Quantum Billiards with Surface Scattering: Ballistic Sigma-Model Approach

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Statistical properties of energy levels and eigenfunctions in a ballistic system with diffusive surface scattering are investigated. The two-level correlation function, the level number variance, the correlation function of wave function intensities, and the inverse participation ratio are calculated. [S0031-9007(98)06025-6]

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The statistical properties of spectra of disordered diffusive systems are now well understood. Using the supersymmetric σ-model approach it has been possible to demonstrate the relevance of the random matrix theory (RMT) and to calculate deviations from its predictions both for the level [1–3] and eigenfunction [4–6] statistics. Generalization of these results to the case of a chaotic *ballistic* system (i.e., quantum billiard) has become a topic of great research interest. For ballistic disordered systems the σ model has been proposed [7], with the Liouville operator replacing the diffusion operator in the action. It has also been conjectured that the same σ model in the limit of vanishing disorder describes statistical properties of spectra of an individual classically chaotic system. This conjecture was further developed in [8,9] where the σ model was obtained by means of energy averaging, and the Liouville operator was replaced by its regularization—the Perron-Frobenius operator.

However, a straightforward application of the results of Refs. [2–4,6] to the case of an individual chaotic system is complicated by the fact that the eigenvalues of the Perron-Frobenius operator are unknown, while its eigenfunctions are extremely singular. For this reason the σ-model approach has so far failed to provide explicit results for any particular ballistic system.

To overcome this difficulty, we consider a model of a billiard with surface disorder leading to diffusive scattering of a particle in each collision with the boundary. This models behavior of a quantum particle in a box with a rough boundary which is irregular on the scale of the wavelength. Since the particle loses memory of its direction of motion after a single collision, this model describes a limit of an "extremely chaotic" ballistic system, with typical relaxation time being of order of the flight time. (This should be contrasted with the case of a relatively slight distortion of an integrable billiard [10].) One might naively think that all results for such a model could be obtained by setting $l \approx L$ in a system with bulk disorder. In fact, the level statistics in a system with bulk disorder and arbitrary relation between mean free path l and system size L were studied in [11]. However, our results are qualitatively different in some respects, which shows that systems with bulk and surface disorder are not equivalent. On the other hand, our findings are in agreement with general expectations for chaotic billiards based on the trace formula treatment [12].

To simplify the calculations, we consider a circular billiard. A similar problem was studied numerically in Ref. [13] for a square geometry. We consider only the case of unitary symmetry (broken time-reversal invariance); generalization to the orthogonal case is straightforward. The level statistics for the same problem were independently studied in Ref. [14].

Properties of the Liouville operator.—Our starting point is the σ-model for ballistic disordered systems [7]. The effective action for this model has the form

$$F[g(\boldsymbol{r},\boldsymbol{n})] = \frac{\pi\nu}{4}\int d\boldsymbol{r}\,\mathrm{Str}\Big(i\omega\Lambda\langle g(\boldsymbol{r})\rangle - \frac{1}{2\tau(\boldsymbol{r})}\langle g(\boldsymbol{r})\rangle^2 - 2v_F\langle\Lambda U^{-1}\boldsymbol{n}\nabla U\rangle\Big). \quad (1)$$

Here a 8×8 supermatrix g depends on the coordinate $\boldsymbol{r}$ and direction of the momentum $\boldsymbol{n}$. The angular brackets denote averaging over $\boldsymbol{n}$: $\langle\mathcal{O}(\boldsymbol{n})\rangle = \int d\boldsymbol{n}\,\mathcal{O}(\mathbf{n})$ with the normalization $\int d\boldsymbol{n} = 1$. The matrix g is constrained by the condition $g(\boldsymbol{r},\boldsymbol{n})^2 = 1$, and can be represented as $g = U\Lambda U^{-1}$, with $\Lambda = \mathrm{diag}(1,1,1,1,-1,-1,-1,-1)$; see [1,9] for more detailed definitions. Since we are interested in the clean limit with no disorder in the bulk, the second term in the action (1) containing the elastic mean free time τ is zero everywhere except at the boundary where it modifies the boundary condition (see below).

Many statistical properties of energy levels [2,3] and eigenfunctions [4,6] are governed by the structure of the action in the vicinity of the homogeneous configuration of the g field, $g(\boldsymbol{r},\boldsymbol{n}) = \Lambda$. Writing $U = 1 - W/2 + \cdots$, we find the action in the leading order in W,

$$F_0[W] = -\frac{\pi\nu}{4}\int d\boldsymbol{r}\,d\boldsymbol{n}\,\mathrm{Str}[W_{21}(\hat{K} - i\omega)W_{12}], \quad (2)$$

where the indices $1,2$ refer to the "advanced-retarded" decomposition of W, and the Liouville operator

$\hat{K} \equiv v_F \boldsymbol{n}\nabla$. This "linearized" action has the same form as that of a diffusive system, with the diffusion operator being replaced by the Liouville operator. This enables us to use the results derived for the diffusive case by substituting the eigenvalues and eigenfunctions of the operator $\hat{K}$ for those of the diffusion operator.

