Thermodynamics of chaotic scattering at abrupt bifurcations

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Tamás Tél * Institut für Festkörperforschung, Forschungszentrum Jülich, D(W)-5170 Jülich, Federal Republic of Germany

Thermodynamic and multifractal spectra of chaotic scattering are investigated at abrupt bifurcations leading from fully developed chaotic to regular scattering as the particle energy E passes through a critical value E_m . For processes with uniform scaling, the spectra of Lyapunov exponents, entropies, and partial dimensions diverge, stay constant, and vanish, respectively, when the energy approaches E_m from below. To characterize processes also having scattering angles close to 90°, a new quantity is introduced, the partial topological entropy depending on the concentration of single scatterings with angles close to 90°. Multifractal spectra are proved to be universal in the sense that they depend on topological properties only. In particular, the generalized dimensions scale as $D_q = d_q / |\ln (E_m - E)|$ for q of order $1 / |\ln (E_m - E)|$, otherwise, D_q is finite and zero in the negative and positive q ranges, respectively. Our approach thus justifies a conjecture of Bleher, Ott, and Grebogi [Phys. Rev. Lett. 63, 919 (1989)] for q=0, and yields explicit expressions for the coefficients d_q . Phase transitions arising at the bifurcation point are analyzed.

I. INTRODUCTION

Chaotic scattering processes are common in the realm of unbounded Hamiltonian systems¹⁻³⁸ (for reviews see Refs. 10, 28, and 35). As a system parameter, most typically the particle energy E, is varied, transitions between classically regular and chaotic behavior might take place. In two-degree-of-freedom potential scattering one of the main scenarios leading to chaos is the abrupt bifurcation described in Ref.18. In this bifurcation a strange chaotic set (repeller) underlying the classical scattering process arises abruptly as E decreases from above a critical value, E_m , to below. E_m is one of the maxima of the potentialenergy function which is supposed to consist of several potential hills. Below the critical value, the strange set is hyperbolic and bounded orbits can be coded by a complete symbolic dynamics on a finite number of symbols; the chaotic scattering is fully developed.¹⁸

We investigate the behavior of thermodynamic and multifractal properties of scattering processes around abrupt bifurcations. In general, these properties can be studied by measuring the deflection function or the delay time distribution as a function of the impact parameter, and analyzing their singularities which sit on a fractal set.²³ The fractal dimension of this set—which coincides with the partial fractal dimension of the chaotic repeller—can also be extracted from differential-crosssection data.37 (Certain classical characteristics like the average lifetime of chaotic trajectories or the fractal dimension can be deduced even from quantum cross-section measurements lying in the semiclassical regime.^{8,20,37}) Unfortunately, the region around abrupt bifurcations is difficult to access experimentally or in a numerical simulation due to a singular behavior: As the particle energy approaches E_m from below, the chaotic set shrinks

to zero, the average lifetime vanishes, and trajectories become extremely unstable. A theoretical approach is, however, well suited for studying this region, and the results might be used as guides in direct measurements. By means of the thermodynamic formalism we derive how different characteristics scale with the particle energy around E_m . Moreover, certain results are universal in the sense that they depend only on topological properties of the dynamics determined by the arrangement of the potential hills in the scattering center.

A quantity of central interest which reflects the hierarchical organization of chaotic scattering processes is the free energy $F(\beta)$. It characterizes the scaling behavior seen by following trajectories with an increasing number n of collisions inside the scattering center.²³ The free energy is introduced in the spirit of the thermodynamic formalism of dynamical systems 39-42 via the relation

$$\sum_{i} l_{i}^{(n)^{\beta}} \simeq e^{-\beta F(\beta)n},\tag{1}$$

where β is any real number and n >> 1. $l_i^{(n)}$ denotes the lengths of intervals $I_i^{(n)}$ defined along a straight line chosen arbitrarily in the configurational space: Trajectories started out of these intervals with a given velocity vector have at least n collisions with the potential hills (see Fig.1). In other words, $I_i^{(n)}$ are the intervals where the delay function, measuring the number of bounces from hills experienced by the particle, is greater or equal to n. Equivalently, one can also use the length scales generated on a straight line in a Poincaré plane by considering trajectories which do not leave a certain neighborhood of the chaotic set earlier than the nth step.²³ Note that both $l_i^{(n)}$ and $F(\beta)$ depend on the particle energy E as a

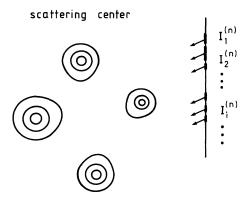


FIG. 1. Schematic diagram for the definition of length scales $l_i^{(n)}$. Contours of the potential hills are shown, as well as a straight line from which particles of unit mass start with a given velocity (arrow). Points belonging to paths with at least n bounces between the hills define the intervals $I_i^{(n)}$ whose lengths are the $l_i^{(n)}$'s. All trajectories starting out of an interval $I_i^{(n)}$ have the same symbolic code up to length n+1.

parameter. Since the scattering is regular for $E > E_m$, the length scales and the free energy are not necessarily defined in this region. In what follows we consider the energy range $E \leq E_m$.

The escape rate κ , which is just the reciprocal value of the average lifetime τ (measured in the number of bounces) in the interaction region, describes the exponential decay of the total interval length $\sum_i l_i^{(n)}$ with n. Consequently,

$$\kappa = \frac{1}{\tau} = F(1). \tag{2}$$

Since the chaotic set is hyperbolic, length scales and natural measures of the intervals are proportional. Therefore, the free energy also contains relevant information concerning metric properties. We shall be interested in the multifractal spectra of Lyapunov exponents 43 $(\lambda_q),$ entropies $^{44-46}$ $(K_q),$ and partial dimensions 47 (D_q) taken with respect to the natural measure of the repeller. Due to the Hamiltonian character of the system, the partial dimensions along both stable and unstable directions coincide, and we consider one of them only. (The total dimension of the chaotic set on a Poincaré plane is simply $2D_q$.) All spectra mentioned above can then be expressed in terms of the free energy according to the rules

$$\lambda_q = \left[\kappa - (1 - q)F(1 - q)\right]/q,\tag{3}$$

$$K_q = \frac{q[F(q) - \kappa]}{q - 1},\tag{4}$$

and

$$\beta F(\beta) \mid_{\beta = q - (q - 1)D_q} = \kappa q \tag{5}$$

as described in Refs. 23 and 29. Quantities with sub-

scripts 0 correspond to the averaged Lyapunov exponent, the topological entropy, and the partial fractal dimension.

