Spectral Statistics and Dynamical Localization: Sharp Transition in a Generalized Sinai Billiard

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We consider a Sinai billiard where the usual hard disk scatterer is replaced by a repulsive potential with $V(r) \sim \lambda r^{-\alpha}$ close to the origin. Using periodic orbit theory and numerical evidence we show that its spectral statistics tends to Poisson statistics for large energies when $\alpha < 2$ and to Wigner-Dyson statistics when $\alpha > 2$, while for $\alpha = 2$ it is independent of energy, but depends on λ. We apply the approach of Altshuler and Levitov [Phys. Rep. **288**, 487 (1997)] to show that the transition in the spectral statistics is accompanied by a dynamical localization-delocalization transition. This behavior is reminiscent of a metal-insulator transition in disordered electronic systems.

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The statistical distribution of quantum mechanical energy eigenvalues is of fundamental interest in diverse areas of physics such as condensed matter, atomic, and nuclear physics [1]. In the strict quasiclassical limit, where the de Broglie wavelength is much smaller than all other length scales, the theory of quantum chaos relates the spectral statistics of a quantum system to the dynamics of its classical counterpart. While chaotic classical dynamics leads to Wigner-Dyson random matrix statistics [2], integrable dynamics generically gives rise to Poisson statistics (uncorrelated eigenvalues) [3]. There is overwhelming evidence, both experimental and numerical, for these results [4]. The spectral statistics of systems with mixed classical dynamics is expected to be described by superposing level sequences with Poisson and random matrix statistics, where the respective mean level spacing is determined from the size of the corresponding phase space volume with regular or chaotic dynamics [5].

However, when the de Broglie wavelength is not the smallest length scale in the system, the spectral statistics is not solely determined by the classical dynamics. For example, the classical motion of an electron in a (three-dimensional) disordered system, such as a metal with substantial impurity scattering, can be regarded as completely chaotic. Nevertheless, upon variation of the disorder strength at a fixed energy (Fermi energy), the spectral statistics undergoes a sharp transition from Wigner-Dyson to Poisson statistics [6]. Note that at the critical point the de Broglie wavelength is of the same order of magnitude as the elastic mean free path, a classical length scale. The transition in the spectral statistics is accompanied by a transition from extended to localized eigenstates (Anderson metal-insulator transition) [7]. In the case of disordered systems, one can therefore attribute the deviation of the spectral statistics from what one would expect on the basis of the classical dynamics to the quantum phenomenon of localization.

A similar effect on the spectral statistics may be caused by *dynamical* localization [8,9]. Dynamical localization occurs, for example, in a circular billiard with a rough boundary, where in a certain range of parameters the quantum eigenstates are localized in angular momentum space despite that the classically chaotic dynamics leads to diffusive spreading of an initial angular momentum distribution [10]. As a function of boundary roughness there is a crossover between localized and extended eigenstates, which takes place when the de Broglie wavelength $\lambda_{\rm dB}$ is of the same order of magnitude as a classical length scale set by the roughness $\langle (dR/d\theta)^2 \rangle / R_0$, where $R(\theta)$ defines the rough circle in polar coordinates, $R_0 = \langle R \rangle$, and the average is over the angle [10]. At the same time the level statistics changes smoothly from Poisson to Wigner-Dyson statistics [10,11].

It is the purpose of the present article to show that a dynamical (nonrandom) system may also display a *sharp transition* in the spectral statistics. This is accompanied by a *dynamical* localization-delocalization transition of the eigenstates and is reminiscent of a metal-insulator transition in disordered systems. We thereby extend the list of analogies between dynamical and disordered systems [7].

We consider a generalization of the well-known Sinai billiard (SB). Sinai proved that the free motion of a classical particle being specularly reflected from a disk of radius R inside a square with periodic boundary conditions is completely chaotic [12]. We modify the SB by replacing the disk with the scattering potential

$$V(r) = \begin{cases} \lambda\left[\left(\frac{R}{r}\right)^{\alpha} - 1\right], & r < R \\ 0, & r > R \end{cases}, \qquad (1)$$

where α and λ are positive parameters (see also Fig. 1). Note that in the limit $\alpha \longrightarrow \infty$ the SB is recovered. In a chaotic billiard, the replacement of a hard wall by a soft potential barrier generically leads to the formation of stable islands [13]; however, in the present case these are hardly visible in a Poincaré surface of section and are not relevant for the effect studied here.

