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Irregular Scattering of Particles Confined to Ring-Bounded Cavities

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The classical motion of a free particle that scatters elastically from ring-bounded cavities is analyzed numerically. When the ring is a smooth circle the scattering follows a regular and periodic pattern. However, for rings composed of N scatterers the flow is irregular, of Lyapunov type. The Lyapunov exponent is found to depend logarithmically with N, which is consistent with the theoretical derivation of Chernov for polygon-shaped billiard systems. The escape time from cavities bounded by a ring of N separated scatterers is demonstrated to follow a geometric distribution as a function of the aperture size. An empirical scaling is proposed between the Lyapunov exponent, the escape time, and N.

KEY WORDS: Irregular scattering; ring-bounded cavities.

1. INTRODUCTION

The study of classical trajectories encountered in scattering problems is interesting because chaotic behavior is observed regardless of the elastic, inelastic, or exchange character of the scattering mechanism.[1,2] Several phenomena in physical systems have to deal with particles that enter a scattering region and are either trapped there or reside in the cavity a certain time before escaping. This class of problems have been approached from classical, semiclassical, and quantum points of view.[3,4] From the scenario of computer simulations, the stability of the classical trajectories of the scattered particles is crucial in determining reliable time averages which require a good sampling of phase space in a moderate computational time.

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When the motion is periodic or quasiperiodic, only restrictive regions of phase space are covered.[5,6] If instead the trajectory samples the phase space in an apparently random manner, the system is ergodic and the computational time needed to achieve good averages is attainable.

A set of semiclassical problems can be modeled by considering the classical counterpart of a free particle trapped in a cavity.[7-9] The motion of the particle is confined by the cavity and determined by the cavity shape. Well-known statistical models of molecular cavities, or trapping sites in solids, consist of systems where moving particles wander inside a region surrounded by spherical scatterers which represent either atoms or molecules. A Lorentz gas is an example. In two dimensions it is possible to design fully closed cavities by packing circles along a boundary. A particle undergoing elastic collisions trapped in such a 2D cavity defines a particular class of dynamical systems called billiard systems.[10,11]

Irregular scattering (IS) problems have recently been revived in connection with their quantum counterpart and their analysis based on random matrices[1-4,7-9] and level fluctuations. Furthermore, it has been stated that whenever IS is observed, the quantum description is such that: (i) the nearest neighbor distribution of the eigenvalues of the trapped particle is a Wigner function; (ii) at a given energy the distribution of the modulus squared of the quantum S-matrix elements between two action states is Poissonian; and (iii) the width of the energy autocorrelation function is proportional to the inverse of the escape time.

In this paper we address statistical issues of a billiard that exhibits irregular scattering (IS). The model is a point particle trapped in a cavity with walls composed of N circular reflecting scatterers. In Section 2, isoenergy trajectories are analyzed as a function of the number of scatterers forming the ring-bounded cavity. In particular, we compare the Lyapunov exponents obtained from the trajectories to an asymptotic formula of Chernov.[11] In Section 3 we discuss the case of particle moving in a cavity surrounded by reflecting scatterers that have gaps between them. A generic feature common to a large class of chaotic scattering problems is that $P(t)$, the probability that the trajectory stays within the confined region for at least the time t, is given by

$$P(t) \sim e^{-\alpha t} \tag{1}$$

when t is large. However, the probability for short times is dependent upon the geometry of the scattering region. Results in this work for cavities surrounded by rings of scatterers corroborate Eq. (1). This is analyzed in Section 3 and compared to a probability model developed from heuristic reasoning. Section 4 gives a brief conclusion.

2. FREE PARTICLE MOTION INSIDE A RING OF SCATTERERS

When a classical point particle moves freely inside a two-dimensional, perfectly reflecting cavity, periodic trajectories can be generated from certain initial conditions. For example, a five-point star trajectory is depicted in Fig. 1a. A slight perturbation of 10^{-2} in the x component of the initial velocity causes the trajectory to precess around an axis passing through the center of the circle as depicted in Fig. 1b. The motion is now quasiperiodic. Quantities will be reported in units of R for distances and number of collisions for time.