The behavior of the free energy around the abrupt bifurcation can be deduced from knowing how the length scales change for $E \to E_m$. For simplicity, we assume that the potential possesses circularly symmetric local maxima. A simple calculation in classical mechanics ¹⁸ yields then a relation between the deflection angle ϕ , impact parameter x_0 , and energy difference with respect to the hill maximum:

$$\tan \phi = \frac{2x_0}{x_0^2 - 2(E_m - E)},\tag{6}$$

valid in the limit when the particle energy approaches the top of a single potential hill with quadratic maximum, and x_0 goes to zero. This shows that the scaling of x_0 depends strongly on whether the deflection angle ϕ is close to 90° or not. If $\tan \phi$ is of order unity,

$$x_0 \simeq (E_m - E) \quad \text{for } \phi \neq 90^{\circ}$$
 (7)

follows from (6), and if $|\tan \phi| >> 1$,

$$x_0 \simeq (E_m - E)^{1/2} \text{ for } \phi \approx 90^{\circ}$$
 (8)

is found.¹⁸ The intervals $I_i^{(n)}$ contain all impact parameter values with given types of collision sequences. Thus, all trajectories starting out from a certain interval possess the *same* symbolic code (of length n+1). The scaling of the lengths $I_i^{(n)}$ can, therefore, be computed by multiplying the energy dependent factors (7) or (8) of each single scattering together.

We shall derive here how the free energy and spectra (3)-(5) scale as $E \to E_m$. For scattering processes with uniform scaling, i.e., when all single scatterings contribute according to (7), it has been shown¹⁸ that $D_q = d_q/|\ln(E_m - E)|$. Our considerations complete this statement by yielding the entropy K_q as the proportionality factor d_q . Furthermore, we point out that the Lyapunov exponents diverge, while the entropies stay E independent when $E \to E_m$ (Sec. II).

Mixed processes where both scaling (7) and (8) appear are of particular interest, since in such cases the scaling is not uniform: to each parameter β or q other subdynamics give the relevant contribution. We propose to characterize this effect by introducing a new kind of multifractal spectrum, that of partial topological entropy belonging to trajectories with a fixed ratio of single scatterings scaling according to (7) and (8). To leading order in $E - E_m$, spectra (3)-(5) turn out to be expressible in terms of the partial topological entropy.

The only statement accessible in the literature which concerns such cases conjectures ¹⁸ that the above rule given for D_q is valid for the fractal dimension (q=0). Our thermodynamic approach of mixed cases (Sec. III) verifies the conjecture, and shows that this rule also holds for generalized dimensions but only in a restricted range where q is of order $1/|\ln(E_m-E)|$, and yields explicit expressions for the coefficients d_q . For q values out of

this range, $D_q = 0$ for q > 0 and D_q is of order unity for q < 0. Similarly, drastically different scaling behaviors in different q ranges follow for the spectra of Lyapunov exponents and entropies. These lead then at $E = E_m$ to nonanalyticities, to so-called phase transitions (Sec. IV). A method for computing the partial topological entropy is given in the Appendix.

II. PROCESSES WITH UNIFORM SCALING

Let us consider first potentials the geometry of which does not allow for the existence of scattering angles near 90° in bounded trajectories around the bifurcation point. The case of three identical Gaussian hills arranged on the vertices of a regular triangle ⁶ provides an example. In such situations each single scattering contributes a factor $E_m - E$, and since each $I_i^{(n)}$ contains initial points of trajectories with n collisions, each $l_i^{(n)}$ is proportional to $(E_m - E)^n$. We can then write

$$l_i^{(n)} = l_{0,i}^{(n)} [\Delta(E)]^n \tag{9}$$

with

$$\Delta(E) \equiv \frac{E_m - E}{E_m - E_0},\tag{10}$$

where $E_0 < E_m$ is an arbitrarily chosen energy value (still close to the critical E_m). This form ensures that $l_{0,i}^{(n)}$ can be interpreted as the interval lengths just at the reference energy E_0 . Substituting (9) and (10) in (1) one finds

$$\beta F(\beta) = \beta | \ln \Delta(E) | + \beta F_0(\beta). \tag{11}$$

 $F_0(\beta)$ denotes here the free energy function belonging to particle energy E_0 . In the limit $E \to E_m$, $\beta F(\beta)$ is a rapidly varying function of the inverse temperature.

At the bifurcation point we obtain from (11)

$$\beta F(\beta) = \begin{cases} -\infty & \text{for } \beta < 0 \\ -K_0 & \text{for } \beta = 0 \\ +\infty & \text{for } \beta > 0. \end{cases}$$
 (12)

The jump in the free energy at $\beta = 0$ can be interpreted as a zeroth-order phase transition (for a discussion see Sec. IV).

For a finite but small energy difference

$$\kappa = |\ln \Delta(E)| + \kappa_0, \tag{13}$$

where κ_0 stands for the escape rate at E_0 . This relation tells us that the average lifetime of chaotic trajectories is decreasing and reaches zero at the bifurcation point.

From relations (3) and (4) we obtain immediately

$$\lambda_q = |\ln \Delta(E)| + \lambda_{0,q}, \tag{14}$$

$$K_q = K_{0,q}, \tag{15}$$

where quantities with subscript zero belong to the reference energy. Note that the E dependence drops out

when taking in (4) the difference $F(\beta) - \kappa$, which leads to (15).

The general dimensions are expected to be small around the bifurcation point; therefore, one can expand Eq.(5) to find an explicit expressions for D_q :

$$(q-1)D_{q}[qF(q)]' = q[F(q) - \kappa]$$
 (16)

from which in the limit $E \to E_m$

$$D_q = \frac{K_q}{|\ln \Delta(E)|} \tag{17}$$

follows. This energy dependence of the order-q dimensions was first derived in Ref.18; our approach specifies also the prefactors as just the order-q entropies.