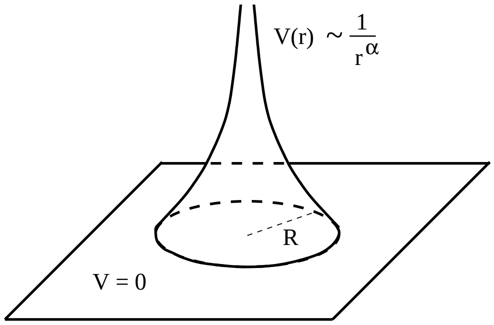

FIG. 1. Potential of the generalized Sinai billiard.

A similar system was considered by Altshuler and Levitov [14]. They focused on the properties of the eigenstates and proved the occurrence of a dynamical localization-delocalization transition. In contrast, the emphasis in the present work is on a transition in the level statistics and on its semiclassical origin. The transition occurs as a function of α at $\alpha = 2$, irrespective of the value of λ. It is a sharp transition in the limit of large energy. Using periodic orbit theory we find that it is caused by a competition between regular ("bouncing ball"-type [15]) and chaotic orbits. In the second part of this article we show that the approach of Altshuler and Levitov may be applied also to the present case. We thereby demonstrate that the transition in the spectral statistics is accompanied by a dynamical delocalization transition of the eigenfunctions.

For large energies, the qualitative quantum dynamics of the generalized Sinai billiard (GSB) is determined by the interplay of three length scales, (i) the de Broglie wavelength λ_{dB}, (ii) the radius $r_c = (E/\lambda + 1)^{-1/\alpha} R$ of the classically forbidden area, and (iii) a typical length $\tilde{l}$ of an orbit before its direction is randomized by scattering from the potential.

When $\alpha > 2$ the potential (1) effectively acts as a hard wall, since the radial wave function then vanishes like $\exp(-c r^{1-\alpha/2})$ with $c = 2\sqrt{\lambda R^{\alpha}}/(\alpha - 2)$ near the origin, i.e., faster than any power. To estimate the behavior of the spectral statistics, we approximate the potential (1) by a hard disk with the energy dependent radius r_c. According to the semiclassical theory [16], the structure in the spectrum on the scale δE is determined by periodic orbits of length $l = hv/\delta E$, where h denotes Planck's constant and v the velocity of the particle. For $l > \tilde{l}$ the chaotic orbits dominate and the spectral statistics will be random-matrix-like, while for $l < \tilde{l}$ the regular orbits dominate, leading to Poisson-like statistics. With $\varepsilon = \delta E/\Delta$ measuring the energy on the scale of the mean level spacing Δ, we expect random-matrix-like behavior on energy scales $\varepsilon < \tilde{\varepsilon}$ and Poisson-like behavior for $\varepsilon > \tilde{\varepsilon}$, where $\tilde{\varepsilon} \sim A/\lambda_{\mathrm{dB}}\, \tilde{l}$ and A denotes the area of the billiard. Now $\tilde{l}$ can be estimated by $\tilde{l} \sim A/r_c$, so that we find $\tilde{\varepsilon} \sim r_c/\lambda_{\mathrm{dB}}$. This ratio scales with energy as $r_c/\lambda_{\mathrm{dB}} \propto E^{(\alpha-2)/2\alpha}$. Consequently, for $\alpha < 2$ and increasing energy, $\tilde{\varepsilon}$ tends to zero, while $\tilde{\varepsilon} \longrightarrow \infty$ for $\alpha > 2$. On this basis we expect a sharp transition between Poisson and random matrix statistics at $\alpha = 2$ in the limit of large energy E. Intuitively, the classically forbidden area becomes invisible to quantum mechanics for $\alpha < 2$, while for $\alpha > 2$ it becomes more and more sizable.

