

Dependence of phase transitions on small changes

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In this contribution, the generalized thermodynamic formalism is applied to a nonhyperbolic dynamical system in two comparable situations. The change from one situation to the other is small in the sense that the grammar and the singularities of the system are preserved. For the discussion of the effects generated by this change, the generalized entropy functions are calculated and the sets of the specific scaling functions which reflect the phase transition of the system are investigated. It is found that even under mild variations, this set is not invariant.

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I. INTRODUCTION

After the discovery that fractal geometry is relevant for the characterization of chaotic systems, much effort was spent on the evaluation of fractal dimensions and related indicators such as Lyapunov exponents and entropies. Many theoretical investigations concentrated on the connection between these quantities. Soon it was realized that, for a refined description, fluctuations should be taken into account [1–8]. Investigations of the fluctuation spectra led then to the discovery of “phase transitions”. This phenomenon, which must be understood in the sense of the thermodynamic formalism [9], is connected with a non-Gaussian fluctuation behavior of the system (in the sense of large deviation theory), such that a nonanalytic dependence of the fluctuation spectrum as a function of the deviation is obtained. The effect has been observed in great variety in model systems and in experiments (chemical systems, laser experiments [10], and semiconductors [11]) and is thought to be of generic nature. Nonhyperbolic maps, such as the intermittent map or the fully developed logistic map, are characteristic models for this effect. Hyperbolic maps are not capable of producing this phenomenon if only finite range correlations are permitted [9].

A striking feature which comes along with a phase transition of a system is the fact that often not all of the specific spectra (among which we have the spectra of Lyapunov exponents, entropies, and fractal dimensions, to name the most prominent ones [10,12] witness the phase transition. It is therefore of interest to discuss in more detail the mechanism which leads to this phenomenon.

For this problem, the usefulness of an approach via the generalized or bi-variate thermodynamical formalism [12–20] is evident. In this approach, the description of a system is realized with the help of symbol sequences. A specific symbol appears with a certain probability. As a consequence of its appearance, the support in the phase space which is compatible with the past of the symbol sequence is scaled down by a length scale associated with that symbol (as a typical example we mention the Cantor

set with measure). The scaling properties due to the length scales are thus interpreted as scaling properties of the support, on which the measure (probability) is distributed according to rules which can be specified by a measure map. As in the “ordinary” thermodynamic formalism, the different contributions obtained from strings of n symbols are interpreted as an ensemble. From its partition function we derive the free energy (or “pressure”) and the associated entropy function (called the generalized entropy function). From the latter, the well-known entropylike scaling functions of generalized Lyapunov exponents and fractal dimensions are obtained by restriction.

In this contribution we investigate the stability of the set of specific entropylike scaling functions which witness the phase transition of a system. As the specific model for our investigation we consider a system for which the scaling of the support is generated by a hyperbolic map of three monotonous, fully extended branches which can be labeled by the symbols A , B , and C . Symbol B is observed with fixed probability. The probability for the other two symbols A and C is chosen according to the elements of the binary partition generated by the fully developed parabola

$$g: x \rightarrow 4(1-x)x, \quad (1)$$

scaled by a factor to normalize the probabilities [19,20]. In this way, the system is provided with an unrestricted ternary grammar (binary grammars can lead to some degeneracies of the generalized entropy function [20]). The nonhyperbolicity of the fully developed parabola leads to a phase transition of the system. We show that, for this system, the set of the specific entropy functions which witness the phase transition is not invariant even under mild changes of the length and the probability scales.

For the generic case of restricted symbolic representations it was shown [17] that calculations based on the “canonical” partition function (2) lead to severe numerical problems. In the case of finite grammatical rules, these can be overcome by the use of appropriate zeta functions. For f and g tent maps, a hyperbolic two-scale

Cantor set with measure is obtained. Note that also for maps from the interval the present approach can be applied. While the behavior of the support is given by the map itself, the measure map has to be determined from additional considerations.