The operator $\hat{K}$ should be supplemented by a boundary condition, which depends on the form of the surface roughness. As a model approximation we consider purely diffusive scattering [15] for which the distribution function $\varphi(\boldsymbol{r}, \boldsymbol{n})$ of the outgoing particles is constant and is fixed by flux conservation:

$$\varphi(\boldsymbol{r}, \boldsymbol{n}) = \pi \int_{(\boldsymbol{N}\boldsymbol{n}')>0} (\boldsymbol{N}\boldsymbol{n}')\varphi(\boldsymbol{r}, \boldsymbol{n}')\, d\boldsymbol{n}', \qquad (\boldsymbol{N}\boldsymbol{n}) < 0\,.$$

Here the point $\boldsymbol{r}$ lies at the surface, and $\boldsymbol{N}$ is an outward normal to the surface. This boundary condition should be satisfied by the eigenfunctions of $\hat{K}$.

The eigenvalues λ of the operator $\hat{K}$ corresponding to angular momentum l obey the equation

$$\tilde{J}_l(\xi) \equiv -1 + \frac{1}{2}\int_0^{\pi} d\theta \sin\theta \exp[2il\theta + 2\xi \sin\theta] = 0\,, \tag{3}$$

where $\xi \equiv R\lambda/v_F$, and R is the radius of the circle. For each value of $l = 0, \pm 1, \pm 2, \ldots$, Eq. (3) has a set of solutions ξ_{lk} with $\xi_{lk} = \xi_{-l,k} = \xi^*_{l,-k}$, which can be labeled with $k = 0, \pm 1, \pm 2, \ldots$ (even l) or $k = \pm 1/2, \pm 3/2, \ldots$ (odd l). For $l = k = 0$ we have $\xi_{00} = 0$, corresponding to the zero mode $\varphi(\boldsymbol{r}, \boldsymbol{n}) = \text{const}$. All other eigenvalues have positive real part $\mathrm{Re}\,\xi_{lk} > 0$ and govern the relaxation of the corresponding classical system to the homogeneous distribution in the phase space.

The asymptotic form of the solutions of Eq. (3) for large $|k|$ and/or $|l|$ can be obtained by using the saddle-point method,

$$\xi_{kl} \approx \begin{cases} 0.66l + 0.14\ln l + 0.55\pi ik, & 0 \le k \ll l\,, \\ (\ln k)/4 + \pi i(k + 1/8), & 0 \le l \ll k\,. \end{cases} \tag{4}$$

Note that for $k = 0$ all eigenvalues are real, while for high values of k they lie close to the imaginary axis and do not depend on l (see Fig. 1).

Level statistics, low frequencies.—We define the level correlation function in a standard way,

$$R_2(\omega) = (\Delta V)^2\langle \nu(\epsilon + \omega)\nu(\epsilon)\rangle - 1\,,$$

where $\nu(\epsilon)$ is the density of states, $\Delta = (V\nu)^{-1}$ is the mean level spacing, and $V = \pi R^2$ is the area. In the range of relatively low frequencies (which for our problem means $\omega \ll v_F/R$; see below) the function $R_2(\omega)$ quite generally has the form [2] ($s = \omega/\Delta$)

$$R_2(s) = \delta(s) - \frac{\sin^2 \pi s}{(\pi s)^2} + A\left(\frac{R\Delta}{\pi v_F}\right)^2 \sin^2 \pi s\,. \tag{5}$$

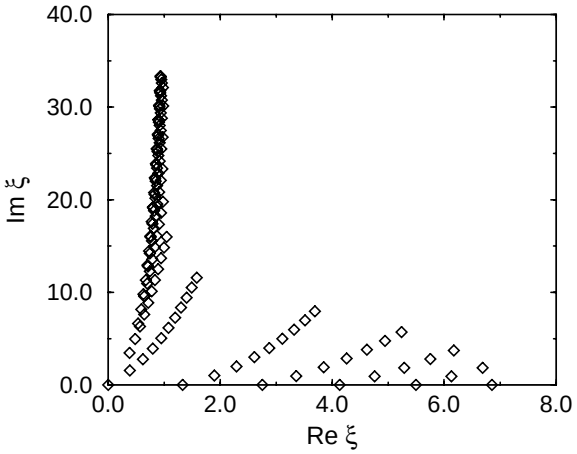

FIG. 1. First 11×11 ($0 \le k, l < 11$) eigenvalues of the Liouville operator $\hat{K}$ in units of v_F/R, as given by Eq. (3).