To see this explicitly, we apply Berry's periodic orbit theory of bilinear spectral statistics [16] to the SB with energy dependent disk radius r_c. The SB has two types of periodic orbits: those that never strike the disk and those that do. The former are marginally stable, occur in one-parameter families, and will be referred to as regular orbits, while the latter are unstable, isolated, and will be referred to as chaotic orbits. In the following, we determine the contribution of the regular orbits to the spectral form factor $K(\tau)$. Denoting the unfolded density of states by $d(\varepsilon)$, the form factor is related to the two-point correlation function

$$R(s) = \left\langle d\left(\varepsilon + \frac{s}{2}\right) d\left(\varepsilon - \frac{s}{2}\right)\right\rangle_{\varepsilon} - 1 \qquad (2)$$

by Fourier transformation, $K(\tau) = \int_{-\infty}^{\infty} ds\, e^{2\pi i s\tau} R(s)$. One way to determine the contribution of the regular orbits to the density of states is to suitably modify the trace formula for the empty billiard. To avoid degeneracies in the spectrum, we use a rectangular instead of a quadratic billiard (sidelengths a and b) and quasiperiodic boundary conditions for the wave function, i.e., $\psi(x + a, y) = e^{i\phi_x}\psi(x, y)$ and analogously for the y direction [17]. The eigenvalues of the rectangle without the disk are $E_{jk} = (2\pi j + \phi_x)^2/a^2 + (2\pi k + \phi_y)^2/b^2$ (here and below $\hbar^2/2m = 1$). Applying the Poisson summation formula to the density of states of the empty rectangle and replacing the resulting Bessel function by its asymptotic form leads to a representation as a sum over periodic orbit families. Each family is specified by two integers, m and n (positive or negative), denoting the number of traversals across the billiard in the x and y direction, respectively. Now including the disk obstructs the path of the orbits that violate the condition $2\, l_{mn} r_c(E) < A$, where $A = ab$ and $l_{mn} = [(ma)^2 + (nb)^2]^{1/2}$ denotes the length of the orbits. The remaining families have to be weighted by the area they cover. The oscillatory part of the regular contribution to the unfolded density of states is then

$$\tilde{d}_{\mathrm{reg}}(\varepsilon) = \sqrt{\frac{2}{\pi}} \sum_{(m,n)'} f_{mn}(E) \sum_{j=1}^{\infty} \frac{\cos(jS_{mn} - \frac{\pi}{4})}{(j\, l_{mn})^{1/2} E^{1/4}}, \quad (3)$$

where the first sum is over all primitive orbits and the second over repetitions. In Eq. (3) we have introduced the actions $S_{mn} = l_{mn}\sqrt{E} + m\phi_x + n\phi_y$ and the orbit selection function $f_{mn}(E) = [1 - 2r_c(E)\, l_{mn}/A]\,\theta(A - 2r_c(E)\, l_{mn})$, and set the mean level density to its large energy limit, so that $\varepsilon = AE/4\pi$. This formula is a simple generalization of the expression for the usual SB given in Ref. [18]. Substituting Eq. (3) into (2) and retaining only the diagonal terms in the double sum over periodic orbits (the diagonal approximation is justified by the energy average and known to be exact for regular systems [16]) yields the contribution of the regular orbits to the form factor

$$K_{\text{reg}}(\tau) = \sum_{(m,n)'} f_{mn}^2(E) \sum_{j=1}^{\infty} \frac{\delta(\tau - j\, l_{mn}/A\sqrt{E})}{2\pi j\, l_{mn}\sqrt{E}}. \quad (4)$$

This expression may be evaluated approximately by replacing the sums over primitive orbits and repetitions by a single sum over all orbits (m,n). In the large E limit,

$$K_{\text{reg}}(\tau) \sim (1 - cE^{(\alpha-2)/2\alpha}\tau)^2\, \theta(1 - cE^{(\alpha-2)/2\alpha}\tau), \quad (5)$$

with $c = 2R\lambda^{1/\alpha}$. Equation (5) shows that the contribution of the regular orbits to the form factor tends to zero for $\alpha > 2$, while for $\alpha < 2$ the Poisson limit $K(\tau) = 1$ is attained. The contribution of the chaotic orbits assures that for $\alpha > 2$ GOE statistics of random matrix theory is reached. To see this explicitly would require going beyond the diagonal approximation.