II. THERMODYNAMICS

The generalized entropy function, from which we wish to discuss the phase transitionlike effects, is built on the partition function [1]:

$$Z_G(q, \beta, n) = \sum_{j \in (1, \dots, M)^n} l_j^\beta p_j^q \tag{2}$$

Here, M denotes the number of symbols used for the symbolic description, l_j the size of the j th region R_j of the partition, and p_j the probability of falling into this region. If local scaling of l and p in n is assumed (where n denotes the "level" of the partition), the length scale l and the probability p give rise to exponents ϵ and α through

$$l_j = e^{-n\epsilon_j} \tag{3}$$

$$p_j = l_j^{\alpha_j} \tag{4}$$

With the partition function, the generalized free energy F_G can be associated [10,12]:

$$F_G(q, \beta) = \lim_{n \rightarrow \infty} \frac{1}{n} \ln \sum_{j \in (1, \dots, M)^n} e^{-n\epsilon_j(\alpha_j q + \beta)} \tag{5}$$

where \ln denotes the natural logarithm. Note that for $G(\beta, q) = -(1/\beta)F_G(q, \beta)$, the term "Gibbs potential" is used. In the presence of phase transitions, it is useful to consider the following iterative equation instead:

$$\lambda(q, \beta) Q_{n+1}(x, y) = \sum_{\epsilon = A, B, C} \frac{Q_n(f_\epsilon^{-1}(x), g_\epsilon^{-1}(y))}{|f'_\epsilon(f_\epsilon^{-1}(x))|^\beta |g'_\epsilon(g_\epsilon^{-1}(y))|^q} \tag{6}$$

(the "generalized" or "bivariate Frobenius-Perron equation" [15,19-23]). Here, ϵ labels the choice being made between the inverses of the maps f and g . While iterating, the sum is performed for f and g over the same symbolic substrings. Starting from any smooth density $Q_0(x, y)$ in $(0, 1) \times (0, 1)$, a unique eigenvalue $\lambda(q, \beta)$ ensures convergence towards a finite $Q(x, y)$. The dependence on x, y disappears for large n , for x, y in the invariant set. The free energy arises then as the largest eigenvalue of the associated Frobenius-Perron operator

$$L(Q(x, y)) = \lambda(q, \beta) Q(x, y) \tag{7}$$

In order to derive the generalized free energy or Gibbs potential, the relation

$$\lambda(q, \beta) = \exp[F_G(q, \beta)] \tag{8}$$

can be used. The properties of the eigenvalues and associated eigenfunctions provide the key tool in understanding phase transitions.

As mentioned before, we are interested in the generalized entropy function which will show characteristic,

generic properties for our model. The generalized entropy $S_G(\alpha, \epsilon)$ is related to the generalized free energy F_G via [10,12,15]

$$S_G(\alpha, \epsilon) = F_G(q, \beta) + (\alpha q + \beta)\epsilon \tag{9}$$

In this formula, those values of α and ϵ which lead to the maximum of the Z_G have been chosen (as a function of given q and β). The free energy F_G or the generalized entropy S_G describe in this way the scaling behavior of the dynamical system equivalently. By restriction, several specific entropy functions are obtained. For $q=0$, we obtain the thermodynamic formalism, which is based on length scales only [3-8]. In this case the associated free energy and entropy are denoted by $F_G(\beta)$ and $S_G(\epsilon)$, respectively. The generalized Lyapunov exponents can be calculated from $F_G(q, \beta)|_{q=1}$; we denote the associated scaling function by $\phi(\lambda)$. Furthermore, the fractal dimensions [1,24,25] are given by the zeros $\beta_0(q)$ of $F_G(q, \beta)$ for given q . They give rise to the entropylike function $f(\alpha)$ [1].

In the thermodynamic formalism introduced by Ruelle, Eq. (5) can be interpreted as the isobar-isotherm partition function of an elastic Ising chain with long-range, multispin interaction. Accordingly, points of nonanalytical behavior of the thermodynamic function are interpreted as phase transitions. The separation between two phases is characterized as the set of points where F_G is not real analytic as a function of the parameters q and β .