The first two terms correspond to the zero-mode approximation and are given by RMT, while the last one is the nonuniversal correction to the RMT results. The information about the operator $\hat{K}$ enters through the dimensionless constant $A = \sum' \xi_{kl}^{-2}$, where the prime indicates that the eigenvalue $\xi_{00} = 0$ is excluded. The value of A, as well as the high-frequency behavior of $R_2(s)$ (see below), can be extracted from the spectral function [16]

$$S(\omega) = \sum_l S_l(\omega); \qquad S_l(\omega) \equiv \sum_k (\lambda_{kl} - i\omega)^{-2}. \tag{6}$$

According to the Cauchy theorem, S_l can be represented as an integral in the complex plane,

$$S_l(\omega) = \left(\frac{R}{v_F}\right)^2 \frac{1}{2\pi i}\oint_C \frac{1}{(z - i\omega R/v_F)^2}\,\frac{\tilde{J}_l'(z)}{\tilde{J}_l(z)}\,dz\,,$$

where the contour C encloses all zeros of the function $\tilde{J}_l(z)$. Evaluating the residue at $z = i\omega R/v_F$, we find

$$S_l(\omega) = -(R/v_F)^2 \frac{d^2}{dz^2}\bigg|_{z=i\omega R/v_F} \ln \tilde{J}_l(z)\,. \tag{7}$$

Considering the limit $\omega \to 0$ and subtracting the contribution of $\lambda_{00} = 0$, we get

$$A = -19/27 - 175\pi^2/1152 + 64/(9\pi^2) \approx -1.48\,. \tag{8}$$

In contrast to the diffusive case, this constant is negative: the level repulsion is enhanced with respect to the result for RMT. Equation (5) is valid as long as the correction is small compared to the RMT result, i.e., provided ω is below the inverse time of flight, v_F/R.

Level statistics, high frequencies.—In the range $\omega \gg \Delta$ the level correlation function can be decomposed into the smooth Altshuler-Shklovskii (AS) part $R_2^{\mathrm{AS}}(\omega) = (\Delta^2/2\pi^2)\,\mathrm{Re}S(\omega)$ [16] and the part R_2^{osc} which oscillates on the scale of the level spacing. Evaluating the asymptotic behavior of $S_l(\omega)$ from Eq. (7), we find in the high-frequency regime when $\omega \gg v_F/R$,

$$R_2^{\rm AS}(\omega) = \left(\frac{\Delta R}{v_F}\right)^2 \left(\frac{v_F}{2\pi\omega R}\right)^{1/2} \cos\left(4\frac{\omega R}{v_F} - \frac{\pi}{4}\right). \tag{9}$$

The oscillating part of the level correlation function $R_2^{\rm osc}(s)$ for frequencies $\omega \gg \Delta$ is given by [8]

$$R_2^{\rm osc}(s) = (1/2\pi^2)\cos(2\pi s)D(s), \tag{10}$$

where $D(s)$ is the spectral determinant,

$$D(s) = s^{-2} \prod_{kl\neq(00)} (1 - is\Delta/\lambda_{kl})^{-1}(1 + is\Delta/\lambda_{kl})^{-1}.$$

Since $\Delta^{-2}\partial^2 \ln D(s)/\partial s^2 = -2\,\mathrm{Re}\,S(\omega)$, we can restore $D(s)$ from Eqs. (6) and (7) up to a factor of the form $\exp(c_1 + c_2 s)$, with c_1 and c_2 being arbitrary constants. These constants are fixed by the requirement that Eq. (10) in the range $\Delta \ll \omega \ll v_F/R$ should reproduce the low-frequency behavior (5). As a result, we obtain

$$D(s) = \left(\frac{\pi}{2}\right)^6 \frac{1}{N} \prod_l \frac{1}{\tilde{J}_l(isN^{-1/2})\tilde{J}_l(-isN^{-1/2})}. \tag{11}$$

Here $N = (v_F/R\Delta)^2 = (p_F R/2)^2$ is the number of electrons below the Fermi level. For high frequencies $\omega \gg v_F/R$ this yields the following expression for the oscillating part of the level correlation function:

$$R_2^{\rm osc}(\omega) = \frac{\pi^4}{128}\left(\frac{\Delta R}{v_F}\right)^2 \cos\left(\frac{2\pi\omega}{\Delta}\right). \tag{12}$$

It is remarkable that the amplitude of the oscillating part does not depend on frequency. This is in contrast to the diffusive case, where in the AS regime (ω above the Thouless energy) the oscillating part $R_2^{\rm osc}(\omega)$ is exponentially small [3].