Next, we verify the above theoretical prediction of a transition in the spectral statistics of the GSB numerically. For $\alpha < 2$, the eigenvalues of the GSB may be calculated by diagonalizing the Hamiltonian in the eigenbasis of the empty billiard. However, for $\alpha \geq 2$ the matrix elements diverge and it is natural to work in the eigenbasis of the $1/r^{\alpha}$-potential [19]. In this regime we chose to apply the Korringa-Kohn-Rostoker method, as described in Ref. [18] for the case of the ordinary SB. The difference with respect to Ref. [18] is that in the present case the scattering phase shifts of the potential have to be determined by solving the radial Schrödinger equation numerically, while they can be expressed in terms of Bessel functions for the usual SB. This makes the present case computationally more demanding.

Figure 2 shows the cumulative spacing distribution $N(s) = \int_0^s dx\, P(x)$, with $P(s)$ denoting the nearest-neighbor spacing distribution, for $\alpha = 1$ and 4 (we used $\lambda = 8$ for the former, $\lambda = 0.01$ for the latter, and in both cases $R = 1$ with a billiard of area 4π). Each curve is displayed with two reference curves, $N(s) = 1 - e^{-s}$ for Poisson statistics and the Wigner surmise $N(s) = 1 - \exp(-\frac{\pi}{4}s^2)$ for the GOE. We observe a clear movement of $N(s)$ towards the Poisson curve with increasing energy for $\alpha = 1$ and towards the Wigner surmise for $\alpha = 4$. Considering the relatively weak energy dependence of the spectral statistics, see Eq. (5), the limiting distributions are not expected to be reached within the available spectra. We verified that for $\alpha = 2$ the spectral statistics is independent of energy in accordance with Eq. (5).

We turn to the properties of the eigenfunctions of the GSB. To keep the discussion general, we consider the GSB in $d \geq 2$ dimensions. Following Ref. [14]

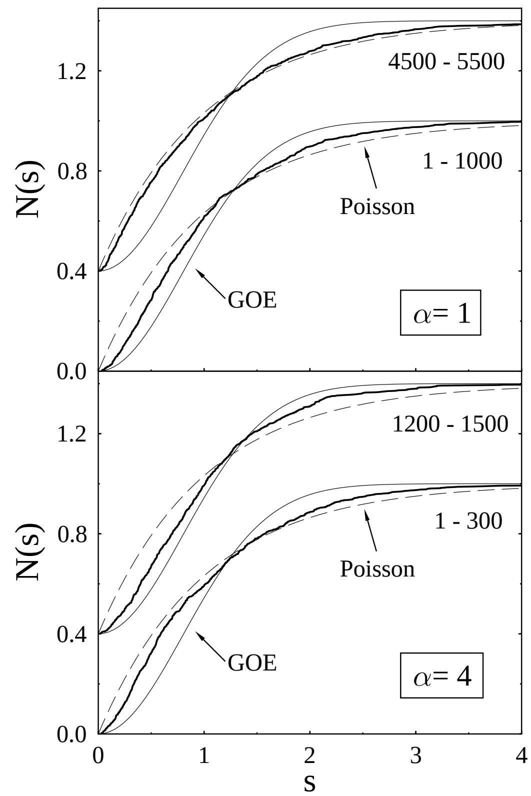

FIG. 2. Cumulative nearest-neighbor spacing distribution for the generalized Sinai billiard. The energy levels that were used are indicated below the curves (for $\alpha = 4$ an average over three different aspect ratios a/b at constant area $ab = 4\pi$ was taken). With increasing energy a clear movement towards Poisson statistics for $\alpha = 1$ and towards GOE statistics for $\alpha = 4$ is visible.

we map the Schrödinger equation for the GSB on a localization problem. Applying Levitov's criterion of a diverging number of resonances [20] we then show that $\alpha = 2$ corresponds to a critical point associated with a delocalization transition.