For the numerical evaluation, the application of Eq. (6) is straightforward [19,26] [for nonhyperbolic systems, Eq. (6) still holds, but its derivation needs more care]. The nonhyperbolicity of the support, or of the measure (as in our example), respectively, usually comes from the ex-

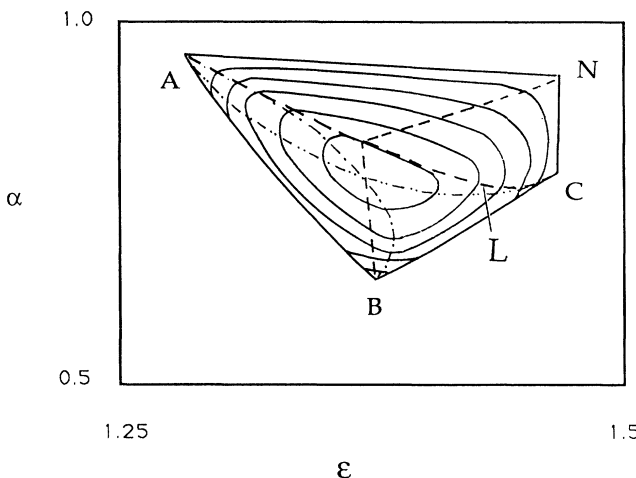


FIG. 1. Support of $S_G(\alpha, \epsilon)$ for the first set of parameter values. The lines are indicated along which the functions $S_G(\epsilon), g(\Lambda)$ (the Legendre transform of the Renyi entropies) and $f(\alpha)$ are evaluated (dash-double-dotted, dashed, and dash-dotted lines, respectively). The corner point generated by the nonhyperbolicity is indicated by N . Contour lines are shown. The critical line is denoted by L .

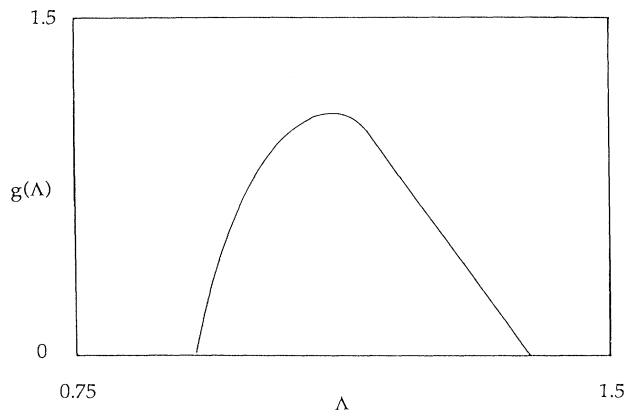


FIG. 2. Graph of $g(\lambda)$ (the Legendre transform of the Renyi entropies): Note the straight-line tail which is characteristic for phase transitions.

istence of a local maximum of these maps or from singularities in their invariant sets. By iteration of such a system, in addition to $\lambda_s(q, \beta)$, obtained from smooth, singularity free eigenfunctions $Q(x, y)$, additional eigenvalues $\lambda_n(q, \beta)$ are obtained when starting from singular initial functions [22,23]. The system chooses its free energy from the requirement $F_G = \max(F_{Gn}, F_{Gs})$, where both contributions to the generalized free energy are smooth functions of their arguments. As the two individual functions intersect, a first-order phase transition is created. Due to the smoothness of the arguments, points of such a nonanalytical behavior must be connected. In this way they form the "critical line" [19,20].

III. STABILITY OF PHASE TRANSITIONS

Earlier [16–18] the form of the generalized entropy function for hyperbolic models, its relation to the more specific entropy functions $S_G(\varepsilon)$, $\Phi(\lambda)$, and $f(\alpha)$, and the connection with experimentally obtained scaling functions were elucidated [10,11,15]. Hyperbolic systems lead to strictly convex specific entropy functions, whereas in

the more relevant nonhyperbolic case linear segments are obtained [27–33]. As for the free energy, in the surface of the generalized entropy function a critical line is obtained [20].

