Chaotic Diffusion and the Statistics of Universal Scattering Fluctuations

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(Received 4 November 1993)

The general properties of quantum transport fluctuations associated with classical chaotic diffusion are analyzed in the framework of chaotic scattering on a simple dynamical model exhibiting universal transmission fluctuations. Quasiclassical approximations for S-matrix correlations are found, and a connection between correlation width and average conductance is demonstrated on numerical data.

PACS numbers: 05.45.+b, 72.15.Rn

Recent investigations on quantum manifestations of classical chaos have given birth to a general semiclassical approach to quantum transport fluctuations, based on classical chaotic scattering [1]. Application of such ideas to conduction in mesoscopic electronic devices of size comparable to the elastic mean free path has led to prediction of Ericson-like transmission fluctuations connected with classical chaotic dynamics [2]. Less studied is the problem of chaotic scattering when the classical dynamics in the interaction region is not only chaotic but also diffusive [3]. In the particular problem of electronic conduction, this situation occurs in the metallic Ohmic regime and gives rise to universal conductance fluctuations [4], which appear to stem from a subtle interplay between diffusion and weak localization. On the other hand, chaotic deterministic diffusion is a rather general aspect of classical chaotic motion, and occurs in a variety of different situations. A prototype is the celebrated standard map, also known as kicked rotor (KR), which has provided highlights for the study of diffusive excitation occurring in many time-dependent problems. The quantum version of the KR exhibits a dynamical localization effect, and it was upon recognizing the affinity of this effect to Anderson localization that the first link between quantum chaology and solid state physics was historically established [5]. It is nowadays known that dynamical localization appears in many relaxation processes in which the decay of metastable states is classically determined by a chaotic diffusion [6].

Does the similarity between Anderson and dynamical localization extend so far as to entail an equivalent for universal conductance fluctuations? This is the starting question of this paper, in which scattering fluctuations associated with chaotic diffusion are studied in the context of the quantum-classical correspondence. To this end we use a one-dimensional toy model closely related to the KR, which has been presented elsewhere [7]. Though physically artificial, this model retains the basic ingredients of classical and quantum transport and, compared to more physical models, offers the advantage of a much easier numerical investigation, both in the quantum and in the classical version. Here we present an analysis of scattering fluctuations in the diffusive regime. First we provide evidence for universal transmission fluctuations in quantitative agreement with theoretical predictions for quasi-one-dimensional disordered solids [8,9]. This result confirms the validity of our model for the quantum diffusive regime and is introductory to the core of this paper, where correlation functions of S-matrix elements (CFS) at different (quasi)energies are investigated. Such correlations play a central role in the theory of chaotic scattering, because they are quasiclassically related to the classical law ruling the decay in time of the survival probability in the interaction region [1,10]. If the latter is exponential at large times, then a Lorentzian form is expected for the squared moduli of CFS at small energies, with a correlation width given by the classical decay rate. Our results for diffusive transport confirm this expectation for the CFS of transmission S-matrix elements, but show instead non-Lorentzian CFS for reflection elements. We explain these results by means of quasiclassical approximations based on the diffusion equation; moreover, we introduce a "local" definition of correlation width that can be estimated in classical terms in all cases. A natural connection between transmission correlation widths and average conductance in the diffusive regime is demonstrated by our numerical results.

Our present description of the model will be a rather compact one; we defer the reader to Ref. [7] for a detailed presentation. We consider a particle moving on a line with coordinate q and momentum k. The interaction region (the "sample") is defined by $q_0 \leq q \leq q_0 + L$. The

0031-9007/94/72(11)/1463(4)$06.00

discrete-time dynamics of our particle is defined by an area-preserving map, which inside the interaction region takes the form

$$\bar{q} = q - H'(k), \quad \bar{k} = k + \bar{q}\tau. \tag{1}$$

Instead, outside the interaction region, i.e., in the "leads," k is constant and q changes according to Eq. (1). Thus free motion is the stroboscopic evolution defined by the Hamiltonian $H(k)$, that is a uniform motion at a constant speed $H'(k)$. If the free Hamiltonian is taken in the form $H(k) = b\cos k$, then the dynamics inside the interaction region is described by the standard map (SM). As is well known, in the strongly chaotic regime ($b\tau \gg 1$) k is completely randomized and (1) gives rise to diffusive transport in q, according to the Fokker-Planck (FP) equation:

$$\frac{\partial f(q,t)}{\partial t} = \frac{D}{2}\frac{\partial^2 f(q,t)}{\partial q^2} \tag{2}$$

