Scattering Involving Prompt and Equilibrated Components, Information Theory and Chaotic Quantum Dots

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We propose an information-theoretic statistical model to describe the universal features of those chaotic scattering processes characterized by a prompt and an equilibrated component. The model, introduced in the past in nuclear physics, incorporates the average value of the scattering matrix to describe the prompt processes, and satisfies the requirements of flux conservation, causality, and ergodicity. We show that the model successfully describes electronic transport through chaotic quantum dots. The predicted distribution of the conductance may show a remarkable two-peak structure.

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The scattering of waves by complex systems has been a problem of longstanding interest in physics.

Scattering of waves by a disordered medium has been studied, for instance, in optics for a long time \cite{1}. Interest in this problem has been revived, for electromagnetic waves and for electrons, in relation with the phenomenon of localization, with a host of exciting new features \cite{2,3}. Here, the diffusion time throughout the medium is the single important characteristic time.

Examples of quantum-mechanical scattering by complex systems can also be found in nuclear and molecular physics. It is amazing that one can describe the scattering of a nucleon by an atomic nucleus—a complicated many-body problem—in terms of two distinct time scales: a prompt response arising from direct processes and a time-delayed one arising from the formation of an equilibrated compound nucleus. The prompt response is slowly varying in energy and is described by the energy averaged, or optical, scattering amplitudes; the equilibrated response is the difference from this energy average and is amenable to a statistical analysis \cite{4}. Further examples of physical processes of this type, and studied in terms of similar notions, can be found in molecular physics, with interesting applications to chemistry \cite{5}.

Most remarkably, features similar to those appearing in scattering from nuclei also occur in quantum-mechanical scattering from simple one-particle systems \cite{6,7}. An example is a particle scattering from a cavity of dimensions larger than the wavelength, in which the classical dynamics is chaotic. One experimental realization of such systems are the ballistic quantum dots \cite{8,9,10}, microstructures in which both the phase-coherence length and the elastic mean free path exceed the system dimensions; the dot acts as a resonant cavity and the leads as electron waveguides. Previous work on these systems has implicitly assumed the absence of any prompt response.

Our purpose is to propose a model describing the universal features that appear in any chaotic scattering process involving a prompt and an equilibrated component. This model was introduced in the past in the context of nuclear physics, using an information-theoretic approach \cite{11} based on the mathematical development in Ref. \cite{12}. Here we show that the same theoretical framework is successful in the description of electronic transport through ballistic quantum dots. We build on previous work which used this model in describing chaotic scattering \cite{13} and in simulating phase-breaking in quantum dots \cite{14}.

Semiclassical \cite{7,9}, field-theoretic \cite{15}, and random-matrix \cite{16,17,18} approaches have been used to describe quantum transport through ballistic quantum dots. In Refs. \cite{16,17} the statistics of the problem was described by assigning to the quantum scattering matrix \( S \) an “equal a priori distribution”, consistent with the symmetry requirements. This “invariant measure” \cite{18} defines the “circular ensemble” of \( S \) matrices. The results for the ensemble average, variance and probability density of the conductance were found, in Ref. \cite{16}, to agree with a statistical analysis of the numerically obtained conductance of a chaotic cavity connected to two waveguides, sampled along the energy axis. It was assumed that one could neglect “direct processes” caused by short trajectories that would give a nonvanishing energy averaged, or optical, \( S \)-matrix; this was enforced in the simulations with two stoppers which block direct transmission between the leads and whispering-gallery trajectories. Although the general problem may contain a range of relevant “time delays”, we present below an improvement on the above model in terms of two very different time scales, in a vein similar to the nuclear scattering problem above. We first summarize the information-theoretic approach \cite{11}.

Information-Theoretic Approach—A quantum scattering problem is described by its \( S \) matrix, which, for scattering involving two leads, each with width \( W \) and \( N \) transverse modes or channels, is \( n = 2N \)-dimensional.
and has the structure
\[
S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}.
\] (1)

Here, \(r, t\) are the \(N \times N\) reflection and transmission matrices for incidence from the left and \(r', t'\) from the right. Current conservation requires \(S\) to be unitary, \(SS^\dagger = I\); for time-reversal symmetry (as is realized in the absence of a magnetic field) and no spin, \(S\) is symmetric.