Results (14), (15), and (17) illustrate the fact that although the spectra λ_q , K_q , and D_q are not independent (all are derivable from the free energy), they describe completely different aspects of the dynamical system and exhibit completely different behavior around the bifurcation point. Lyapunov exponents characterize the instability of the chaotic set. Their divergence at E_m for all q means that all bounded hyperbolic orbits are infinitely unstable just when they appear, and become more stable with decreasing particle energy. Entropies reflect properties of the strange set's symbolic organization and of the symbol sequence distribution. Their energy independence shows the robustness of these properties around the bifurcation. Dimensions describe fractal aspects. Equation (17) tells us that the chaotic repeller is completely rarified when created, and becomes less sparse as the energy is decreased.

III. MIXED PROCESSES

A. General setup

To describe the scaling of processes including single scatterings with angles close to 90° one has to know some details concerning the symbolic organization of the strange set. The reason is that in view of relations (7) and (8), single scatterings with angles close to 90° yield a scaling factor completely different from those far away from 90° . Consequently, the length scales $l_i^{(n)}$ scale in a different way with particle energy E if trajectories starting out of the corresponding intervals have different numbers of single scatterings with angles close to 90° . As examples we shall consider cases with potential hills of equal heights on the vertices of a rectangle (example I) and of a right-angled triangle (example II) (see Appendix).

In order to achieve a more detailed description, we introduce some new quantities. Let $N^{(n)}(m)$ denote the number of trajectories with n collisions containing exactly m (m = 0, 1, ..., n) single scatterings with angles close to 90°. Similarly, let us divide the length scales $l_i^{(n)}$ into subsets $\{l_{i_m}^{(n)}(m)\}, i_m = 1, 2, ..., N^{(n)}(m)$ according to number m. As a consequence of (7) and (8), the energy dependence is given by

$$l_{i_m}^{(n)} = l_{0,i_m}^{(n)} [\Delta(E)]^{n-m/2}.$$
(18)

At this point we make two conjectures, in the spirit of the theory of large deviations, 48 which will be essential in what follows. We expect for large n and m the scaling behavior

$$N^{(n)}(m) \sim e^{nh(x)},\tag{19}$$

where

$$x \equiv m/n \tag{20}$$

is the concentration of single scatterings with angles close to 90° in bounded trajectories. h(x) is a one-humped function (see Fig.2) and can be interpreted as the partial topological entropy for trajectories with concentration x. The maximum of h is obviously the global topological entropy K_0 . Note that h(x) is a purely geometrical quantity that can be obtained for whole classes of scattering arrangements from combinatorial arguments. The way this can be done is described in the Appendix.

Furthermore, we also expect that the partial partition sum based on the length $l_{0,i_m}^{(n)}(m)$ exhibits a scaling that depends on m through the concentration x only, i.e., for n large

$$\sum_{i_m=0}^{N^{(n)}(m)} \left[l_{0,i_m}^{(n)}(m) \right]^{\beta} \sim e^{-\beta F_0(x,\beta)n}, \tag{21}$$

where $F_0(x,\beta)$ is the partial free energy, at particle energy E_0 , characterizing trajectories with concentration x.

Putting these forms together we find for the total partition sum

$$e^{-\beta F(\beta)n} \sim \sum_{x=0}^{x=x_c} e^{-[(1-x/2)\beta|\ln\Delta(E)|+\beta F_0(x,\beta)]n}.$$
 (22)

Here x_c is the largest possible concentration in the system. It is not obvious that there exist trajectories containing solely single scatterings with angles close to 90°. In fact, in the triangular geometry the highest possible concentration is $x_c = \frac{1}{2}$ provided by a periodic orbit bouncing along the shorter sides of the right-angled triangle. In the rectangular arrangement the maximum concentration is accessible (by an orbit passing around the sides all the time), and $x_c = 1$ in this case.

The free energy $F(\beta)$ is obtained by finding the dominant contribution from sum (22) for $n \to \infty$ [$\Delta(E)$, β fixed]. Since the behavior depends essentially on the ratio of the two terms in the exponent, we have to discuss two regions separately: (i) β is of order unity and (ii) $\beta \mid \ln \Delta(E) \mid$ is of order unity. Although the latter is very narrow for $E \to E_m$, it cannot be neglected because the free energy exhibits a nontrivial behavior there from which quantities like the fractal dimension D_0 or topological entropy K_0 also follow.

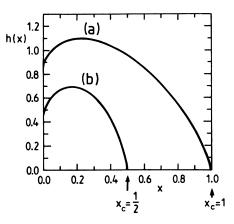


FIG. 2. The partial topological entropy. (a) Example I: rectangular geometry, (b) example II: right-angled triangular geometry. Arrows mark the largest possible concentrations x_c . A good approximation of h(x) is obtained by taking a smooth curve passing through the points $h(m/150) = \ln [N^{(300)}(2m)/N^{(150)}(m)]/150$, m = 0, 1, ..., 150 where $N^{(n)}(m)$ is the numerical solution of recursions (A1)–(A3) and (A6)–(A9).

B. Results for inverse temperatures of order 1

In this range the dominating contribution is determined by the first term in the exponent of (22).

We first consider positive values of β . The largest exponent then belongs to the largest possible x value. Therefore, we have

$$\beta F(\beta) = \left(1 - \frac{x_c}{2}\right)\beta \mid \ln \Delta(E) \mid +\beta F_0(x_c, \beta)$$

for
$$\beta = O(1) > 0$$
. (23)

Consequently, the escape rate is obtained as

$$\kappa = \left(1 - \frac{x_c}{2}\right) |\ln \Delta(E)| + \kappa_0 \tag{24}$$

with $\kappa_0 = F_0(x_c, 1)$. From relations (3)-(5) one then finds

$$\lambda_q = \left(1 - \frac{x_c}{2}\right) | \ln \Delta(E) | + \lambda_{0,q}$$

for
$$(1-q) = O(1) > 0$$
, (25)

where

$$\lambda_{0,q} = \frac{\kappa_0 + (q-1)F_0(x_c, 1-q)}{q},$$

furthermore,

$$K_q = \frac{q(F_0(x_c, q) - \kappa_0)}{q - 1}$$
 for $q = O(1) > 0$, (26)

and

$$D_q = \frac{K_q}{(1 - x_c/2) |\ln \Delta(E)|} \quad \text{for } q = O(1) > 0.$$
 (27)

These results are formally very similar to (14), (15), and

(17), simply a new factor $1-x_c/2$ shows up due to scaling (8). The actual behavior is, however, much simpler, since in typical cases only one single periodic trajectory (or a few equivalent ones) can possess the critical concentration x_c . The free energy for a periodic orbit is independent of β and equal to the Lyapunov exponent of this orbit. Therefore $F_0(x_c, \beta) \equiv \lambda_0$ where λ_0 is the Lyapunov exponent of the trajectory with concentration x_c taken at the reference energy E_0 . As a consequence of (23), $\kappa_0 = \lambda_0 = \lambda_{0,q}$, and both dimensions and entropies vanish:

$$K_q = D_q = 0 \text{ for } q = O(1) > 0$$
 (28)

as follows from (26) and (27).