with the diffusion coefficient $D = \beta D_0$, where β depends in a known way on $K = b\tau$, and D_0 is the quasilinear diffusion coefficient computed from (1) in the random phase approximation. In our case for numerical convenience we chose $H(k) = b\xi^{-1}\arctan(\xi\cos k)$, which yields the SM in the limit $\xi \to 0$. The physical picture underlying our model is that of an ensemble of particles which impinge on the sample with randomly distributed momenta k and diffuse therein according to (1) until they escape from either end. Associated with this picture is a boundary value problem for the diffusion equation (2), defined by nonhomogeneous boundary conditions which, in the SM case, read

$$\begin{aligned} \frac{2\beta-1}{4}D_0 f'(q_0) + \frac{b}{\pi}f(q_0) &= \Phi_{\mathrm{in},1}(t), \\ \frac{2\beta-1}{4D}{}_0 f'(q_0+L) + \frac{b}{\pi}f(q_0+L) &= \Phi_{\mathrm{in},2}(t), \end{aligned} \tag{3}$$

where arbitrarily prescribed incoming fluxes from the left (1) and right (2) boundaries appear on the right-hand side. The left-hand sides of (3) completely define (in statistical terms) the coupling of the sample to the leads, and are dictated by the map (1) [7]. On solving the boundary value problem one gets outgoing fluxes in terms of incoming ones ($i = 1, 2$),

$$\Phi_{\mathrm{out},i}(t) = \sum_{j=1}^{2}\int_0^\infty R_{ij}(\sigma)\Phi_{\mathrm{in},j}(t-\sigma)d\sigma. \tag{4}$$

The kernels $R_{ij}(\sigma)$ are explicitly given in Ref. [11]. Their integrals over the delay σ yield a transmission coefficient if $i \neq j$ and a reflection one if $i = j$; normalized to unit integral they give the conditional probability distributions of first-exit times of particles that exit through the i boundary, having entered through the j one. The transmission coefficient is

$$\eta = \frac{\Phi_{\mathrm{out}}}{\Phi_{\mathrm{in}}} = \frac{\pi D}{2b(\bar{l}+L)}, \quad \bar{l} = \frac{\pi(2\beta-1)D_0}{2b}. \tag{5}$$

At lengths $L \gg \bar{l}$ Ohm's law [12] is therefore valid [13]. Comparison with well-known results of kinetic theory shows that $l_0 = \pi D/2b$ has the meaning of mean free path (mfp). We emphasize that while our microscopic dynamics (1) is artificial on strictly physical grounds, the statistical description summarized by Eqs. (2) and (3) is instead fully generic and is in fact the canonical description of one-dimensional diffusive transport. On such grounds we expect that quantization of the microscopic dynamics will yield likewise generic indications about the quantum counterpart of classical 1D diffusive transport.

In the usual quantization of the SM k is an angle, the conjugate momentum q assumes integer values (we assume $\hbar = 1$), and the quantized model describes motion on a 1D discrete lattice. To the one-step classical evolution (1) we associate the quantum unitary propagator $\hat{U} = \hat{T}\hat{U}_0$, where $\hat{U}_0 = e^{iH(\hat{k})}$ and $\hat{T} = e^{iF(\hat{q})}$. The function $F(q)$ vanishes in the leads and is given by $\frac{1}{2}\tau q^2$ inside the sample [14]. The eigenphases λ of $\hat{U}$ are quasienergies that play in discrete-time quantum dynamics the same role as energies in continuous time. Since $\hat{U}$ is a finite-rank perturbation of $\hat{U}_0$, the free dynamics defined by $\hat{U}_0$ and the interacting one defined by $\hat{U}$ give rise to a well-posed scattering problem and the scattering operator is defined even in the strict mathematical sense. At fixed quasienergy λ, this operator is a finite matrix $S_{\alpha\beta}(\lambda)$ of rank $2b/\pi$ whose indexes α, β label scattering channels. Such channels arise because every quasienergy eigenvalue λ is multiply degenerate: associated with it is a set of free waves whose momenta k_α satisfy $H(k_\alpha) = \lambda(\mathrm{mod}2\pi)$. In order to compute the S matrix we numerically solved an equation of the Lippman-Schwinger type,

$$u - e^{i\lambda}\lim_{\epsilon\to 0+}(\hat{U}_0 - e^{i\lambda+\epsilon})^{-1}(\hat{T}^\dagger - 1)u = u_0,$$

which for any given free wave u_0 yields an interacting eigenfunction u. Having obtained the S matrix in the standard way from interacting eigenfunctions, we could compute various quantities related to quantum transport and fluctuations thereof. Statistical ensembles were generated by moving the "sample" to different positions on the q lattice, i.e., by changing q_0. Under a well-known assimilation of the quantum kicked rotator to a tight binding model [5], this is equivalent to taking different realizations of disorder. The quantum diffusive regime is roughly defined by $l_0 < L < \ell$, where $\ell \sim D$ is the localization length associated with the Anderson-like localization phenomenon occurring in the quantum KR and related models [5].

