Thermodynamics of Irregular Scattering

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(Received 25 July 1989)

It is pointed out that scaling (multifractal) properties of chaotic repellers underlying irregular scattering in two-degree-of-freedom systems can be deduced by measuring simple length scales generated hierarchically along a straight line taken far away from the interaction region, or on the Poincaré plane, and analyzing them in the spirit of the thermodynamic formalism. The method is easier to apply than a periodic-orbit analysis.

PACS numbers: 05.45.+b, 03.20.+i, 05.90.+m

It has recently been recognized that in the realm of scattering processes regular scattering is exceptional and irregular, or chaotic, scattering[1-11] is typical, in a way very analogous to that of integrability and nonintegrability in bounded Hamiltonian systems.[12] The essential feature of irregular scattering is a clustering of initial conditions that leads to a delay in the interaction region, including a fractal set that leads to complete asymptotic trapping (for a review, see Ref. 7). The trajectories that come close to the trapped ones exhibit, on finite time scales, chaotic behavior. It has been pointed out[11] that the phenomenon can be well understood as a special case of transient chaos.[13,14] The set of all bounded periodic orbits plays the role of a chaotic repeller.[14] An adequate description of such scattering processes must therefore also include concepts worked out for dynamical systems. Our aim here is to illustrate how multifractal or, more generally, scaling properties of irregular scattering can be described by means of the so-called thermodynamic formalism,[15,16] which has been applied so successfully to one-dimensional chaotic maps.

We shall show that for irregular scattering taking place in two-degree-of-freedom systems it is sufficient to consider a straight-line intersection of the stable manifolds of the repeller, and the length scales generated on this one-dimensional subspace completely characterize chaotic and multifractal features of the process.

As an illustrative example, we shall use the problem of the scattering off three hard disks centered on the vertices of a regular triangle, introduced in Ref. 5, which has become a standard model of the field.[8,10]

Let us start with a few general comments. In scattering problems with two degrees of freedom, one can always introduce an area-preserving Poincaré map for trajectories having at least one collision with the interaction region. The coordinates of the map can be chosen to be, e.g., the modulus of an angular momentum and an appropriate angle. The elements of the repeller are just the points on which the map can be iterated arbitrary times both forward and backward. Each point of a repeller is expected to be hyperbolic, i.e., possess one-dimensional stable and unstable manifolds. The system is Hamiltonian, and time reversal implies the equivalence of stable and unstable manifolds. Consequently, the fractal properties (e.g., partial dimensions[17]) along both stable and unstable manifolds agree. (In another context, see Ref. 11.) Therefore, in contrast to dissipative cases, it is sufficient to concentrate now on any of the invariant manifolds which makes the problem effectively one dimensional.

Imagine a generating partition[18] on a neighborhood S of the repeller. This is obtained by taking the cross section of the nth images and preimages of S, and letting n go to infinity. The nth image of S contains, roughly speaking, strips which are elongated in the unstable direction but narrow in the stable one (dotted lines in Fig. 1). The nth preimage of S also contains strips but these are elongated in the stable direction. Let $\epsilon_{1,i}^{(n)}$, $i=1,2,\ldots$ denote the widths of these strips. Although

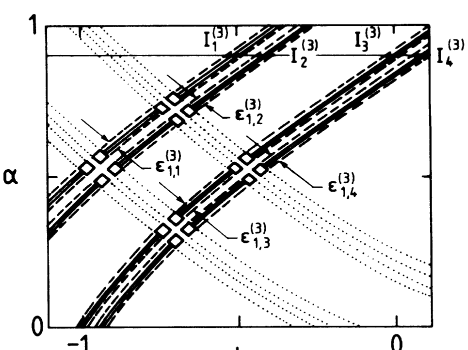

FIG. 1. Part of the Poincaré map in the three-disk problem (disk radius = 1.0, distance between disks $2\sqrt{3}$). b is the angular momentum (with respect to the symmetry center) of the particle with unit mass and velocity; α is the direction of velocity. Dotted and dashed lines denote the third image and preimage of neighborhood S which was taken as the region in phase space from which at least one collision is possible both in the direct and time-reversed motions. The boxes are elements of the generating partition covering the repeller; solid lines represent branches of the stable manifolds of repeller points. The four intervals exhibited correspond to initial conditions with fixed α and allow three successive collisions with the disks.

the actual values of $\epsilon_{1,i}^{(n)}$ depend on the choice of S, the scaling properties in n do not.

