Classical Irregular Scattering and Its Quantum-Mechanical Implications

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(Received 28 September 1987)

We analyze the effect of irregular classical scattering on the corresponding quantum-mechanical scattering matrix. Using semiclassical arguments, we show that the fluctuations in the S matrix and the cross sections are consistent with a random-matrix description (Ericson fluctuations). The results are illustrated by a numerical solution of a simple quantum problem, whose classical counterpart displays irregular scattering.

PACS numbers: 03.80.+r, 05.45.+b, 24.60.Ky

It has been known for many years[1,2] that classical trajectories describing scattering (elastic, inelastic, or exchange) may show extremely complicated ("irregular") and sensitive dependence on the initial conditions. The interest in this phenomenon was recently revived[3-8] when the modern tools developed for the study of chaotic *bounded* trajectories were successfully applied to the analysis of *unbounded* scattering problems, displaying irregular features. Several models of very different physical systems were studied in detail. All exhibit irregular scattering (IS), and have some common basic features which seem to be generic, suggesting that IS is rather common within the manifold of nonintegrable scattering problems.

In the present paper we study the quantum description of systems whose classical analog displays IS. Using semiclassical arguments we show that classical IS implies that the quantum S matrix is fluctuating in a way consistent with the results of the random-matrix scattering theories.[9-15] The relation between random-matrix theory and the fluctuations in the quantal spectra of classically chaotic *bounded* Hamiltonians is well established.[16,17] Our results extend this link to the domain of scattering in *unbounded* systems.

We shall concentrate on nonintegrable Hamiltonians with two freedoms, x and θ, with conjugate momenta p and I. The x motion is unbounded and I (θ) are conjugate action (angle) variables. (Our analysis can be trivially extended to include any number of action-angle variables.) As $|x| \to \infty$ the Hamiltonian depends only on the momenta p and I. Classical trajectories required for the calculation of the $I \to I'$ transition probabilities (cross sections) are constructed in the following way: At $t \to -\infty$ (and $|x| \to \infty$) the initial action I_i is set to the value I, while p_i is set to give the total energy its specified value. For each initial angle θ_i, a solution of the classical equations of motion yields at $t \to +\infty$ ($|x| \to \infty$) the final value of the action, $I_f(\theta_i, I_i = I)$. Each trajectory which satisfies $I_f(\theta_i, I_i) = I'$ contributes to the transition probability a term

$$p_{I \to I'}^{(s)} = (2\pi)^{-1} [\partial I_f(\theta_i, I_i)/\partial \theta_i]^{-1}$$

and the total transition probability is the sum over all the contributing trajectories labeled by the index s.

For further reference we introduce the reduced action[2]

$$\Phi = -\left[\int x\,dp + \int \theta\,dI\right] = \int p\,dx + \int I\,d\theta - [px + I\theta]_i^f \quad (1)$$

calculated along a scattering trajectory. Φ is finite and its derivative with respect to the energy, $\partial\Phi/\partial E$, defines the delay time $T(\theta_i, I_i)$ which measures the extra time spent by the trajectory in the interaction region. Similarly, $\partial\Phi/\partial I_f$ defines the net phase angle $\Theta(\theta_i, I_i)$ acquired during the interaction.

IS manifests itself in the calculation of classical trajectories in the following way:

(i) The function $I_f(\theta_i, I_i)$ fluctuates wildly in some (θ_i, I_i) domains. The fluctuations persist on all scales of either θ_i or I_i, and $I_f(\theta_i, I_i)$ assumes all values I' consistent with energy conservation) infinitely many times (see Fig. 1). In these regions $\Theta(\theta_i, I_i)$ and $T(\theta_i, I_i)$ display unbounded fluctuations, and the trajectories are unstable.[1-8]

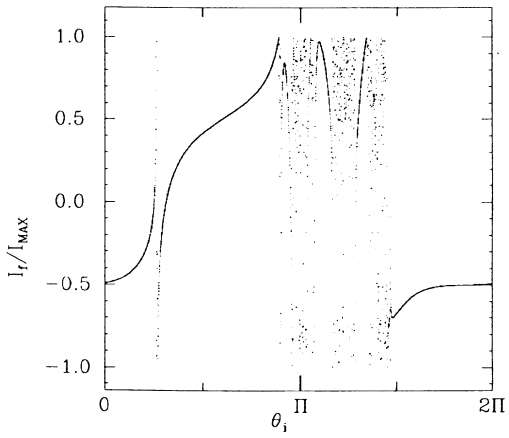

FIG. 1. The function $I_f(\theta_i, I_i = 7\hbar)$ showing IS for $E = 1.7$, $R = 0.1$, and $V = 3.0$.