The level number variance.—The smooth part of the level correlation function can be best illustrated by plotting the variance of the number of levels in an energy interval of width $E = s\Delta$,

$$\Sigma_2(s) = \int_{-s}^{s} (s - |\tilde{s}|)R_2(\tilde{s})\, d\tilde{s}, \tag{13}$$

A direct calculation gives for $s \ll N^{1/2}$

$$\pi^2\Sigma_2(s) = 1 + \gamma + \ln(2\pi s) + As^2/(2N) \tag{14}$$

and for $s \gg N^{1/2}$

$$\pi^2\Sigma_2(s) = 1 + \gamma + \ln\frac{16N^{1/2}}{\pi^2} - \frac{\pi^2}{16}\left(\frac{2N^{1/2}}{\pi s}\right)^{1/2} \cos\left(\frac{4s}{N^{1/2}} - \frac{\pi}{4}\right). \tag{15}$$

Here $\gamma \approx 0.577$ is Euler's constant, and A is defined by Eq. (8). The first three terms on the right-hand side of Eq. (14) represent the RMT contribution (curve 1 in Fig. 2).

As seen from Fig. 2, the two asymptotics (14) and (15) perfectly match in the intermediate regime, $s \sim N^{1/2}$. Taken together, they provide a complete description of $\Sigma_2(s)$. According to Eq. (15), the level number variance saturates at the value $\Sigma_2^{(0)} = \pi^{-2}[1 + \gamma + \ln(16N^{1/2}/\pi^2)]$, in contrast to the behavior found for diffusive systems [16] or ballistic systems with weak bulk disorder [11]. The saturation occurs at energies $s \sim N^{1/2}$, or in conventional units $E \sim v_F/R$. This saturation of $\Sigma_2(s)$, as well as its oscillations on the scale set by short periodic orbits, is expected for a generic chaotic billiard [12]. It is also in good agreement with the results for $\Sigma_2(s)$ found numerically for a tight-binding model with moderately strong disorder on boundary sites [13].

Eigenfunction statistics.—Now we study correlations of the amplitudes of an eigenfunction in two different points. Following Ref. [6], we define

$$\alpha(\boldsymbol{r}_1, \boldsymbol{r}_2, E) = \Delta V^2 \left\langle \sum_\mu |\psi_\mu(\boldsymbol{r}_1)\psi_\mu(\boldsymbol{r}_2)|^2 \delta(E - \epsilon_\mu) \right\rangle,$$

where ψ_μ are the eigenfunctions corresponding to the exact single-particle states μ. A calculation analogous to that of Ref. [6] yields

$$\alpha(\boldsymbol{r}_1, \boldsymbol{r}_2, E) = 1 + \Pi(\boldsymbol{r}_1, \boldsymbol{r}_2), \tag{16}$$

where Π is the Green's function of the operator $\hat{K}$ integrated over directions of momentum, $\Pi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \int d\boldsymbol{n}_1\, d\boldsymbol{n}_2\, g(\boldsymbol{r}_1, \boldsymbol{n}_1; \boldsymbol{r}_2, \boldsymbol{n}_2)$. Here g is a solution of the equation

$$\hat{K} g(\boldsymbol{r}_1, \boldsymbol{n}_1; \boldsymbol{r}_2, \boldsymbol{n}_2) = \frac{1}{\pi\nu}\left[\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\delta(\boldsymbol{n}_1 - \boldsymbol{n}_2) - \frac{1}{V}\right].$$

Direct calculation gives

$$\Pi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \Pi_1(\boldsymbol{r}_1, \boldsymbol{r}_2) + \Pi_2(\boldsymbol{r}_1, \boldsymbol{r}_2), \tag{17}$$