The trajectory deviates with respect to the perfect star as time evolves. This deviation can be best measured by monitoring the time evolution of the Euclidean distance $d(t)$ in phase space between the periodic trajectory (parent) and the perturbed one[12]:

$$d(t) = ((x_o - x_p)^2 + (y_o - y_p)^2 + (v_{xo} - v_{xp})^2 \tau^2 + (v_{yo} - v_{yp})^2 \tau^2)^{1/2} \quad (2)$$

where the o represents the variables of the original parent trajectory and p those of the perturbed trajectory. Hence τ is the unit of time. For small initial deviations, $d(t)$ is a linear function of time indicating the regular and quasiperiodic character of the motion. This is regular scattering.

The motion of the same particle in a two-dimensional, ring-bounded cavity composed of N perfectly reflecting and touching circular scatterers is shown in Fig. 2 for $N = 5$, 9, and 20. The ring boundary allows for initial conditions that give rise to trivially periodic trajectories. An example for $N = 5$ is illustrated in Fig. 2a. For many other initial conditions the trajectory is irregular and tends to cover densely the allowed phase space. The behavior is depicted in Figs. 2b–2d, where trajectories were followed during equal times.

Ring-bounded cavities exhibit irregular scattering. To quantify this statement, the distance $d(t)$ between one parent trajectory and a set of

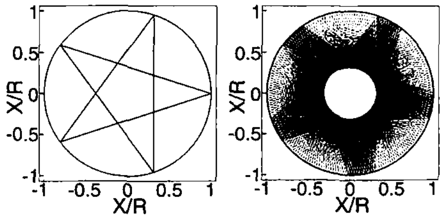

Fig. 1. Trajectories of a free particle confined to move in a smooth circular cavity. (a) Initial conditions satisfy Eq. (2); (b) Initial conditions as in (a) plus a 10^{-2} perturbation in the speed.

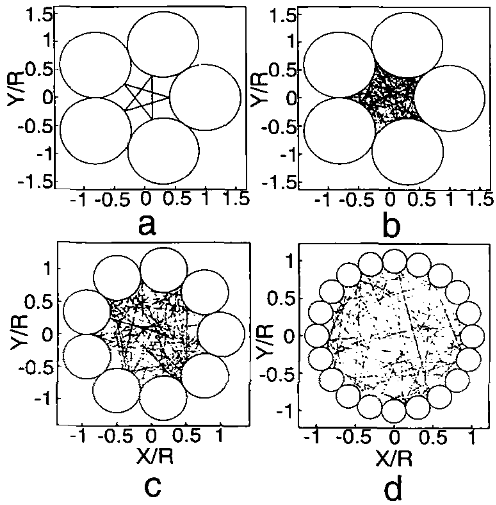

Fig. 2. Trajectories of a free particle confined to cavities bounded by an N-scatterer ring. (a) Five-scatterer-ring boundary; (b) same case as (a), but the initial conditions differ by a slight perturbation of the speed; (c) trajecttory in nine-scatterer ring; (d) trajectory in a 20-scatterer-ring cavity.

perturbed ones was calculated from Eq. (2) for cavities with different values of N. Two types of perturbations were considered. In the first, the x component of the velocity was altered by 10^{-6}. In the second perturbation scheme, the magnitude of the velocity remained fixed, but its direction was perturbed at random within an angular amplitude of 10^{-3} rad. In both cases the instability is of Lyapunov type. Figure 3 illustrates the linear growth of $\ln d(t)$ as a function of time using the first perturbation scheme mentioned above. The various lines in Fig. 3 show a change in the slope as

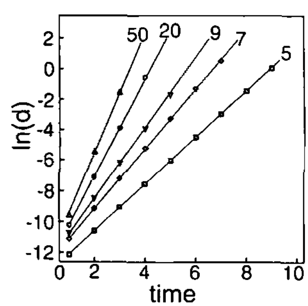

Fig. 3. Distance between parent and perturbed trajectories as a function of time (given in number of collisions). Solid lines are the fits leading to the Lyapunov exponent. Numbers on top indicate the number of scatterers in the ring cavity.

a function of number of boundary scatterers N. In all cases the Lyapunov exponent λ, the slope of the lines, is positive. This indicates that the motion is chaotic and irregular. No major differences were observed in the values of the Lyapunov exponent when calculated from the second perturbation scheme.

The numerical precision achievable in our computers limits the size of the smallest perturbation. Because of this limitation, the exponential correlation is only visible during a small number of collisions. This is clearly seen in Fig. 3, where every curve is stopped at that maximum time after which the exponential correlation is lost. For equal initial perturbations, the exponential correlation is lost faster as N, the number of scatterers, increases. This effect allowed us to carry calculations with N only up to about 50. For larger N the correlation between the two trajectories is lost in less than three collisions, making it impossible to extract a numerical value for λ with the method described here.