Let us fix a straight line in the Poincaré plane sufficiently far away from the repeller. This intersects the stable manifolds of the repeller points in a Cantor set we call C. If trajectories are started out of this line and the intervals $I_i^{(n)}$ are specified from which trajectories do not leave the neighborhood S up to, at least, n steps, we obtain a coverage of the Cantor set with a number, say, $N(n)$ of intervals. Let the length of these intervals be denoted by $l_i^{(n)}$, $i=1,2,\ldots,N(n)$. The intervals are practically the intersections of the straight line with the nth preimage of S; therefore, it is obvious that these lengths are proportional to the lengths obtained in the generating partition along the unstable direction: $l_i^{(n)} \sim \epsilon_{1,i}^{(n)}$. Since the stable manifolds extend smoothly to infinity, the scaling properties of $\{l_i^{(n)}\}$ do not depend on the position and direction of the straight line. Consequently, the fractal dimension of C is nothing but the partial fractal dimension $D_0^{(1)}$ along the unstable direction of the repeller. In view of reversibility, $D_0^{(1)}=D_0^{(2)}$. Branches of the stable manifolds and a few intervals $I_i^{(n)}$ on a straight-line intersection are illustrated in Fig. 1 for the three-disk problem.

It is worth noting that a similar procedure can also be performed in configurational space. Let us fix, as done in Ref. 5, a straight line far away from the interaction region (this corresponds to a line on the Poincaré map, too) and start trajectories from it in a given direction (with constant velocity). Those which do not leave the interaction region up to, at least, n collisions start out from certain intervals $I_i'^{(n)}$, whose lengths will be denoted by $l_i'^{(n)}$. For $n \to \infty$, these intervals approach a Cantor set C'. A smooth transformation connects these intervals with those obtained on the Poincaré map, so the scaling properties of $\{l_i^{(n)}\}$ and $\{l_i'^{(n)}\}$, and the fractal dimension of C and C', are the same. Thus our arguments explain the observation of Refs. 5 and 6 about the independence of the fractal dimension of C' from the choice of the straight line. In what follows, we shall use the set $\{l_i^{(n)}\}$ but keep in mind the equivalence with $\{l_i'^{(n)}\}$.

We are now in a position to work out quantitative relations. In the spirit of the thermodynamic formalism,[15,16] let us associate with each interval the microstate of a fictitious spin chain of length n with energy

$$nE_i = -\ln(l_i^{(n)}) . \tag{1}$$

The quantity $l_i^{(n)\beta}$, where β is a real parameter, the analog of an inverse temperature, plays the role of a Boltzmann factor. The partition sum is expected to scale exponentially with n; therefore, we can write for large n

$$\sum_{i=1}^{N(n)} l_i^{(n)\beta} \sim e^{-\beta F(\beta) n} , \tag{2}$$

where $F(\beta)$ is the free energy (density). This quantity is easy to measure, e.g., by comparing two partition sums at subsequent values of n. There are, in general, several intervals characterized by the same energy value E. Their number grows exponentially with n, like $\exp[S(E)n]$. The easiest way to obtain in practice the entropy function $S(E)$ it to take the Legendre transform of $\beta F(\beta)$: $S(E)=\beta E-\beta F(\beta)$. For our purposes it is sufficient to know the scaling forms (1) and (2), and we shall not use any longer the analogy with spin chains. $F(\beta)$ and $S(E)$ will be considered as characteristics of the repeller which, in principle, can also be determined in classical experiments.