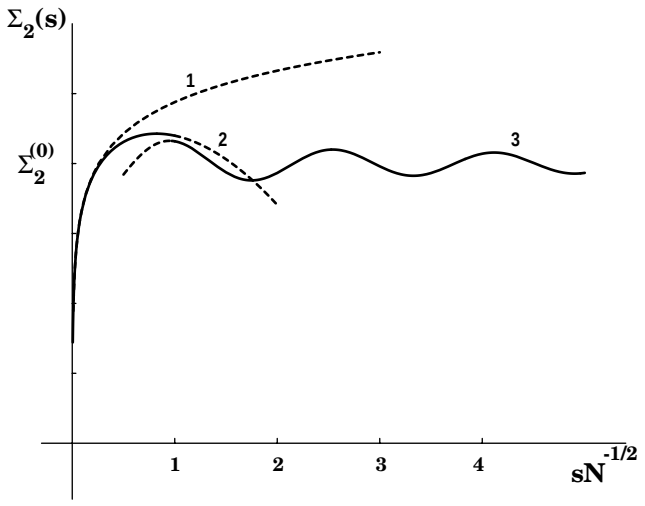

FIG. 2. Level number variance $\Sigma_2(E)$ as a function of energy; $s = E/\Delta$. Curve 1 shows the RMT result, while curves 2 and 3 correspond to asymptotic regimes of low (14) and high (15) frequencies. The saturation value $\Sigma_2^{(0)}$ is given in the text.

$$\Pi_1(\boldsymbol{r}_1,\boldsymbol{r}_2) = \tilde{k}_d(\boldsymbol{r}_1-\boldsymbol{r}_2) - V^{-1}\int d\boldsymbol{r}_1'\,\tilde{k}_d(\boldsymbol{r}_1'-\boldsymbol{r}_2) - V^{-1}\int d\boldsymbol{r}_2'\,\tilde{k}_d(\boldsymbol{r}_1-\boldsymbol{r}_2') + V^{-2}\int d\boldsymbol{r}_1'\,d\boldsymbol{r}_2'\,\tilde{k}_d(\boldsymbol{r}_1'-\boldsymbol{r}_2');$$
$$\Pi_2(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{4\pi p_F R}\sum_{k=1}^{\infty}\frac{4k^2-1}{4k^2}\left(\frac{r_1 r_2}{R^2}\right)^k \cos k(\theta_1-\theta_2), \tag{18}$$

where $\tilde{k}_d(\boldsymbol{r}) = 1/(\pi p_F|\boldsymbol{r}|)$, and (r,θ) are the polar coordinates. This formula has a clear interpretation. The function Π can be represented as a sum over all paths leading from $\boldsymbol{r}_1$ to $\boldsymbol{r}_2$, with possible surface scattering in between. In particular, Π_1 corresponds to direct trajectories from $\boldsymbol{r}_1$ to $\boldsymbol{r}_2$ with no reflection from the surface. Hence, the term Π_1 is insensitive to the geometry of the system. It can be obtained from the RMT-like conjecture that amplitudes of different wave functions are independent Gaussian variables [17]. More precisely, we find that the function [6,17] $k_d(\mathbf{r}_1-\mathbf{r}_2) = J_0^2(p_F|\mathbf{r}_1-\mathbf{r}_2|)$ is replaced in Eq. (18) by its smoothed version, $\tilde{k}_d(\mathbf{r}_1-\mathbf{r}_2) = 1/(\pi p_F|\mathbf{r}_1-\mathbf{r}_2|)$. This is because our semiclassical approach is valid on scales much larger than the wave length. Thus, one has to replace $\tilde{k}_d(\mathbf{r})$ by $k_d(\mathbf{r})$ in the expression (18) for Π_1. The contribution Π_2 is due to the surface scattering. The first term in the numerator $4k^2-1$ comes from trajectories with only one surface reflection, while the second sums up contributions from multiple reflections. A formula analogous to (16) was proposed recently for a generic chaotic system [18].

Finally, we calculate the inverse participation ratio, $\langle P_2\rangle \equiv V^{-2}\int d\boldsymbol{r}\,\alpha(\boldsymbol{r},\boldsymbol{r})$, which characterizes the degree of spatial uniformity of eigenfunctions. The RMT prediction for this quantity $P_2^{(0)} = 2/V$ is recovered from Eqs. (16) and (18) if we take into account the first term in the expression for Π_1, since $k_d(0) = 1$. The leading correction comes from the single-reflection contribution to the term Π_2, and is equal to

$$\delta P_2 = V^{-1}(4\pi p_F R)^{-1}\ln(p_F R) \sim P_2^{(0)} N^{-1/2}\ln N.$$

In conclusion, we have used the ballistic σ-model approach to study statistical properties of levels and eigenfunctions in a billiard with diffusive surface scattering, which exemplifies a ballistic system in the regime of strong chaos. We have found that the level repulsion and the spectral rigidity are enhanced compared to RMT. In particular, the level number variance saturates at the scale of the inverse time of flight, in agreement with Berry's prediction for a generic chaotic system [12]. As another manifestation of the strong spectral rigidity, the oscillating part of the level correlation function does not vanish at large level separation. We have also considered correlations of eigenfunction amplitudes in different spatial points and calculated the deviation of the inverse participation ratio from the RMT value.

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