(ii) Denote by S_T the set of initial conditions (θ_i, I_i) at a given energy E for which $T(\theta_i, I_i) \geq T$. Then (a) the measure $\mu(S_T)$ decreases as $\mu(S_T) = A\exp(-\gamma T)$, and (b) in the limit of large T, $S_{T\to\infty}$ is a Cantor set.[3]

We shall use the semiclassical reaction theory[2] to write the S matrix in the form

$$S_{I\to I'}(E) = \sum_s [p^{(s)}_{I\to I'}]^{1/2} \exp(i\Phi^{(s)}/\hbar - \tfrac{1}{2} i\pi\alpha_s). \quad (2)$$

The sum extends over all the contributing classical trajectories and α_s is the Maslov index.[18] The semiclassical theory relies on the assumption that the actions $\Phi^{(s)}$ for different trajectories with the same boundary conditions are separated by more than $\hbar$. The validity of this statement was never checked in the context of IS, where there exist infinitely many trajectories which contribute to the sum, all lying in close vicinity in phase space. We shall justify the use of the form (2) in the sequel.

We shall denote by $S^{(d)}_{I\to I'}(E)$ and $\tilde{S}_{I\to I'}(E)$ the contributions to the S matrix from the regular and irregular trajectories, respectively Consider the autocorrelation function

$$C_{II'}(\epsilon) = \langle \tilde{S}^*_{II'}(E)\tilde{S}_{II'}(E+\epsilon)\rangle_E, \quad (3)$$

where $\langle\ \rangle_E$ denotes the average over a classically small energy interval ΔE, whose size will be discussed below. Substituting (2) in (3), we get to lowest order in ϵ

$$C_{II'}(\epsilon) = \langle \sum_s p^{(s)}_{I\to I'}(E) \exp(i\epsilon\hbar^{-1}\partial\Phi^{(s)}/\partial E)\rangle_E + \langle \sum_{s\neq s'} [p^{(s)}_{I\to I'}(E) p^{(s')}_{I\to I'}(E)]^{1/2} \exp[i(\Phi^{(s)} - \Phi^{(s')})/\hbar - \tfrac{1}{2} i\pi(a_s - a_{s'})]\rangle_E. \quad (4)$$

The phase factor in the second term involves differences of classical actions from different trajectories. If we choose ΔE such that the variation of the classical actions will be large on the quantum scale, the contribution of the double sum in Eq. (4) averages out. In the first term we replace $\partial\Phi^{(s)}/\partial E$ by $T^{(s)}$, and, using the delay time to label the trajectories, we get

$$C_{II'}(\epsilon) = \int dT \langle P_{II'}(E,T)\rangle_E \exp(i\epsilon T/\hbar). \quad (5)$$

$P_{II'}(E,T)$ is the classical probability that an $I \to I'$ transition occurs while the delay is in the interval $[T, T+dT]$. According to (i) and (ii) above, $P_{II'}(E,T) \sim \exp[-\gamma(E)T]$ (see Fig. 2), and is independent of I or I'. If ΔE is chosen sufficiently small on the classical scale that the variation of γ in the interval can be neglected, we get

$$C_{II'}(\epsilon) = C_{II'}(0)\gamma/(\gamma - i\epsilon/\hbar). \quad (6)$$

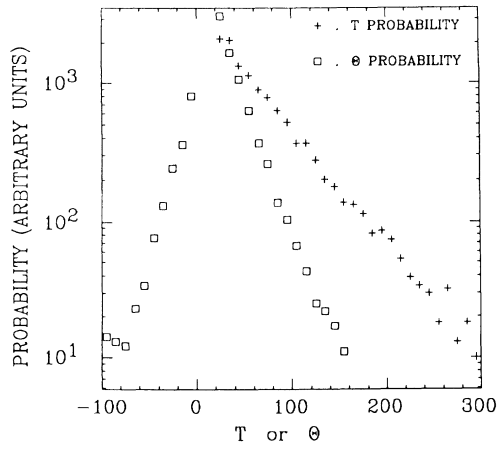

FIG. 2. Probability distributions $P_{I_i I'}(E,T)$ and $P_{I_i I'}(E,\Theta)$ averaged over I'. Same potential parameters as in Fig. 1.

This equation is valid if the classical and quantum energy scales are sufficiently different and ΔE is chosen in the intermediate range.