We next consider negative values of the inverse temperature. The dominant contribution to sum (22) is then given by the maximal exponent belonging to x = 0. Thus,

$$\beta F(\beta) = \beta | \ln \Delta(E) | + \beta F_0(0, \beta)$$

for
$$\beta = O(1) < 0$$
. (29)

This is simply the free energy of a restricted dynamics in which no single scattering with angle close to 90° occurs, and is formally of the same type as Eq. (11). Since, however, the escape rate differs from (13), we now obtain in the limit $E \to E_m$ for spectra (3)-(5):

$$\lambda_q = \left(1 - \frac{x_c}{2q}\right) |\ln \Delta(E)| + \lambda_{0,q}$$
for $(1 - q) = O(1) < 0$ (30)

where $\lambda_{0,q}$ is given as in (25) but F_0 is taken now at x=0,

$$K_q = \frac{x_c q/2}{q-1} | \ln \Delta(E) | + \frac{q[F_0(0,q) - \kappa_0]}{q-1}$$

for
$$q = O(1) < 0$$
, (31)

and

$$D_q = \frac{x_c q/2}{q-1} + \frac{q \left[(1 - x_c/2) F_0(0, q(1 - x_c/2)) - \kappa_0 \right]}{|\ln \Delta(E)| (q-1)}$$

for
$$q = O(1) < 0$$
. (32)

We see that for negative values of q the entropies diverge and the dimensions stay finite around the bifurcation point, which is a completely new effect in comparison with uniform scaling (Sec. II).

C. Results around zero inverse temperature

The free energy changes very rapidly at $\beta=0$ if the particle energy is close to the critical value. This behavior, however, cannot be linear in the present case, as can be seen by comparing (23) and (29). Thus, a nontrivial free energy is expected to exist in the range where β is of order $1/|\ln \Delta(E)|$.

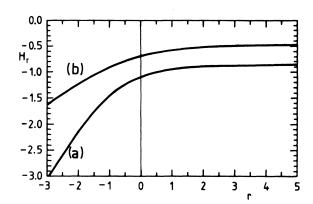


FIG. 3. The Legendre transform H_r of the partial topological entropy h(x) obtained via (36): (a) example I, (b) example II.

It is worth enlarging this region formally by introducing a rescaled inverse temperature b via

$$\beta = \frac{b}{|\ln \Delta(E)|} \tag{33}$$

and assume that b is of order unity. Since β is small, the partial partition sum (21) is practically the number $N^{(n)}(m)$ of trajectories with concentration x. Therefore, in this range

$$\beta F_0(x,\beta) = -h(x),\tag{34}$$

the free energy is of entropic origin, and $\beta F_0(\beta)$ is temperature independent. Consequently, the total partition sum (22) appears as

$$e^{-\beta F(\beta)n} \sim \sum_{x=0}^{x=x_c} e^{-[(1-x/2)b-h(x)]n}$$
 (35)

It is clear from this form that the x value belonging to the dominant contribution for $n \to \infty$ will now be determined essentially by the parameter b, since both terms in the exponent are of the same order. This means that, depending on b, different symbolic subdynamics that are neccessarily incomplete yield the mean contribution to the free energy. It is also clear that the total free energy is specified by h(x) and b in this range and is, therefore, independent of metric properties.

To be more specific, let us introduce the Legendre transform H_r of h(x) as

$$H_r = xr - h(x), \qquad \frac{dh(x)}{dx} = r. \tag{36}$$

 H_r is a monotonically increasing function that goes to saturation for $r \to \infty$ (see Fig.3) since h(x) is finite at the origin. For large negative r, $H_r = x_c r$.

By applying the saddle-point approximation to sum (35) we find that the main contribution comes from a term where h' = -b/2. Thus, the free energy turns out to be expressible with the Legendre transform of h as

$$\beta F(\beta)_{|\beta=b/|\ln\Delta(E)|} = b + H_{r=-b/2}.$$
 (37)

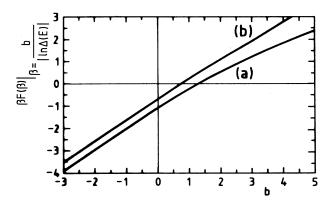


FIG. 4. The free energy (37). (a) Example I, (b) example II.

Note that the right-hand side at $\beta=0$ is $-K_0$, as expected, since the maximum of h is just the global topological entropy. The asymptotic slopes for large positive and negative b values are 1 and $1-x_c/2$, respectively, ensuring smooth interpolation to formulas (23) and (29) (see also Fig.4).

The spectra (3)-(5) can then all be expressed in terms of H_r . Since β is restricted to be of order $1/|\ln \Delta(E)|$, the variables q are to be scaled accordingly. We thus find the generalized Lyapunov exponents and entropies as

$$q\lambda_q = \kappa + k - H_{r=k/2} \quad \text{for} \quad q - 1 = \frac{k}{|\ln \Delta(E)|}$$
 (38)

and

$$K_q = -x_c \frac{k}{2} - H_{r=-k/2}$$
 for $q = \frac{k}{|\ln \Delta(E)|}$, (39)

respectively, where the parameter k is of order unity. An implicit condition follows for the dimension from (5). By writing

$$D_q = \frac{d_k}{|\ln \Delta(E)|} \text{ for } q = \frac{k}{|\ln \Delta(E)|}$$
 (40)

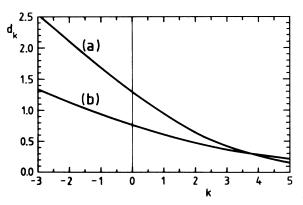


FIG. 5. The reduced dimension d_k defined by (40). (a) Example I, (b) example II.

one obtains an equation for the reduced dimensions d_k in the form

$$(H_r - 2r)_{|r = -(k+d_k)/2} = \left(1 - \frac{x_c}{2}\right)k. \tag{41}$$

The spectrum d_k is shown in Fig.5. Note that for $x_c = 0$ all results of this section must coincide with those obtained for the uniform case.