Our starting point is \(d\mu^{(\beta)}(S)\), the invariant measure under the symmetry operation for the universality class \(\beta\) in question. The operation is \(S' = U_0 SV_0\), where \(U_0, V_0\) are arbitrary fixed unitary matrices in the case of unitary \(S\) matrices [the circular unitary ensemble (\(\beta = 2\))], with the restriction \(V_0 = U_0^\dagger\), in the case of unitary symmetric \(S\) matrices [the circular orthogonal ensemble (\(\beta = 1\))]. \(d\mu^{(\beta)}(S)\) can be written explicitly in several different representations \([12, 14, 17]\).

The ensemble average of \(S\), and hence the prompt component, vanishes when evaluated with the invariant measure. Ensembles in which \(\langle S \rangle\) is nonzero contain more information than the circular ensembles; they are constructed by multiplying the invariant measure by a function of \(S\) to give the differential probability
\[
dP^{(\beta)}(S) = p^{(\beta)}(S) \ d\mu^{(\beta)}(S).
\] (2)
The information \(I\) associated with the above probability distribution is defined as \([14]\)
\[
I[p(S)] = \int p(S) \ln[p(S)] \ d\mu(S).
\] (3)

Far from channel thresholds, the \(S\)-matrix is analytic in the upper half of the complex-energy-plane (causality). We also require that the ensemble be ergodic \([20]\), so that energy averages can be replaced by ensemble averages. These analyticity-ergodicity requirements (AE) imply the reproducing property
\[
f(\langle S \rangle) = \int f(S) dP(S)\),
\] (4)
for a function \(f(S)\) analytic in its argument (expandable in a power series in \(S\) not involving \(S^\dagger\)). The probability density known as Poisson’s kernel,
\[
p^{(\beta)}(S) = V_\beta^{-1} \left[ \frac{\det(I - \langle S \rangle S^\dagger)}{\det(I - S') \langle S S^\dagger \rangle} \right]^{(\beta n - 2 - \beta)/2} \] (5)
where \(V_\beta\) is a normalization constant, satisfies the reproducing property Eq. \([12]\), and the associated information is less than or equal to that of any other probability density satisfying the AE requirements for the same \(\langle S \rangle\) \([11]\). Recently, this probability density for the \(S\)-matrix has been derived from a statistical distribution for the Hamiltonian \([21]\), explaining the coincidence noticed between the two approaches \([11]\). Thus, Poisson’s kernel describes those physical situations in which (a) the details are irrelevant except for the average \(S\)-matrix and (b) the requirements of flux conservation, time-reversal invariance (when applicable), and AE must be met.

For \(n = 1\), when the system is a cavity connected to the outside by only a one-mode lead and \(S = e^{i\theta}\) describes reflection back into the same lead, the ensemble is uniquely determined by AE and a specified value of \(\langle S \rangle\) and is given by Poisson’s kernel \([22]\). For \(n > 1\) the additional minimum-information criterion explained above is needed to determine the ensemble.

Transport through Quantum Dots—In terms of the \(S\) matrix, the conductance for spinless particles is \([3]\)
\[
G = \frac{(e^2/h)T}{(e^2/h)\text{Tr}[tt^\dagger]}.
\] (6)
Thus, in applying Poisson’s kernel Eq. \([3]\) to electronic transport through quantum dots, we need the probability distribution \(w(T)\) of the total transmission \(T\); i.e.
\[
w(T) = \int \delta(T - \text{Tr}[tt^\dagger]) p^{(\beta)}(S) \ d\mu^{(\beta)}(S). \] (7)
We study below the case \(n = 2\), for which there is only one mode in each lead.