The ring of N scatterers might be used to model the *roughness* of a boundary.[12,13] Within the limits of numerical validity of our simulations, Fig. 4 illustrates the change in λ due to the number of scatterers N in the ring boundary. The best functional fit to the numerical values can be cast in the following expression:

$$\lambda = 1.125 \ln\left(\frac{N}{1.25}\right) \tag{3}$$

which is depicted by the broken line in Fig. 4. This formula is reminiscent of a theoretical formulation due to Chernov.[11] His example concerned a chain of identical touching semicircles placed along a polygon-shaped

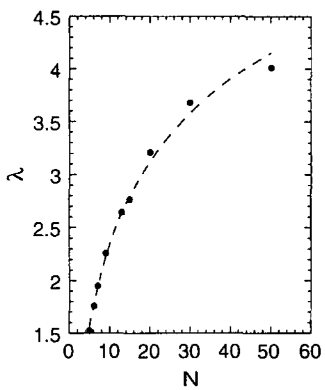

Fig. 4. Lyapunov exponent as a function of the number of scatterers in the right-bounded cavity. Dashed line corresponds to the fit proposed in Eq. (4).

billiard. In the limit of an infinite number of semicircles, $N \to \infty$, Chernov's formula expresses the entropy (equal in this case to the largest Lyapunov exponent) as

$$h = c_1 \ln(N/c_2) \tag{4}$$

which matches the empirical functional form (3) found in our study.

Summarizing, we show that the roughness of a ring boundary that confines a particle is responsible for quantitative changes in IS. When no roughness occurs (plain circular cavity), the motion is regular, periodic, with no chaos. When the ring that bounds the cavity is rough ($N > 3$), the motion is irregular, chaotic, and the flow is of Lyapunov type. This irregular motion might be associated with an indirect coupling between the particle degrees of freedom induced by the boundary shape.[13-15] Usually it is difficult to model this coupling by a Hamiltonian.

3. ESCAPE TIME FROM A BROKEN RING-BOUNDED CAVITY

In most scattering problems the moving particle enters a scattering region and resides within it only a finite time. This residency time is referred to as the scattering delay time[3,4] or escape time.[7] The class of ring-bounded cavities described in the previous section may be generalized by considering an open ring configuration with gaps between the scatterers. This situation is typical in three-dimensional cavities surrounded by hard-sphere scatterers.

Consider a plane geometry where small disks are arranged along the circumference of a large circle and separated by equal gaps g. We calculate numerically the escape time of a moving particle inside the cavity as a function of the gap size and of the number of scatterers. We define the gap g in relative terms as

$$g = \frac{D - 2r}{D} \tag{5}$$

where D is the distance between the centers of two contiguous scatterers of radius r located along the ring boundary. This g corresponds approximately to the ratio of the total aperture along the boundary ring to the entire boundary perimeter. Figure 5 shows a histogram of the escape time from a five-scatterer ring for 104 trajectories. The different trajectories were started from the same position, with the same energy, but random initial directions of motion. As is apparent from the histogram, the distribution is exponential, Poisson type, except at very short times. The short-time behavior is specific to the geometry of the cavity. A Poisson distribution is

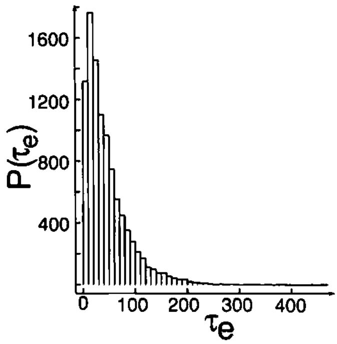

Fig. 5. Distribution of the escape times based on 104 trajectories for a particle confined in a five-scatterer ring cavity with $g = 0.0204$.

characteristic of a chaotic scattering mechanism in which there is no correlation between the gap and the dynamical variables. In Fig. 5 the scale of time shows the number of collisions with the boundary before escape.

The numerical process was repeated for different relative gap sizes. As expected, the smaller the gap, the more dominant the short-time behavior, and therefore the Poisson-like distribution is washed out. Under these circumstances it is best to obtain the numerical average of the escape time as a function of the gap size. Figure 6 illustrates the calculated averages (dots) of the escape time as a function of the gap size for the case $N = 5$. It is found that the average escape time decreases exponentially as the gap is increased. This behavior is the same irrespective of the value of N.