D. Multifractal spectra to leading order

The multifractal spectrum $f(\alpha)$ (Ref. 49) belonging to the generalized dimensions D_q (q arbitrary) can even be expressed explicitly with the partial topological entropy h(x). To see this, let us recall that the natural measure of an interval $I_i^{(n)}$ is proportional to the length of this interval times $\exp{(\kappa n)}$.²³ Using (24) and the scaling $l^{(n)}(m) \sim \left[\Delta(E)\right]^{n(1-x/2)}$ [see (18)], we conclude that the measure for intervals belonging to concentration x is proportional to $\left[\Delta(E)\right]^{n(x_c-x)/2}$. The crowding index α is the ratio of the logarithms of measure and length, so that we find in leading order

$$\alpha = \frac{x_c - x}{2 - x}.\tag{42}$$

Furthermore, as the number of intervals with crowding index α (or concentration x) is proportional to $l^{(n)}(m)^{-f(\alpha)}$, and this is the same as $N^{(n)}(m)$, we conclude that

$$f(\alpha) = \frac{1}{|\ln \Delta(E)|} \left(\frac{h(x)}{1 - x/2} \right) \Big|_{x = (x_c - 2\alpha)/(1 - \alpha)}. \tag{43}$$

Results obtained for examples I and II are plotted in Fig.6.

In particular, since the maximum of f is the fractal dimension D_0 , it follows from here that the reduced fractal dimension d_0 [cf. (40)] is just the maximum of h(x)/(1-x/2):

$$d_0 = \left(\frac{h(x)}{1 - x/2}\right)_{\text{max}}.\tag{44}$$

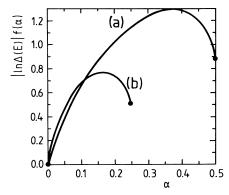


FIG. 6. The $f(\alpha)$ spectrum obtained via relation (43). (a) Example I, (b) example II. Dots at the end of the spectra illustrate that the crowding indices $\alpha_{\min} = 0$ and $\alpha_{\max} = x_c/2$ belong to a continuum of q values (see text).

By means of relation (44), we found in example I that $d_0=1.30$ (see Appendix). This value is consistent with a direct numerical computation of the fractal dimension for a square-symmetric, four-hill potential with equal hill maxima [see Fig. 5(b) of the first item of Ref.18 and take into account error bars]. It is worth emphasizing, however, that the same reduced fractal dimension d_0 holds for all rectangular geometries with circularly symmetric local maxima and does not even depend on the widths of hills, as follows from the definition of h(x). In example II $d_0=0.76$ is obtained for all three-hill problems (with cylindrical hills of equal heights) on right-angled triangles.

We mention that Eq. (44) implies that the fractal dimension is still connected with some kind of topological entropy but now the *partial* topological entropy is relevant. For $x_c = 0$, $d_0 = K_0$ follows.

Taking the Legendre transform of $f(\alpha)$ one recovers (41) if q is supposed to be of order $1/|\ln \Delta(E)|$. This assumption, however, has not been used in the above argument, and Eq.(43) is expected to be the complete multifractral spectrum in leading order for $\Delta(E) \to 0$. In fact, for q of order unity, we must distinguish two cases. For negative q values there is a single crowding index $\alpha_{\max} = x_c/2$, yielding in leading order $D_q = x_c q/[2(q-1)]$, in agreement with (32). For positive q values $\alpha_{\min} = 0$ from which $D_q = 0$ follows.

Similarly, $f(\alpha)$ -like spectra belonging to entropies and Lyapunov exponents can also be expressed, in leading order, in terms of h(x). Here we give only the dynamical multifractal spectrum 46,50 $f_0(\alpha_0)$, the Legendre transform of $(q-1)K_q$. One obtains

$$f_0(\alpha_0) = h(x) \mid_{x = x_c - 2\alpha_0/|\ln \Delta(E)|}$$
 (45)

This is consistent with (39). For q values of order unity it yields $K_q = x_c q/[2(q-1)]|\ln \Delta(E)|$ and $K_q = 0$ for q < 0 and q > 0, respectively.

We conclude that the multifractal spectra in leading order depend only on the partial topological entropy. This is a consequence of an anomalous property of the free energy: It exhibits completely different E dependence in regions where trajectories having no single scatterings with angles close to 90° are relevant and where one periodic orbit with maximal concentration x_c gives the dominant contribution. Furthermore, the energy dependence is so strong that it suppresses the contribution coming from the length scales $l_{0,i}^{(n)}$ for $\beta < 0$. The universality we find is, therefore, a special feature of mixed cases and is not present in scatterings with uniform scaling.

IV. DISCUSSION

It is useful to discuss the singularities (phase transitions) that arise in the spectra when $E \to E_m$ and to compare them with ones known to exist in dissipative systems.^{50–55}

The function $\beta F(\beta)$ develops a jump at $\beta = 0$, expressed by (12), in both uniformly scaling and mixed cases [see Eqs. (23) and (29)]. This is due to the fact

that the length scales vanish, leading to an energy dependence proportional to $\beta | \ln \Delta(E) |$. A similar kind of transition has been found in one-dimensional maps with complete topology containing a fixed point with infinite slope 51,55 since the length scale belonging to this fixed point has a much faster decrease then the others. Therefore, $\beta F(\beta) = -\infty$ for negative β but, in contrast to our case, $\beta F(\beta)$ is finite in the range $\beta \geq 0$ for such maps.

No singularity shows up in spectra (3)–(5) of scattering processes with uniform scaling since the escape rate and the free energy $F(\beta)$ possess exactly the same E dependence. Consequently, the natural measure of boxes becomes independent of the particle energy. Thus no interval can have an extremely small or large measure.