We first discuss \(\beta = 2\). Denote the elements of \(\langle S \rangle\) by
\[
\langle S \rangle = \begin{pmatrix} x & w \\ z & y \end{pmatrix}
\] (8)
where \(w, x, y, z\) are complex numbers with \(X \equiv |x| \leq 1\), etc. If there is no prompt transmission, \(w = z = 0\), we can perform the integrations analytically, yielding
\[
w(T) = (1 - X^2)^2(1 - Y^2)^2 \times \{1 - (1 - T)(X^2 + Y^2)(1 - 6X^2Y^2 + X^4Y^4) \\
- \langle 4X^2Y^2(1 + X^2Y^2) \rangle + (1 - T)^2(1 + X^2)(6X^2Y^2 - X^4 - Y^4) \\
- \langle 4X^2Y^2(2X^2 + Y^2) \rangle + (1 - T)^3(2X^2Y^2)(X^2 - Y^2)^2 \}
\times \{1 - (X^2Y^2)^2 - 2(1 - T)(1 + X^2Y^2)(X^2 + Y^2) \\
- 4X^2Y^2 \}
\times (1 - X^2Y^2)^2 - 5/2. \] (9)
For \(x = y\) the above result reduces to
\[
w(T) = (1 - X^2)^2 \times (1 - X^4)^2 + 2X^2(1 + X^4) + 4X^4T^2 \times \langle (1 - X^2)^2 + 4X^2T \rangle^{5/2}. \] (10)
Calling \(\Gamma = 1 - X^2\), Eq. \([14]\) gives, in the limit \(\Gamma \ll 1\), the result of Ref. \([24]\). In the opposite case of no prompt component to the reflection, \(x = y = 0\), \(w(T)\) is related to that of Eq. \([10]\) by the replacements \(x \rightarrow w, y \rightarrow z, \ldots\)
For nonzero \(x, y, w, z\), we can express the result in terms of a single angular integration; it will not be given here because of lack of space.

We now discuss the case \(\beta = 1\). When \(\langle S \rangle\) is diagonal and \(y = 0\), one finds (see Eq. (5.13) of Ref. [1])

\[
w(T) = \frac{(1 - X^2)^{3/2}}{2\sqrt{T}} F\left(\frac{3}{2}, \frac{3}{2}; 1; (1 - T)X^2\right)
\]

where \(F\) is a hypergeometric function. When \(\langle S \rangle\) is diagonal and \(x = y\), we find

\[
w(T) = \frac{C}{\sqrt{T}} \left\langle \frac{F\left(\frac{3}{2}, \frac{3}{2}; 1; E^2\right)}{1 + (1 - T)X^2 - 2\sqrt{1 - TX \cos \psi}\sqrt{2}} \right\rangle_\psi,
\]

where \(\langle \rangle_\psi\) indicates an average over \(\psi \in [0, 2\pi]\) and

\[
E^2 = X^2 \frac{1 - T + X^2 - 2\sqrt{1 - TX \cos \psi}}{1 - TX^2 + X^2 - 2\sqrt{1 - TX \cos \psi}}.
\]

When \(\langle S \rangle\) is off-diagonal \((x = y = 0)\) with \(w = z\), we find

\[
w(T) = (1/2)(1 - Z^2)^{3/2}T^{-1/2}\left\langle (1 + 2(2T - 1)Z^2 + Z^4 - 4\sqrt{X^2 \cos \psi + 4Z^2 \cos^2 \psi} - 3/2) \right\rangle_\psi.
\]

For several cases, these complicated distributions are plotted in Fig. 1 and will be discussed in connection with the numerical results below.

**Numerical Results**—We have computed the conductance for several stadium billiards, sketched in Fig. 1, using the methods of Ref. [23]. \(w(T)\) was found by sampling in an energy window much larger than the energy correlation length but smaller than the interval over which the prompt response changes (so that “stationarity”, a condition for ergodicity [20], is attained) and by using several slightly different structures. Typically we used 200 energies in k\(W/\pi\) \(\in [1.6, 1.8]\) and 10 structures found by changing the height or angle of the convex “bumper” in Fig. 1. Thus we rely on ergodicity to compare the numerical distributions to the ensemble averages of random-matrix theory. In each case the optical \(S\)-matrix was extracted directly from the numerical data; in this sense the theoretical curves shown below are parameter free.