Another important correlation function is

$$F_{II'}(\eta) = \langle \tilde{S}^*_{II'}(E)\tilde{S}_{II''}(E)\rangle_I$$

where $\eta = I'' - I'$, and $\langle\ \rangle_I$ denotes the average over a classically small domain of I and I', with η constant. Using similar reasoning as above, we find

$$F_{II'}(\eta) \sim \langle \sum_s p^{(s)}_{I\to I'} \exp(i\hbar^{-1}\eta\,\partial\Phi^{(s)}/\partial I_f)\rangle \sim \int d\Theta \langle P_{I\to I'}(\Theta)\rangle_I \exp(i\hbar^{-1}\eta\Theta). \quad (7)$$

$P_{II'}(E,\Theta)$ is analogous to $P_{II'}(E,T)$ where the net angle Θ replaces the delay time. $P_{II'}(E,\Theta)$ is peaked at some mean angle Θ_0, and falls as $\exp(-\alpha|\Theta - \Theta_0|)$ (see Fig. 2) and is independent of I and I'. Therefore $F_{II'}(\eta) \sim F(0)(1 - i\eta/\hbar\alpha)^{-1}$. $\eta/\hbar$ can assume only integer values. Hence, if $\alpha < 1$, the $\tilde{S}_{II'}$ are uncorrelated and their mean square is independent of I and I'. If $S^{(d)} \sim 0$, $\tilde{S}$ is only constrained to be unitary and symmetric, suggesting that its properties are completely determined by the corresponding properties of Dyson's orthogonal ensemble.[14] Hence, we have the following.

(a) The nearest-neighbor distribution of the eigenvalues on the unit circle is a Wigner function.

(b) At a given energy, the distribution of $|S_{II'}|^2$ is Poissonian.

(c) Since the probability of $S_{II'}$ to be small is largest, the energy dependence of the cross section for a given transition, $\sigma_{II'}(E)$, will show a typical fluctuation pattern (Ericson fluctuations).[9]

(d) Because of (6), the $\langle \sigma_{II'}(E)\sigma_{II'}(E+\epsilon)\rangle_E$ should be a Lorentzian, whose width is $\hbar\gamma$.

These features are modified if $S^{(d)} \neq 0$,[10] but we shall

not discuss this point here because of lack of space.

To justify the semiclassical approximation we observe that the problem of coalescence of actions $\Phi^{(s)}$ becomes more acute as the delays $T^{(s)}$ are longer. The corresponding probability densities decrease exponentially and hence this regime of T (and Θ) values will have little effect on the correlation functions.

To illustrate these results we computed the S matrix for a simple Hamiltonian:

$$H(p,x,I,\theta)=\tfrac{1}{2}p^2+\tfrac{1}{2}RI^2+V\cos\theta\sum_{m=0,\pm1}\exp[-(x-m\xi)^2]. \tag{8}$$

We shall show results for two values of V. For $V=3.0$ classical phase space is dominated by IS, whereas for $V=0.3$ the classical phase space is mostly regular. The range of energies considered was $1.5\le E\le 2.3$ and we chose $R=0.1$ and $\xi=10$. The probabilities $P_{II'}(E,T)$ and $P_{II'}(E,\Theta)$ were calculated by means of a Monte Carlo integration procedure and the decay constants γ and α were deduced, $\gamma=0.023\pm0.001$ and $\alpha=0.045\pm0.005$. Within the statistical uncertainty the values of γ and α were found to be independent of the energy (within the considered range) and of the actions I and I'. In Fig. 1 we show the function $I_f(\theta_i,I_i)$, and in Fig. 2 we show $P_{I_iI'}(E,T)$ and $P_{I_iI'}(E,\Theta)$ averaged over all I' values.

The Schrödinger equation was written in the basis of the free-rotor eigenstates, truncated to include all "open channels" with $|I|<I_{\max}=(E/2R\hbar^2)^{1/2}$, and we chose $\hbar^2=\frac{1}{5}$. The Hamiltonian is symmetric with respect to the operation $\theta\to-\theta$. Hence symmetric and antisymmetric combinations of rotational states $|I^{(\pm)}\rangle=(1/\sqrt{2})\{|I\rangle\pm|-I\rangle\}$ do not couple. Further reduction is possible because of the symmetry $x\to-x$. In each subspace we checked the properties (a) and (b) mentioned above. We accumulated sufficient statistics by adding to the same histogram the contributions from a range of energies. Figure 3(a) shows the computed nearest-neighbor distribution. Figure 3(b) shows the probability distribution of $|S_{II'}|^2$. The full histograms were calculated for $V=3$ (classical IS) and the dashed histograms correspond to $V=0.3$ (regular case). The solid curves show the expectation from random-matrix theory. The E dependence of the inelastic transmission probability accompanied by the $|7^{(-)}\rangle\to|9^{(-)}\rangle$ transition is shown in the inset of Fig. 4 for $V=3$ (classical IS). It displays a typical fluctuation pattern, while the same quantity when calculated for $V=0.3$ is monotonic in E (not shown). The corresponding S-matrix autocorrelation function [Eq. (3)] is also shown in Fig. 4 together with the expected Lorentzian [Eq. (6)], whose width $\hbar\gamma=0.01$ was extracted from the classical calculations. The fluctuating part of the S matrix was obtained after the subtraction of the smooth part of $S_{II'}(E)$, which was taken to be the energy average of the S matrix over five correlation lengths. The shape of the autocorrelation functions of the other S-matrix channels closely resem-