The situation is different in mixed cases. As a consequence of inhomogenous scaling, the natural measure of intervals with concentration x scale as $[\Delta(E)]^{n(x_c-x)/2}$. The crowding indices are, therefore, of order unity. The least and most probable intervals are thus characterized by a crowding index $\alpha_{max} = x_c/2$ and $\alpha_{min} = 0$, respectively. Since $f(\alpha)$ vanishes for $E \to E_m$, one has at the bifurcation point

$$D_q = \begin{cases} x_c q / [2(q-1)] & \text{for } q \le 0 \\ 0 & \text{for } q > 0 \end{cases}$$
 (46)

expressing the coexistence of two phases with α_{\min} and α_{\max} . The q/(q-1) dependence seems to be general for all systems possessing a nontrivial crowding index on a set of zero dimension. An elementary example 56,49,54 is a function of type $x^{-1+z}, z > 0$. At the singularity the crowding index is z, and is 1 otherwise, so that $(q-1)D_q = \min(zq, q-1)$. In our case, when a periodic trajectory with concentration x_c dominates, it has a Dirac- δ -like measure with a vanishing α_{\min} and, therefore, $D_q = 0$ for q positive.

As another consequence of having intervals with very small measures, one finds the entropy spectrum at the bifurcation point to have the form [see Eqs. (28) and (31)]:

$$K_{q} = \begin{cases} \infty & \text{for } q < 0 \\ K_{0} & \text{for } q = 0 \\ 0 & \text{for } q < 0. \end{cases}$$
 (47)

The phase q < 0 is familiar from one-dimensional fully developed chaotic maps with an infinite slope at one of the fixed points 51 and is due to the fact that the symbolic code belonging to this fixed point is much less probable than all others.

The singularities in dimensions and entropies express the fact that the measure is rather unevenly distributed on the repeller when it is created. These phase transitions show that the chaotic set *cannot* be considered to be hyperbolic at the bifurcation point, although it is hyperbolic for all particle energies below E_m .

Interestingly, there is no singularity in the spectrum of Lyapunov exponents: $\lambda_q = \infty$ expressing that all periodic orbits are infinitely unstable at the bifurcation point.

In conclusion, we have worked out how thermodynamic

and multifractal characteristics of chaotic scattering processes scale with the particle energy around abrupt bifurcations. Mixed cases containing single scatterings with angles close to 90° required a special approach. It has been useful to introduce a new spectrum, that of partial topological entropies having a universal character which is transferred to other quantities, too. This approach illustrates that the thermodynamic formalism can be a powerful tool also for deducing how properties of chaotic systems scale with an external parameter, in our case the particle energy.

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APPENDIX: COMPUTATION OF THE PARTIAL TOPOLOGICAL ENTROPY

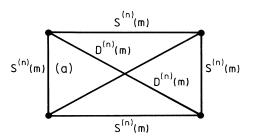
In general, one cannot hope to find an exact expression for $N^{(n)}(m)$, and we have not been able to derive a closed equation for this quantity. It is useful, however, to consider a somewhat more detailed description and specify trajectories according to their final position. This is always possible since the rule of the symbolic dynamics is simple: around abrupt bifurcations leading to fully developed chaotic scattering the global topology is complete. At this level, a closed set of recursions can be found which can be solved numerically.

Example I. The case of four hills of equal maxima arranged on the vertices of a rectangle (of arbitrary aspect ratio). We introduce the number $D^{(n)}(m)$ and $S^{(n)}(m)$ of trajectories ending along one of the diagonals and along one of the sides, respectively, after the last (nth) single scattering. Here m = 0, 1, ..., n is the number of single scatterings with angles close to 90°. Trajectories ending along a diagonal can proceed either along the diagonal or along two of the sides. The next single scattering has, therefore, in all of these cases an angle different from 90°. Trajectories ending along a side can proceed along one of the diagonals, can be reflected, or can be scattered with an angle close to 90° towards a hill along another side [see Fig.7(a)]. Thus, one can write down a closed set of recursions for the numbers $D^{(n)}(m)$ and $S^{(n)}(m)$. Starting from any of the hills, we find $D^{(1)}(0) = 3$, $D^{(1)}(1) = 0$, $S^{(1)}(0) = 4$, $S^{(1)}(1) = 2$, and

$$D^{(n+1)}(m) = D^{(n)}(m) + S^{(n)}(m), \tag{A1}$$

$$S^{(n+1)}(m) = S^{(n)}(m-1) + S^{(n)}(m) + 2D^{(n)}(m).$$
(A2)

The total number $N^{(n)}(m)$ is simply



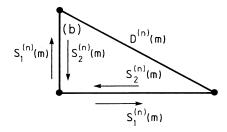


FIG. 7. The geometry of the examples and hint for defining the recursion yielding $N^{(n)}(m)$. (a) Example I, (b) example II.

$$N^{(n)}(m) = 4[D^{(n)}(m) + S^{(n)}(m)]. \tag{A3}$$

One can easily be convinced that both $D^{(n)}(m)$ and $S^{(n)}(m)$ have the same scaling for large n as $N^{(n)}(m)$, i.e., $D^{(n)}(m)$, $S^{(n)}(m) \sim \exp{[nh(x)]}$. For m = 0 one finds

$$D^{(n+2)}(0) - 2D^{(n+1)}(0) - D^{(n)}(0) = 0$$
 (A4)

from which $h(0) = \ln(1 + \sqrt{2}) = 0.88$ follows. Using Taylor expansions, recursions (A1) and (A2) can be converted into a differential equation for h(x):

$$e^{2h-2xh'} - e^{h-(x+1)h'} - 2e^{h-xh'} + e^{-h'} - 1 = 0.$$
 (A5)

The main advantage of this form is that it yields the maximium value of h (for h' = 0) as $\ln 3$, so that $K_0 = \ln 3$ as expected. Furthermore, assuming that the slope is infinite at x = 0 but xh' vanishes, one recovers the above value of h(0).