The important question we would like to address is the following: What kind of parameter variations are needed to change the set of the specific entropylike scaling functions which witness the phase transition of the system? Clearly an additional nonhyperbolicity will be sufficient, if appropriately chosen. However, we would like to know whether a change in the length and probability scales only can be sufficient too (this could be done with preservation of the already existing singularities and grammar). The generalized entropy function depends in a nontrivial way on the length and on the probability scales. Therefore, the occurrence of phase transitions in the specific entropy spectra is not determined by the critical line alone, but also depends from the range which is accessible for the scaling variables α and ε . This can be illustrated by two examples provided by our model. For the first model, as parameters the length scales $l_{A,B,C}^{-1} = 4.0, 3.5, 4.5$ and the probabilities $p_{A,B,C} = 0.3, 0.4, 0.3$ are chosen. Note that $p_A + p_C = 0.6$ is the total probability for obtaining a measure designed by the fully developed parabola. The "internal" conditional probabilities are assigned according to the partition of the interval as generated from the preimages of the critical point of the parabola. The generalized entropy function, which reflects the scaling properties of the system, then has the following form (cf. Fig. 1): Emanating from the nonhyperbolicity labeled by N , a sheet touches the hyperbolic part along the critical line L . Those of the specific entropy functions $S_G(\varepsilon)$, $\phi(\lambda)$, and $f(\alpha)$ which cross the critical line inherit the phase-transition effect. For the present situation, this is the case only for the Legendre transform of the Renyi entropies (Fig. 2). Note the linear part on the right-hand side of the function. The Lyapunov scaling function, the scaling function belonging to the "usual free energy" based on length scales, and $f(\alpha)$ show no phase transitions. Their graphs are strictly convex. A refined explanation can be given, taking into account the range of the underlying variables: (1) Since point A is higher than the nonhyperbolicity N ,

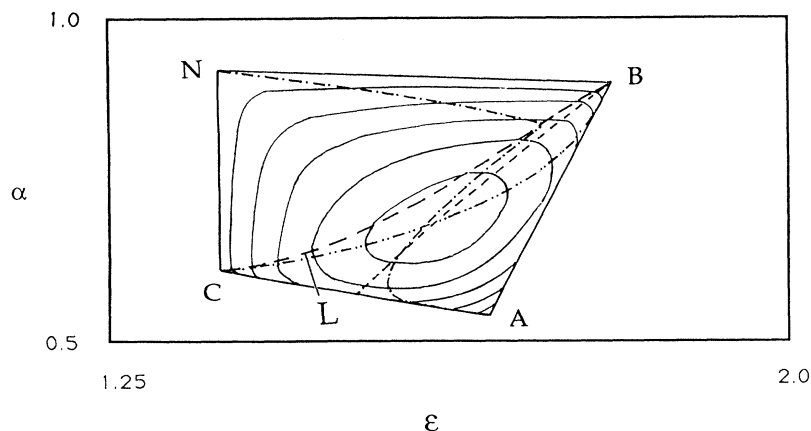


FIG. 3. Support of $S_G(\alpha, \varepsilon)$ for the second set of parameter values. The lines are indicated along which the functions $S_G(\varepsilon)$, $g(\lambda)$ (the Legendre transform of the Renyi entropies), and $f(\alpha)$ are evaluated (dash-double-dotted, dashed, and dash-dotted lines, respectively). Contour lines are shown; the critical line is denoted by L , the corner point generated by the nonhyperbolicity by N .

