all periodic orbits which never hit σ, and are the complement of the set of all periodic orbits which do hit it. Hence (8) and (15) express a *reordering* of the Gutzwiller sum: $d(E)$ (sum over all periodic orbits) equals $d_R(E)$ (sum over periodic orbits which miss σ) plus $\zeta^{sc}(E)$ (sum over periodic orbits which hit σ). This observation provides an *a posteriori* justification to our statement that (2) is a semiclassical secular function. Indeed, starting from (2) we derived (15), which was shown to be a natural reordering of the Gutzwiller sum for $d(E)$.

We can connect the above results to the experimental determination of spectra of chaotic billiards by means of microwave absorption in the following way. It has been shown [18] that the reflectivity of a weakly absorbing cavity can be written as

$$\Gamma(E) = \frac{1}{L}\mathrm{Tr}[S^{\dagger}(E+i\alpha)S(E+i\alpha)]$$
$$\approx \exp\left(-2\frac{\alpha}{L}\sum_{l=1}^{L}\frac{\partial\theta_l(E)}{\partial E}\right) = \exp[-2\alpha\tau(E)]\,, \tag{16}$$

where $\alpha \ll \gamma$ stands for the effective absorption rate. Measuring the reflectivity therefore amounts to measuring the resonance density $\tau(E)$, which is a smooth function composed of Lorentzians centered at the resonance energies. As long as the resonances are well separated, $\tau(E)$ approximates the spectral density. However, even in such cases some of the resonances may acquire a large width. These resonances contribute to the smooth background of $\tau(E)$, and do not show up as well-defined peaks. This may provide a partial explanation for Stöckmann's failure to identify some 15% of the eigenenergies in his experiment [2] (the finite frequency resolution can also account for some missing values, as he mentions). In contrast to that, knowledge of the scattering *amplitudes* enables one to extract information concerning the eigenvalues of the system, even in the regime of highly overlapping resonances, at least within the context of the semiclassical approximation.

In summary, we would like to make the following comments. The present formalism can be generalized to other systems, which differ either in the form of the scattering potential or in the nature of the free propagation. However, care must be taken to write $Z^{sc}(E)$ in the proper form. The most general form for $Z^{sc}(E)$ is

$$Z^{sc}(E) = \det[S(E) - S_0(E)]\,, \tag{17}$$

where $S_0(E)$ depends on the way in which we choose to close our scattering system. $S_0(E)$ would usually be chosen so that the sytsem would be closed along a coordinate surface, in the coordinate basis we find most convenient. In our case, the system was closed by imposing Dirichlet boundary conditions along the $x=0$ line in the waveguide. Consequently $S_0(E) = -I$, giving us the condition $\det[S(E)+I]=0$. If instead we impose Neumann boundary conditions, we get $S_0(E)=I$, and (2) becomes $\det[S(E)-I]=0$.

The theory presented here bears some likeness to Bogomolny's recent formulation of the spectral secular function in terms of the semiclassically unitary operator analog of a Poincaré map [19]. In the present formalism, we use the S matrix which is always unitary and which is the quantum-mechanical analog of the Poincaré scattering map. The analytical properties of $Z^{sc}(E)$ are similar to those of Bogomolny's secular function, since in both cases they arise from the special form of (7). Finally, we note that the connection made between the spectral density and the scattering matrix indicates a possible link between the statistical properties of the spectral functions and the distribution of the eigenphases of the S matrix. We are currently investigating this connection.

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