To obtain the whole function it is convenient to iterate recursions (A1) and (A2) up to $n \sim 300$ and read off h via relation (19). This is how Fig.2 was generated. For the maximum of h/(1-x/2) we found numerically the value $d_0 = 1.30$. The crowding index associated with the fractal dimension is $\alpha_0 = 0.37$, while the concentration belonging to the maximum value of h is obtained as $x_0 = 0.22$

Example II. The case of three hills of equal maxima arranged on the vertices of a right-angled triangle [Fig. 7(b)]. Here three different numbers have been introduced: $D^{(n)}(m)$ for trajectories ending along the hypotenuse (orientation irrelevant), as well as, $S_1^{(n)}(m)$ and $S_2^{(n)}(m)$ for trajectories ending along the two short sides pointing away and towards the vertex with 90°, respec-

tively. Both D and S_1 induce at the next level trajectories of type D and S_2 . S_2 , however, generates two trajectories of type S_1 one of them with a scattering angle close to 90°. The initial conditions are $D^{(1)}(0) = 4$, $D^{(1)}(1) = 0$, $S_1^{(1)}(0) = 2$, $S_1^{(1)}(1) = 2$. The recursions, thus, read

$$D^{(n+1)}(m) = D^{(n)}(m) + S_1^{(n)}(m), \tag{A6}$$

$$S_1^{(n+1)}(m) = S_2^{(n)}(m-1) + S_2^{(n)}(m)$$
 (A7)

with

$$D^{(n)}(m) \equiv S_2^{(n)}(m). \tag{A8}$$

The total number is

$$m=0$$
 we find

(A9)

For m = 0 we find

$$D^{(n+2)}(0) - D^{(n+1)}(0) - D^{(n)}(0) = 0$$
 (A10)

yielding $h(0) = \ln \left[(\sqrt{5} + 1)/2 \right] = 0.48$. The differential equation now has the form

 $N^{(n)}(m) = D^{(n)}(m) + S_1^{(n)}(m) + S_2^{(n)}(m)$

$$e^{2h-2xh'} - e^{h-xh'} - e^{-h'} - 1 = 0 (A11)$$

and implies that the maximum h value is $\ln 2 = K_0$. For the reduced fractal dimension we found in this case numerically $d_0 = 0.76$. The crowding index and concentration belonging to the maximum of $f(\alpha)$ and h(x) is now $\alpha_0 = 0.16$ and $x_0 = 0.17$, respectively.

- *On leave of absence from Institute for Theoretical Physics, Eötvös University, Budapest, Hungary.
- ¹C. C. Rankin and W. H. Miller, J. Chem. Phys. 55, 3150 (1971); L. Gottdiener, Mol. Phys. 29, 1585 (1979); D. W. Noid, S. K. Gray and S. A. Rice, J. Chem. Phys. 84, 2649 (1986); S. K. Gray, S. A. Rice, and M. J. Davis, J. Phys. Chem. 90, 3470 (1986); S. K. Gray and S. A. Rice, Faraday Discuss. Chem. Soc. 82, 307 (1986); M. Berblinger and C. Schlier, Chem. Phys. Lett. 145, 299 (1988).
- ²J. Froyland, Phys. Rev. D 27, 943 (1983).
- ³ J. M. Petit and M. Hénon, Icarus 66, 536 (1986).
- ⁴H. Aref, Ann. Rev. Fluid Mech. 15, 345 (1983); S. V. Manakov and L. N. Schur, Pis'ma Zh. Eksp. Teor. Fiz. 37, 45 (1983) [JETP Lett. 37, 54 (1983)]; B. Eckhardt, Europhys. Lett. 5, 107 (1988); B. Eckhardt and H. Aref, Philos. Trans. R. Soc. A 326, 655 (1988).
- ⁵C. Jung, J. Phys. A **19**, 1345 (1986); **20**, 1719 (1987); in Finite Dimensional Integrable Nonlinear Dynamical Systems, edited by P. G. L. Leach and W. H. Steeb (World Scientific, Singapore, 1988).
- ⁶B. Eckhardt and C. Jung, J. Phys. A 19, L829 (1986); C. Jung and H. J. Scholz, ibid. 20, 3607 (1987); 21, 2301 (1988).
- ⁷B. Eckhardt, J. Phys. A **20**, 5971 (1987).
- ⁸R. Blümel and U. Smilansky, Phys. Rev. Lett. 60, 477
- 9S. Bleher, C. Grebogi, E. Ott, and R. Brown, Phys. Rev. A 38, 930 (1988).
- ¹⁰B. Eckhardt, Physica D **33**, 89 (1988).
- ¹¹M. Hénon, Physica D 33, 132 (1988).
- ¹²W. J. Firth, Phys. Rev. Lett. **61**, 329 (1988); S. A. Trugman, ibid. 62, 579 (1989).
- ¹³B. Mirbach and H. J. Korsch, Nonlinearity 2, 327 (1989).
- ¹⁴G. Troll and U. Smilansky, Physica D **35**, 34 (1989).
- ¹⁵P. Gaspard and S. A. Rice, J. Chem. Phys. **90**, 2225 (1989); 90, 2242 (1989); 90, 2255 (1989).
- ¹⁶T. Tél, J. Phys. A 22, L691 (1989).
- ¹⁷P. Cvitanović and B. Eckhardt, Phys. Rev. Lett. 63, 823
- ¹⁸S. Bleher, E. Ott, and C. Grebogi, Phys. Rev. Lett. 63, 919 (1989); S. Bleher, C. Grebogi, and E. Ott, Physica D 46, 87 (1990).
- ¹⁹C. Jung and S. Pott, J. Phys. A 22, 2925 (1989); 23, 3729 (1990); C. Jung, ibid. 23, 1217 (1990).