The results shown in Fig. 6 suggest a probabilistic interpretation based on the following arguments. Assume an infinite two-dimensional box with an opening of size g on one of the walls. A particle moving ergodically and

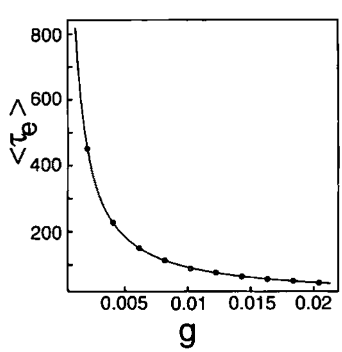

Fig. 6. Average escape time as a function of the relative aperture g for a five-scatterer ring cavity. Dots correspond to the simulation and the line represents Eq. (7) with $\alpha = 1.067$.

uniformly inside the box has a probability $p = \alpha g$ to escape without colliding with the wall that has the opening and a probability $1 - p$ to collide with the other wall. The probability for the particle to escape after exactly m collisions is then

$$P_m = p(1-p)^{m-1} \tag{6}$$

The expected value of the escape time τ_e (measured in number of collisions) is

$$\langle \tau_e \rangle = \langle m \rangle = \sum_{m=1}^{\infty} m P_m = \frac{1}{p} = \frac{1}{\alpha g} \tag{7}$$

The proportionality parameter α is related to the geometry of the wall close to the aperture and thus it depends on N. In the ideal case of a planar wall, $\alpha = 1$. However, our rough boundary is made of convex pieces irrespective of the number of scatterers. The value of α is obtained by equating the left-hand side of Eq. (7) to the calculated averages given in Fig. 6. Results of this fit give rise to the solid line in Fig. 6 for the case $N = 5$. As the boundary becomes rougher, $N \to \infty$, the parameter α is found to reach a saturation value as shown in Fig. 7. This behavior is not trivial. For the type of cavities considered in this work, the empirical dependence shown in Fig. 7 is a property of the cavity shape that characterizes the roughness of its boundary.

We have presented some cases of classical IS for which the quantum mechanical counterpart needs to be formulated. We have provided accurate results of the escape time (or delay time) in these IS cases. Universality relations of trajectories characterized by their Lyapunov exponent λ have been discussed in the literature.[16] Relevant to this work is the determination of the Hausdorff dimension d_f of classical trajectories. For the class of

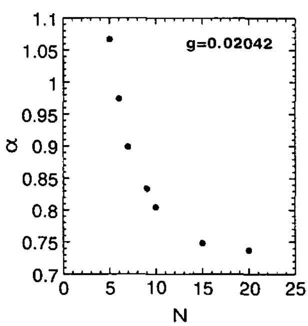

Fig. 7. Dependence of the parameter α of Eq. (7) on the number of scatterers in the ring-bounded cavity for $g = 0.02042$.

problems discussed here $d_f = 2$. For some other applications of free particle motion the dimensionality of the trajectory might have values lower than two, as is the case in zeolites,[17] where $d_f = 1$. From our results it is possible to establish an empirical relation connecting the roughness (represented by N), the Lyapunov exponent λ, and the escape time τ_e in an N-scatterer cavity with a fixed aperture g:

$$d_f \ln(N) = \tau_e \lambda - \ln(b) \tag{8}$$

where $b = 0.1786$ for $g = 0.0204$. This equation indicates the correlation between the ring roughness and the dynamical variables for $3 < N < 50$. In fact, ring-boundary confinement has been used to simulate the mean square displacement of small molecules and ions diffusing in zeolites. The role of structural disorder is important in zeolites, where 10- and 12-scatterer rings have been used to model silicalite and faujasite.[18] Both of these situations correspond to rough boundary conditions with IS of Lyapunov type.

4. CONCLUSION

In conclusion, we have analyzed the classical dynamics of a class of IS problems in two-dimensional N-scatterer ring-bounded cavities. The dynamical motion is irregular when the ring is rough ($N > 3$). The flow is of Lyapunov type. We have demonstrated that the Lyapunov exponent increases logarithmically with N. In addition, we have found that the mean escape time from ring cavities with gaps is proportional to the inverse of a typical gap aperture. The Hausdorff dimension of the trajectories is confirmed to be two. From empirical results we propose the scaling of Eq. (8) between the number of scatterers, the expected value of the escape time, and the Lyapunov exponent.

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