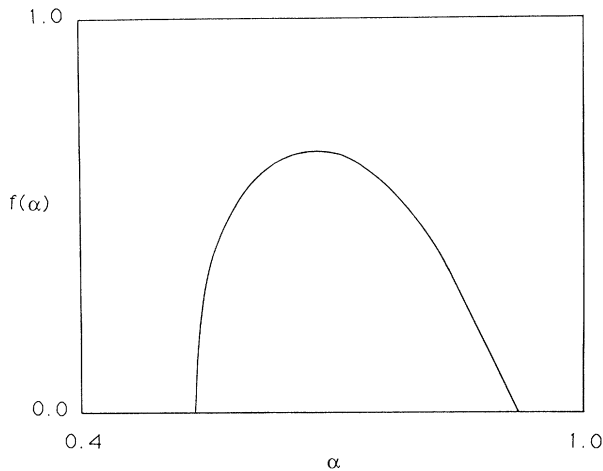


FIG. 4. Graph of $f(\alpha)$ for the second parameter set. The function is no more strictly convex, but indicates the phase transition of the system (straight-line behavior on the right-hand side).

$f(\alpha)$ shows no phase transition [because α is the relevant variable for $f(\alpha)$]. (2) $S_G(\varepsilon)$ has no phase transition. This inherent property of the model is reflected by the fact that N is on a vertical line with C . (3) $g(\Lambda)$ has a phase transition since $\varepsilon\alpha_N > \varepsilon\alpha_A, \varepsilon\alpha_B$ [the relevant scale for $g(\Lambda)$ is $\varepsilon\alpha$].

In order to generate a phase transition in $f(\alpha)$, we would like to have N at a higher α value than point A . This can be achieved by different “crossover” transitions which preserve the number of the elements of the partition and the type of the singularities, but change the order of the sizes of the scales. For example, the choice of the second parameter set ($l_{A,B,C}^{-1} = 5.5, 6.0, 4.5$ and probability scales $p_{A,B,C} = 0.4, 0.2, 0.4$) leads to the desired situation. Figure 3 shows the generalized entropy function for the changed parameter values. As can be seen, $f(\alpha)$ now crosses the critical line and obtains a phase transition (cf. Fig. 4); the phase transition in the Renyi entropies is no longer present (Fig. 5). This is due to the relation $\varepsilon\alpha_N < \varepsilon\alpha_B$, which holds for the new parameter values. For completeness we mention that the appearance of additional hyperbolic scaling elements can lead to similar effects.

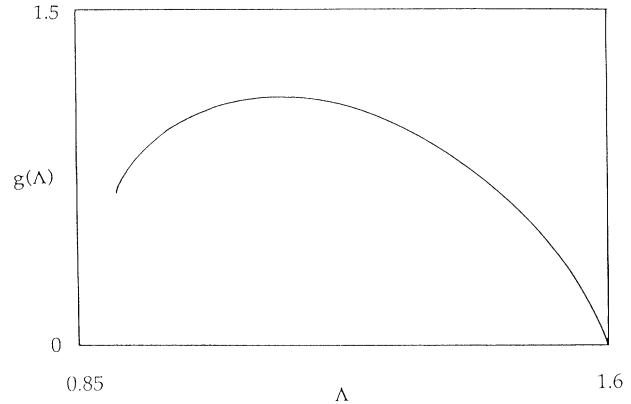


FIG. 5. Graph of $g(\Lambda)$ for the second parameter set, showing the absence of phase transitions in this spectrum.

IV. CONCLUSIONS

In this contribution, it has been shown that a small variation of external parameters may lead to a change of the set of entropy functions which witness the phase transition of the system. An improved explanation of the occurrence of phase transitions has been given from the point of view of the generalized entropy function. The explanation goes beyond the existence of a critical line. It shows that for a complete characterization of the phase transition properties of a system the generalized (in the sense of bivariate) thermodynamic formalism can be used with profit. The insight gained leads to a better understanding of the changes in a system under variation of external parameters. For experimental systems, first progress towards a partition of the phase space by using periodic orbits has already been achieved [34]; the length scales and the probabilities obtained from that approach can then be used as the input for the generalized thermodynamic formalism. In this sense, the results and tools outlined in this contribution are also of interest for experimental systems. They may, e.g., help to direct experimental systems towards working conditions for which phase transitions appear in specific spectra.

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