We first consider a simple half-stadium with collinear leads at low magnetic field \((BA/\phi_0 = 2, r_c = 55 W, A\) is the area of the cavity, \(r_c\) is the cyclotron radius, and \(W\) is the width of the leads): \(w(T)\) is nearly uniform [Fig. 1(a)], and \(\langle S \rangle\) is small because direct trajectories are negligible in this large structure. We thus obtain good agreement with the circular unitary ensemble prediction, as in previous work [14].

In order to increase \(\langle S \rangle\) we modify the situation in three ways: (1) introduce potential barriers at the openings of the leads into the cavity (dashed lines in structures of Fig. 1), (2) increase the magnetic field, and (3) extend the leads into the cavity. The barriers (chosen so that the transmission of each barrier is 1/2) increase the direct reflection and thus skew the distribution towards small \(T\) [Fig. 1(b)]. The large magnetic field \((BA/\phi_0 = 80, r_c = 1.4 W)\) increases one component of the direct transmission—the one corresponding to skipping orbits along the lower edge—and thus skews the distribution towards large \(T\) [Fig. 1(c)]. Finally, extending the leads into the cavity increases the direct transmission in both directions and thus also skews the distribution towards large \(T\) [Fig. 1(d)]. Note the excellent agreement with the information-theoretic model. In panels (b)-(d) the curve plotted is the analytic expression of Eq. (4) and the corresponding one for direct transmission.

By combining several of these modifications, different \(\langle S \rangle\) and so different distributions can be produced. First, by using extended leads with barriers at their ends, one can cause both prompt transmission and reflection: this case, Fig. 1(e), is in good agreement with the prediction of the full Poisson’s kernel. Finally, increasing the magnetic field in this structure produces a large average transmission and a large average reflection. The resulting \(w(T)\), Fig. 1(f), has a surprising two-peak structure: one peak near \(T = 1\) caused by the large direct transmission and another near \(T = 1/2\). Even in this unusual case, the prediction of the information-theoretic model is in excellent agreement with the numerical result. In these last two cases (e,f) the analysis was performed independently over four intervals of 50 energies each (since the four intervals show slightly different \(\langle S \rangle\)’s) and the four sets of theoretical and numerical data were then superimposed.

**Discussion**—In addition to the structures shown in Fig. 1 we have studied cavities whose level density is not large enough for stationarity, and hence ergodicity, to hold. In this case, a sample taken across independent cavities for a fixed energy shows excellent agreement with Poisson’s kernel. This suggests that the reproducing property Eq. (4) may be valid even in the absence of ergodicity; the reason for this is not understood.

In Ref. [4] we found that increasing the magnetic flux through the structure beyond a few flux quanta spoiled the agreement with the circular ensemble; we now know that a nonzero \(\langle S \rangle\) is generated and that the present model describes the data very well. The excellent agreement found here with a flux as high as 80 suggests extending the analysis to the quantum Hall regime.

We close by noting that the above \(w(T)\)’s should be experimentally accessible in structures where phase-breaking is small enough. Experimentally one can sample the conductance distribution by varying the energy or shape of the structure with an external gate voltage [23], much as we did in collecting the numerical results. The barrier at the opening of the leads can be realized by designing a pincher gate and, of course, obtaining a sufficiently high magnetic field is standard.
FIG. 1. The distribution of the transmission coefficient for $N = 1$ in a simple half-stadium (top row) and a half-stadium with leads extended into the cavity (bottom row). The magnitude of the magnetic field and the presence or absence of a potential barrier at the entrance to the leads (marked by dotted lines in the sketches of the structures) are noted in each panel. Cyclotron orbits for both fields, drawn to scale, are shown on the left. The squares with statistical error bars are the numerical results; the lines are the predictions of the information-theoretic model, parametrized by an optical S-matrix extracted from the numerical data. The agreement is good in all cases.
Figure 1.