The free energy or the entropy contains relevant information concerning the scaling properties of the system. To illustrate this, we first consider quantities that are independent of an invariant measure. The escape rate κ describes the exponential decay of the number of trapped trajectories with n. Since the total length of the intervals defined above must, therefore, decrease as $\exp(-\kappa n)$, we immediately find

$$F(1)=\kappa . \tag{3}$$

Note that $1/\kappa$ is just the average lifetime of trapped trajectories. A central result of the thermodynamic formalism says[15] that the free energy vanishes exactly at the value of β which agrees with the fractal dimension. Therefore, the partial fractal dimension $D_0^{(1)}$ is determined by the relation

$$F(D_0^{(1)})=0 . \tag{4}$$

The number $N(n)$ of the intervals tells us how many different trajectories of length n stay inside the interaction region. This number should grow as $\exp(K_0 n)$, where K_0 can be called the topological entropy of the scattering process. Consequently,

$$\beta F(\beta)\,|_{\beta=0} = -K_0 . \tag{5}$$

Let us now turn to metric properties. Among different invariant measures on the repeller, the most important one is the so-called natural measure. It can be determined by letting several trajectories start and concentrating on those which are trapped for sufficiently long time, in the same manner as described for dissipative cases in Ref. 14. The natural measure possesses a smooth density on a refining generating partition, as is the case for hyperbolic systems in general. This means that considering a strip of finite width along the unstable direction, the natural measure $P_i^{(n)}$ belonging to a box which has a size $\epsilon_{1,i}^{(n)}$ in the generating partition is proportional to this size. By taking into account normalization, we find

$$P_i^{(n)} \sim \frac{\epsilon_{1,i}^{(n)}}{\sum \epsilon_{1,i}^{(n)}} \sim e^{\kappa n}\epsilon_{1,i}^{(n)} \sim e^{\kappa n} l_i^{(n)} , \tag{6}$$

where in the last equality the fact has been used that the ϵ's are proportional to the l's. It is essential for what follows that a connection has thus been found between length scales $l_i^{(n)}$ and natural measures $P_i^{(n)}$. Being interested first in the scaling properties along the unstable direction, we introduce a partial crowding index[19] α_1 by

$$P_i^{(n)} \sim l_i^{(n)\alpha_1} . \tag{7}$$

Using (1) and (6), one immediately finds $P_i^{(n)} \sim \exp(-E\alpha_1 n) \sim \exp[(\kappa - E)n]$, i.e.,

$$\alpha_1 = 1 - \kappa/E \tag{8}$$

for each interval with energy E. Since this relation is unique, the number of intervals with a given α_1 is the same as that with $E = \kappa/(1-\alpha_1)$, i.e., $\exp[S(E)n]$. Furthermore, using the language of the $f(\alpha)$ formalism,[19] this number should behave as $l^{-f_1(\alpha_1)}$, where l is the interval length and where $f_1(\alpha_1)$ is the multifractal spectrum along the unstable direction, i.e., the fractal dimension of intervals with crowding index α_1. But because of (1), $l = \exp(-En)$; therefore, $S(E)$ and $Ef_1(\alpha_1)$ are equal. Thus, f_1 can be expressed in terms of the entropy function as

$$f_1(\alpha_1) = \left.\frac{S(E)}{E}\right|_{E=\kappa/(1-\alpha_1)} . \tag{9}$$

By taking the Legendre transform of f_1, we find an implicit equation for $D_q^{(1)}$:

$$\beta F(\beta)\,|_{\beta = q-(q-1)D_q^{(1)}} = \kappa q . \tag{10}$$

Note that Eq. (10) is the extension of (4). Since stable and unstable directions are equivalent $D_q^{(1)} = D_q^{(2)}$. The global dimension D_q appears as a sum of the partial ones:[17]

$$D_q = 2D_q^{(1)} . \tag{11}$$

The quantity $P_i^{(n)}$ is also proportional to the path probability of a given type of trajectories. Let us recall that the sum $\sum P_i^{(n)q}$ should scale[20] as $\exp[(1-q)K_q n]$ from which we obtain for the generalized entropies K_q

$$K_q = \frac{q[F(q) - F(1)]}{q-1} , \tag{12}$$

providing an extension of relation (5). The derivative of $\beta F(\beta)$ at $\beta = 1$ is just the averaged Lyapunov exponent on the repeller.