- ²⁰R. Blümel and U. Smilansky, Physica D **36**, 111 (1989); Phys. Rev. Lett. 64, 241 (1990).
- ²¹P. Gaspard and S. A. Rice, J. Phys. Chem. 93, 6947 (1989); S. H. Tersigni, P. Gaspard, and S. A. Rice, J. Chem. Phys. 93, 1670 (1990).
- ²²B. Eckhardt and D. Wintgen, J. Phys. B 23, 355 (1990).
- ²³Z. Kovács and T. Tél, Phys. Rev. Lett. **64**, 1617 (1990).
- ²⁴C. Jung and P. Richter, J. Phys. A 23, 2847 (1990).
- ²⁵Q. Chen, M. Ding, and E. Ott, Phys. Lett. A 147, 450 (1990).
- ²⁶O. Legrand and D. Sornette, Europhys. Lett. 11, 583 (1990).
- ²⁷P. Gaspard and G. Nicolis, Phys. Rev. Lett. **65**, 1693 (1990).
- ²⁸Ù. Smilansky, in *Chaos and Quantum Physics*, edited by M.-J. Giannoni et al. (Elsevier, New York, 1990).
- ²⁹T. Tél, in *Directions in Chaos*, edited by Bai-lin Hao (World Scientific, Singapore, 1990), Vol. 3, pp. 149-221.
- ³⁰G. Troll, Physica D (to be published).
- ³¹M. Ding, C. Grebogi, E. Ott, and J. A. Yorke, Phys. Lett. 153A, 21 (1991); Phys. Rev. A 42, 7025 (1990); Y-T. Lau, J. M. Finn, and E. Ott, Phys. Rev. Lett. 66, 978 (1991).
- ³²L. Wiesenfeld, Phys. Lett. A **144**, 467 (1990); Comments At. Mol. Phys. 25, 335 (1991).
- 33C. Jung (unpublished); Y-C. Lai and C. Grebogi (unpub-
- ³⁴P.Eckelt and E. Zienicke, J. Phys. A **24**, 153 (1991); Z. Lu, J. F. Heagy, M. Vallieres, and J. M. Yuan, Phys. Rev. A 43, 1118 (1991).
- ³⁵R. Blümel, in *Directions in Chaos*, edited by H. Bai-lin, D. H. Feng, and J. M. Yuan (World Scientific, Singapore, in press), Vol. 4.
- ³⁶P. Gaspard, K. Nakamura, and S. A. Rice, Comments At. Mol. Phys. (to be published); S. A. Rice, P. Gaspard, and K. Nakamura (unpublished); A. Bringer (unpublished).
- ³⁷C. Jung and T. Tél, J. Phys. A (to be published).
- ³⁸M. L. Roukes and O. L. Alerhand, Phys. Rev. Lett. 65, 1651 (1990); R. A. Jalabert et al., ibid. 65, 2442 (1990); E. Doron, U. Smilansky, and A. Frenkel, ibid. 65, 3072 (1990); (unpublished).
- ³⁹D. Ruelle, Thermodynamic Formalism (Addison-Wesley, Reading, MA, 1978); D. H. Mayer, Lect. Notes Phys. 123,
- ⁴⁰M. J. Feigenbaum, M. H. Jensen, and I. Procaccia, Phys.

- Rev. Lett. 56, 1503 (1986).
- ⁴¹T. Bohr and D. Rand, Physica D 25, 387 (1987).
- ⁴²M. Kohmoto, Phys. Rev. A 37, 1345 (1987); T. Bohr and T. Tél, in *Directions in Chaos*, edited by U. Bai-lin Hao (World Scientific, Singapore, 1988), Vol. II; A. Arneodo and M. Holschneider, J. Stat. Phys. 50, 995 (1988); M. J. Feigenbaum, *ibid.* 52, 527 (1988); T. Tél, Z. Naturforsch. 43a, 1154 (1988); R. Badii, Riv. Nuovo Cimento 12, N3, 1 (1989); A. B. Chhabra, R. V. Jensen, and K. R. Sreenivasan, Phys. Rev. A 40, 4593, 1989; R. Artuso, E. Aurell, and P. Cvitanović, Nonlinearity 3, 325 (1990); 3, 361 (1990); C. Beck, Physica D (to be published).
- ⁴³H. Fujisaka, Prog. Theor. Phys. 70, 1264 (1983); 71, 513 (1984); P. Grassberger, in *Chaos*, edited by A. Holden (Manchester University Press, Manchester, 1986).
- ⁴⁴P. Grassberger and I. Procaccia, Phys. Rev. A 28, 2591 (1983).
- ⁴⁵J. P. Eckmann and D. Ruelle, Rev. Mod. Phys. **67**, 617 (1985).
- ⁴⁶J. P. Eckmann and I. Procaccia, Phys. Rev. A **34**, 659 (1986).
- Ar P. Grassberger and I. Procaccia, Physica D 13, 34 (1984).
 R. S. Ellis, Entropy, Large Deviations, and Statistical Me-
- chanics (Springer, Berlin, 1985); Y. Oono, Prog. Theor. Phys. Suppl. 99, 165 (1990).

- ⁴⁹T. C. Halsey et al., Phys. Rev. A 33, 1141 (1986).
- ⁵⁰P. Grassberger, R. Badii, and A. Politi, J. Stat. Phys. **51**, 135 (1988).
- ⁵¹ A. Csordás and P. Szépfalusy, Phys. Rev. A **39**, 4767 (1989).
- 52P. Cvitanović, in Group Theoretical Methods in Physics, edited by R. Gilmore (World Scientific, Singapore, 1987);
 P. Szépfalusy and T. Tél, Phys. Rev. A 35, 477 (1987);
 D. Katzen and I. Procaccia, Phys. Rev. Lett. 58, 169 (1987);
 R. Badii and A. Politi, Phys. Rev. A 35, 1288 (1987);
 Phys. Scr. 35, 243 (1987); 36, 3525 (1987);
 M.H.Jensen and T.Bohr, ibid. 36, 4904 (1987);
 H. Hata et al., Prog. Theor. Phys. 80, 809 (1988);
 T. Yoshida et al., ibid. 82, 879 (1989).
- ⁵³E. Ott, C. Grebogi, and J. A. Yorke, Phys. Lett. **135A**, 343 (1988); M. Feigenbaum, I. Procaccia, and T. Tél, Phys. Rev. A **39**, 5359 (1989); A. Csordás and P. Szépfalusy, *ibid*. **40**, 2221 (1989); X.-J.Wang, *ibid*. **39**, 3214 (1989); **40**, 6647 (1989); J. Bene, P. Szépfalusy, and A. Fülöp, *ibid*. **40**, 6719 (1989).
- ⁵⁴C.Beck, Physica D 41, 67 (1990).
- ⁵⁵P.Szépfalusy, T. Tél, and G. Vattay, Phys. Rev. A 43, 681 (1991).
- ⁵⁶E. Ott, W. D. Withers, and J. Yorke, J. Stat. Phys. **36**, 687 (1984).