In this regime the average quantum transmission coefficient depends on L according to the classical law (5) [7]. A dimensionless conductance G can be formally de-

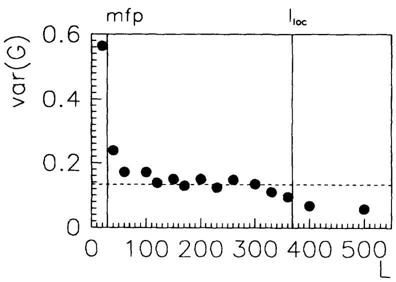

FIG. 1. Variance of the dimensionless conductance G, computed over 100 samples, versus sample length L, for $b = 45, \xi = 1.5, b\tau = 10$ (18 scattering channels). The dashed horizontal line corresponds to the theoretical value 2/15. mfp and localization length are shown by vertical lines.

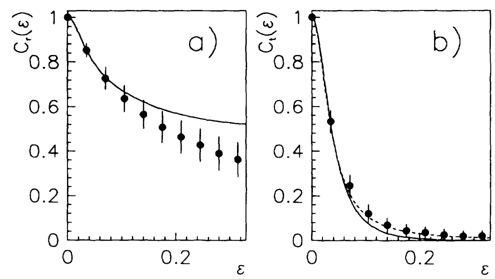

FIG. 2. Normalized squared moduli of correlations between S-matrix elements at quasienergy 0 and ϵ; reflection (a) and transmission (b) for the same parameter values as in Fig. 1 and $L = 200$. Full lines show classical results from the diffusion equation. The dashed line in (b) is a Lorentzian fit. Error bars show the dispersion of correlations obtained for individual matrix elements.

fined from the S matrix according to the many-channel generalization of the Landauer formula, which gives G as the sum of squared moduli of all transmission elements in one direction. Universal conductance fluctuations are demonstrated by a plot of the variance of G versus the sample length (Fig. 1), which clearly shows a plateau in the diffusive range [8], around an average value quite close to the random-matrix theoretical value 2/15 [15–17].

We have studied correlations of S-matrix elements at different quasienergies:

$$\mathcal{C}_{\alpha\beta}(\lambda, \epsilon) = \left\langle S^{*}_{\alpha\beta}(\lambda)\, S_{\alpha\beta}(\lambda + \epsilon)\right\rangle , \tag{6}$$

where the brackets denote disorder averaging. In the semiclassical domain such functions have a dynamical interpretation, which can be derived either from semiclassical arguments [1] or from the observation [7] that a prescribed incoming flux in channel β produces an average outgoing flux in channel α given by

$$\langle \Phi_{\mathrm{out},\alpha}(t)\rangle = \int_0^\infty \check{\mathcal{C}}_{\alpha\beta}(\sigma)\, \Phi_{\mathrm{in},\beta}(t - \sigma - t_f)\, d\sigma, \tag{7}$$

where the inverse Fourier transform (in ϵ) of (6) appears, and t_f is the free-flight time. If an incoherent homogeneous distribution of incoming fluxes from the left is assumed, then (7) shows that the inverse Fourier transform of (6), averaged either over transmission elements or over reflection ones, plays the same role as the kernels $R_{21}(\sigma), R_{11}(\sigma)$ (respectively) in Eq. (4), *as long as* $\sigma \gg t_f$. We therefore expect correlations (6) to be quasiclassically reproduced by Fourier transforms of the classical kernels R_{ij} on (quasi)energy scales smaller than the one related to fast direct transitions across the sample. This conclusion was confirmed by our numerical simulations. In order to filter out nonfluctuating contributions, correlations were computed not for the original S matrix but for its fluctuating part $S^{\mathrm{fl}}_{\alpha\beta} = S_{\alpha\beta} - \langle S_{\alpha\beta}\rangle$. The squared moduli of such correlations were averaged over all transmissions (respectively, all reflections), and the functions of ϵ thus obtained were normalized to unit value at $\epsilon = 0$. Classical counterparts for the functions $C(\epsilon)$ computed in this way were provided by squared moduli of Fourier transforms of R_{ij}, normalized to 1 at $\epsilon = 0$. Results are shown in Fig. 2. For both transmission and reflection, classical and quantum curves closely agree when ϵ is on the order of the Thouless energy D/L^2 or less, but are different in the tails. Correlation curves for transmission elements are very close to Lorentzian curves, but they are quite different for reflection; in fact reflection, although diffusive, is on the average a much faster process than transmission, and the corresponding energy scale is comparable to the "direct" one. For this reason, we found the "curvature width" $\epsilon_0 = \sqrt{2}|C''(0)|^{-1/2}$ to provide a more convenient measure of correlation widths than the usual "half-width" $\epsilon_{0.5}$ defined by $C(\epsilon_{0.5}) = 0.5$. The curvature width is the half-width of a Lorentzian osculating the given curve at $\epsilon = 0$, and has a simple dynamical meaning: in fact the memory kernel in Eq. (7) defines a distribution of first-exit times, and ϵ_0 is the width of this distribution *as given by its rms deviation.* ϵ_0 may be a useful quantity in other problems, too, when the "chaotic" and the "direct" energy scales are not neatly separated. In Fig. 3 we show the dependence of both widths on the sample length. For transmission $\epsilon_{0.5}$ and ϵ_0 are close to each other, reflecting the closeness of the corresponding correlations to Lorentz curves; moreover they are close to the corresponding classical quantities, analytically computed from $R_{ij}(\sigma)$. The latter classical widths are asymptotically given, at large L, by the first eigenvalue of the diffusive boundary-value problem: $\epsilon_0 \approx \pi^2 D/2L^2$. Comparing this with $\langle G\rangle \approx D/L$ [which follows from (5) at large L on neglecting weak-localization corrections] we get $\epsilon_0 \approx \pi \langle G\rangle\, \delta\lambda/4$ where $\delta\lambda = 2\pi/L$ is the average spacing of quasienergy levels in the sample. If the correlation width is taken as a measure of the "level width," this connection between average conductance and correlation width is just Thouless' formula (apart from a numerical coefficient), and its validity is also demonstrated in Fig. 3.