We applied the method presented here to the three-disk problem at the parameter value used in Ref. 5. The free energy was determined by measuring the length scales $\{l_i^{(n)}\}$ at generations $n = 9, 10, 11$ numerically. The convergence was very fast, and an accuracy of six digits has been reached by $n = 11$. From relations (3) and (4), $\kappa = 1.464771(4)$ and $D_0^{(1)} = 0.320781(1)$ were obtained, much more accurately than in Ref. 5. The function $\beta F(\beta)$ vs β has at this parameter value a weak curvature only. Therefore, we present rather the entropy function $S(E)$ [Fig. 2(a)]. The multifractal spectrum was evalu-

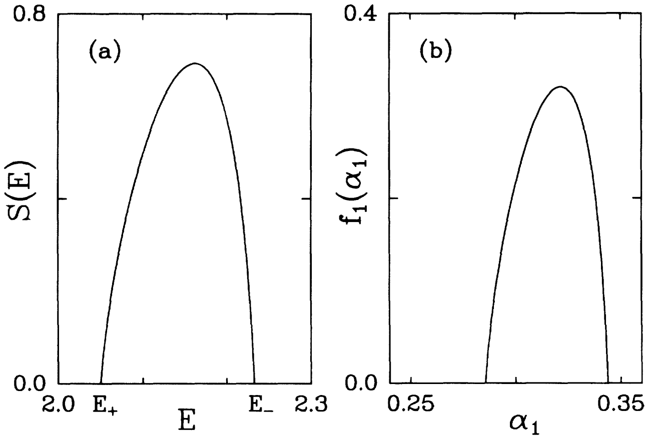

FIG. 2. The thermodynamics of the three-disk problem (disk radius 0.7). (a) The entropy function $S(E)$ obtained as the Legendre transform of $\beta F(\beta)$. The extremal energy values are $E_+ = 2.050104$ and $E_- = 2.232301$. (b) The partial multifractal spectrum $f_1(\alpha_1)$.

ated via relation (9) [Fig. 2(b)], with a relative error of 10^{-4}.

As an independent check, we performed the periodic-orbit analysis of the three-disk problem. All cycles of length n up to $n = 15$ have been determined by using the PIM triple method of Ref. 21 (where PIM denotes proper interior maximum) which could be improved in our case by the complete knowledge of the allowed symbol sequences. From the (largest) eigenvalues of these orbits, the multifractal spectra can be deduced via the formalism described in Ref. 11. We have found an agreement better than 0.2% with the data obtained from the length scales. The amount of computational efforts is, however, considerably increased not only because of the search for the cycles but also because of slower convergence and stronger finite-size effects. Recently, a new approach has been worked out based on the cycle expansion of the zeta function[10,15,22] which provides fast convergence even for short cycles. The convergence seems, however, to be nonuniform in β. The method requires determining zeros of a β-dependent polynomial of order equal to the largest cycle length used. At intermediate β values ($\beta \sim 6$ at $n = 6$), we found that roots tend to accumulate making numerics unreliable. Simultaneously, the root having been relevant for smaller β values disappeared. This disturbing region can be shifted toward large values by increasing the cycle length. Thus, a reliable evaluation of $F(\beta)$ in a region, say, $|\beta| \le 15$, also requires considerable computational effort by using the cycle expansion of the zeta function.

We emphasize that the method presented is not at all restricted to the three-disk problem. It has been shown that a topologically similar repeller exists also in scattering processes defined by smooth potentials.[23] The measurement of length scales and their analysis in the spirit of the thermodynamic formalism as described above has also recently been applied to such cases.[24] We recall that in practical, e.g., experimental, applications the Poincaré map need not be constructed. One might work with the scales $\{l_i'^{(n)}\}$ generated on a straight line in the configurational space as explained in the text. Finally, it is worth mentioning that in smooth-potential cases an interesting new phenomenon can occur. At energy values where quasiperiodic trajectories are present, the "stickiness" of the tori[25] may lead to a phase transition in the scaling properties, just like in bounded Hamiltonian systems.[26]

The authors are indebted to P. Cvitanović and B. Eckhardt for useful discussions. One of us (T.T.) would like to thank G. Eilenberger for the kind hospitality at the Kernforschungsanlage Jülich. This work was partially supported by grants provided by the Hungarian Academy of Sciences (Grants No. OTKA 819).

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