Using periodic boundary conditions and a billiard of unit volume, the Schrödinger equation in momentum representation takes the form

$$E_{\mathbf{k}}\, c_{\mathbf{k}} + \sum_{\mathbf{k}' \neq \mathbf{k}} V_{\mathbf{k}-\mathbf{k}'} c_{\mathbf{k}'} = E\, c_{\mathbf{k}}, \quad (6)$$

where $\mathbf{k}$ denotes a site in the reciprocal lattice, $c_{\mathbf{k}}$ the Fourier coefficients of the wave function, $V_{\mathbf{k}}$ those of the potential, and $E_{\mathbf{k}} = \mathbf{k}^2 + V_{\mathbf{0}}$. Equation (6) may be interpreted as the Schrödinger equation of a particle on a lattice with on-site energies $E_{\mathbf{k}}$ and hopping amplitudes $V_{\mathbf{k}}$. Considering an eigenfunction with energy E, one finds [14] that its Fourier coefficients are nonvanishing only in an energy shell $E - \delta E < E_{\mathbf{k}} < E + \delta E$, where δE is proportional to λ, which is assumed to be much smaller than E. Within this quasi-$(d-1)$-dimensional shell, the on-site energies $E_{\mathbf{k}}$ are uniformly distributed quasirandom numbers. Since $V_{\mathbf{k}} \propto 1/k^{d-\alpha}$ for large k, one may interpret Eq. (6) as an Anderson model with long-range power-law hopping within the energy shell [14]. A delocalization transition occurs when the mean number of *resonances* per site diverges [20]. A resonance is defined as a pair of sites $\mathbf{k},\mathbf{k}'$ that fulfill the condition $|V_{\mathbf{k}-\mathbf{k}'}| > |E_{\mathbf{k}} - E_{\mathbf{k}'}|$. If two sites are in resonance, the eigenstates of the corresponding two by two eigenvalue problem have amplitudes $c_{\mathbf{k}},c_{\mathbf{k}'}$ that are comparable in magnitude. Informally, they can then be considered as "linked" and an eigenstate can spread along this link. If the mean number of resonances per site is infinite, there can be no localization, irrespective of the hopping strength.

Noting that for $V_{\mathbf{k}-\mathbf{k}'} \ll \delta E$ [21] the probability that the sites $\mathbf{k}, \mathbf{k}'$ are in resonance is simply $|V_{\mathbf{k}-\mathbf{k}'}|/\delta E$, the mean number of resonances $\mathcal{N}$ with a fixed site $\mathbf{k}$ can be estimated by summing the probability over the energy shell,

$$\mathcal{N} = \frac{1}{\delta E} \sum_{\mathbf{k}' \in \delta E} |V_{\mathbf{k}-\mathbf{k}'}| \sim \frac{1}{\sqrt{E}} \int_0^{\sqrt{E}} dk\, k^{d-2}\, V_k \,. \tag{7}$$

The sum is estimated by an integration over a flat region of radius $\sqrt{E}$ (we used $\Delta k = \delta E/2\sqrt{E}$ for the width of the energy shell and dropped an energy independent factor). Substituting the asymptotic form of V_k for large k into Eq. (7) we find that the mean number of resonances per site diverges in the limit of large energy when $\alpha > 2$, independent of the dimension. In the case that was considered by Altshuler and Levitov [14] the same consideration leads to a critical α of one. For α below the critical value, the eigenstates are localized with a power-law tail due to direct hopping, independent of λ when $d \leq 3$ (because the effective lattice, i.e., the energy shell, is two-dimensional for $d = 3$), and also for small λ when $d > 3$.

In summary, we have shown that the GSB displays a sharp transition in the spectral statistics, which is caused by a competition between chaotic and regular orbits. It is accompanied by a dynamical delocalization transition of the eigenstates. The investigation helps to clarify the relation between disordered systems and quantum chaos.

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