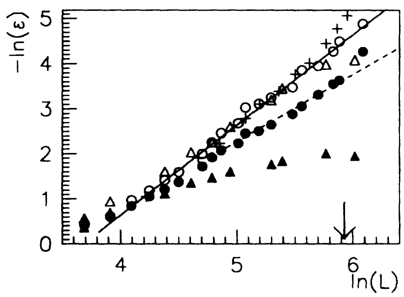

FIG. 3. Inverse correlation widths versus sample length, for the same parameter values as in Figs. 1 and 2. Open symbols are for transmissions, full ones for reflections; circles are for local widths ϵ_0, triangles for half-widths $\epsilon_{0.5}$. Lines are theoretical results from the classical diffusion equation. The arrow on the lower margin shows the value of the localization length. Crosses were obtained by inserting the numerically computed conductance into $\epsilon_0 = \pi \langle G \rangle \delta\lambda/4$.

For reflection, ϵ_0 again agrees with the corresponding classical value, for which the following asymptotic formula at large L was derived from the formulas reported in Ref. [11]:

$$\epsilon_0 \approx 0.25\pi^2 D l_0^{-1/2} L^{-3/2}.$$

The half-width $\epsilon_{0.5}$ is instead quite different from ϵ_0. It cannot be compared to the classical half-width, because the latter is comparable or even larger than the direct energy scale. Moreover, the classical reflection curve does not shrink indefinitely as $L \to \infty$ but converges instead to a certain limit curve. Quantum data indicate an analogous saturation; however, at large L localization effects come into play which make numerical computations quite problematic. These very effects are responsible for a sharp uprising of the ϵ_0 curves observed at large L. The saturation of the half-widths of reflection curves, along with the steady decrease of ϵ_0, indicate that in the limit of an infinitely long sample $C(\epsilon)$ should have an angle at $\epsilon = 0$, as observed in Ref. [7].

We have thus shown that the second order statistics of S-matrix fluctuations in quantum one-dimensional diffusive transport can be efficiently analyzed in the framework of chaotic scattering. In closing we wish to remark that the agreement between numerical quantum data and theoretical results from the FP equation can also be taken as a striking, if unusual, test of the validity of the diffusive approximation for the dynamics of chaotic classical maps.

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$$R_{ij}(\sigma) = \frac{\delta_{ij}\delta(\sigma)}{1-2\beta} - \frac{2\beta}{1-2\beta}\sum_{n=1}^{\infty}(-1)^{(i-j)n} f_n,$$

$$f_n = a\lambda_n e^{-\lambda_n \sigma}\left(a^2 + a + \nu_n^2\right)^{-1}, \quad a = L(2\beta-1)\beta^{-1} l_0{}^{-1},$$

where λ_n are the eigenvalues of the homogeneous boundary-value problem, given by $(n \geq 1)$

$$\lambda_n = 2D\nu_n^2 L^{-2}, \quad \tan(\nu_n) = (-1)^{n+1}(a/\nu_n)^{(-1)^{n+1}}.$$

[12] This denomination is somewhat abusive in the absence of a classical definition of conductance. We use it for brevity, because the law (5) for the *quantum* transmission coefficient would imply Ohm's law via the Landauer formula.

[13] The length $\bar{l}$ is determined by the boundary conditions, i.e., by the coupling to the leads; its role was discussed in [9]. Such a length must necessarily appear in any well-posed formulation of the diffusive transport problem. In our case $\bar{l} \leq l_0$, the mfp.

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