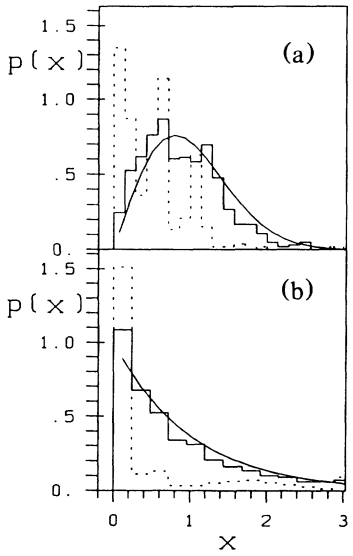

FIG. 3. (a) Nearest-neighbor distribution and (b) the distribution of $|S_{II'}|^2$. The full histogram is for $V=3.0$, the dashed histogram for $V=0.3$, and the smooth curves are the predictions of random-matrix theory. The height of the first bin in the dashed histogram of (b) was truncated at 1.5 for a clearer presentation (the true value is 2.93).

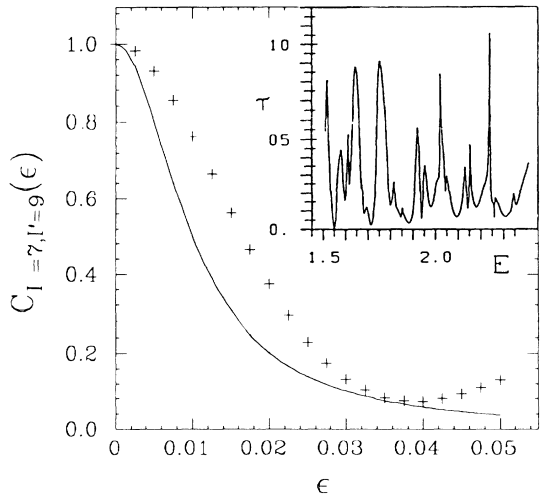

FIG. 4. Absolute square of the energy autocorrelation function for the S matrix elements corresponding to the $|7^{(-)}\rangle\to|9^{(-)}\rangle$ transition for $V=3.0$. The smooth curve is obtained from Eq. (6), with $\hbar\gamma=0.01$. Inset: Inelastic transmission probabilities, for the same transition, as a function of the total energy.

bles the one in Fig. 4 and their widths are within 50% of the expected result ($\hbar\gamma=0.01$).

We can summarize the numerical study by stating that whenever the classical dynamics shows IS, the corresponding quantum description follows the predictions (a)–(d). These results strongly support the simple semiclassical arguments presented above, and the suggested link between classical IS and the quantal random-matrix theory for scattering.

Fluctuations of the kind discussed here were first observed in the measurements of nuclear reactions and were interpreted by Ericson[9] and others[10] as due to the contributions of many resonances with widths which exceed the mean level spacing. Further analysis in terms of the random-matrix model were carried out later.[11-13] In the present work we have established for the first time that such fluctuations may exist in very simple systems and we have unraveled their dynamical origin—the presence of classical IS trajectories. The width of the energy autocorrelation function is proportional to γ, the inverse of the mean classical delay time. Its relation to the Hausdorff dimension of the fractal $S_{T\to\infty}$ was discussed in Ref. 8. γ is a classical quantity, and hence the width of the autocorrelation function is $O(\hbar)$. The mean level spacing in our two-dimensional model is $O(\hbar^2)$. Hence in the semiclassical limit, the conditions assumed for the validity of Ericson's analysis always prevail.

Fluctuating cross sections are expected to occur whenever the relevant freedoms are not decoupled as a result of very different characteristic time scales, or some symmetry which renders the dynamics separable. These fluctuations should be observed in experiments in which the initial and final conditions (quantum numbers and the energy) are well resolved. Such high resolutions are now becoming available in the study of atomic and molecular reactions.

We would like to thank Dr. Bruno Eckhardt for very illuminating discussions. One of us (U.S.) is grateful for the hospitality extended by Professor H. Walther during his stay at the Max Planck Institute for Quantum Optics.

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