Bivariate thermodynamic formalism and anomalous diffusion

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(Received 7 July 1993; revised manuscript received 17 March 1994)

Anomalous diffusion, generated by intermittent systems, is investigated from the point of view of a bivariate thermodynamic formalism. We show that the phenomenon is related to the occurrence of phase transitions. Detailed numerical calculations are performed.

PACS number(s): 05.45.+b, 05.70.Ce, 05.70.Fh

I. INTRODUCTION

The scaling behavior [1–12] of dynamical systems is characterized by several invariants which are to some extent mutually independent. In addition, fluctuation properties provide a refined description of the scaling behavior. Dynamical systems often have the property of being nonhyperbolic. This then leads to the occurrence of the well-known phenomenon of phase transitions [7,12] in their flucutation spectra. In the case of mappings on a grid of unit cells, nonhyperbolicity may also give rise to the phenomenon of anomalous diffusion. It is one aim of this paper to elucidate the relation between the two phenomena described above. For diffusion [13–22], the characteristic quantity to be investigated is the mean-squared displacement r as a function of the time t (or of the number of iterations n in the discrete case). In most cases it is found to scale as $\langle r^2(t)\rangle \sim t^{\alpha}$. Characteristic of Brownian motion is an exponent $\alpha=1$, in which case the diffusional behavior is called regular or linear. Then the diffusion can be described by $\langle r^2(t)\rangle \cong Dt$, where D is the diffusion coefficient. However, $\alpha\neq 1$ is frequently found in experiments. The sublinear diffusion $\alpha<1$ has been found, e.g., for motion on fractal structures [15]. Superlinear diffusion $\alpha>1$ has been observed primarily in Hamiltonian systems. It has been shown that Lévy walks [19] are an appropriate approach for the description of this effect.

Instead of following the common probabilistic approach, we will exploit the thermodynamic formulation of the problem. This description of a dynamical system uses as a starting point a suitable generating partition of the phase space. Then the partition function [1] is used to calculate the thermodynamic averages. From the partition function, the generalized free energy and the associated entropy can be evaluated. From either of these functions, all relevant information on the invariants of the system, such as the spectrum of fractal dimensions $f(\alpha)$ [1], and of Lyapunov exponents $\phi(\lambda)$ [or $g(\gamma)$], is available [5,11,12]. As usual, points of nonanalytical behavior of these functions are interpreted as phase transitions. Generically, a first-order phase transition appears if there is an element of the partition which shows a power-law dependence upon iteration. An analogous situation holds for anomalous diffusion. Once the diffusion properties can be included in the partition function, nonanalytical dependence of the thermodynamic function on the associated weighting exponent can be related to the occurrence of anomalous diffusion. However, it will be pointed out that higher-order phase transitions play a distinct role in connection with diffusional behavior.

II. GENERATING ANOMALOUS DIFFUSION FROM ONE-DIMENSIONAL MAPS

A typical map which eventually leads to anomalous diffusion can be obtained by suitably piecing together intermittent generating branches [16]

$$f(x)=(1+\varepsilon)x+\bar{a}x^{\bar{z}},\quad 0<x<\tfrac{1}{2}, \tag{1}$$

where the parameter $\bar{a}$ is chosen to be $\bar{a}=2^{\bar{z}}(1-\varepsilon/2)$. For $\varepsilon=0$, a marginally stable fixed point arises. This fixed point is responsible for the nonhyperbolicity of the system and for the intermittent behavior. If the branches are put together as shown in Fig. 1(a), a map is generated

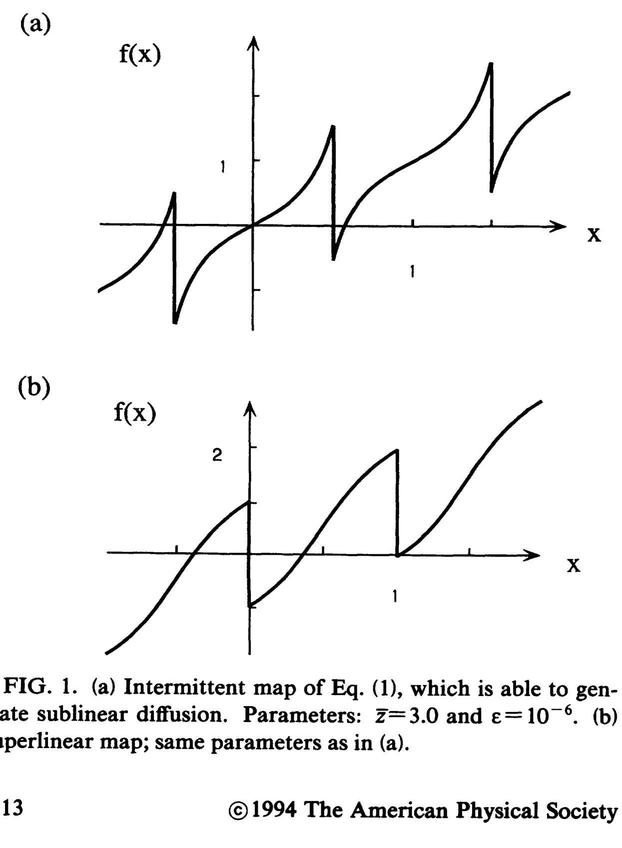

FIG. 1. (a) Intermittent map of Eq. (1), which is able to generate sublinear diffusion. Parameters: $\bar{z}=3.0$ and $\varepsilon=10^{-6}$. (b) Superlinear map; same parameters as in (a).

which will spend most of the time in the vicinity of its fixed points on the diagonal. In this case, there will not be much transport. For the map of Fig. 1(b) the situation is entirely different: Here most orbits will lead from one peak of the map to another, thus causing a great deal of transport. Clearly, the extent to which the orbits are concentrated and remain in the vicinity of the nonhyperbolic points is of great importance for the amount of diffusion. However, the information about the concentration of orbits, which may be investigated with the help of the reduced maps, is most sufficient to aid in understanding anomalous diffusion. It cannot explain the fact that anomalous diffusion does not appear simultaneously for the two variants of maps when the intermittency exponent $\bar{z}$ is increased. It is one aim of this contribution to elucidate by which mechanism the diffusional anomality is triggered. In our work, the maps displayed in Figs. 1 are used as motivating examples for a generic behavior of intermittent maps; they are not the primary focus of our study. The general diffusional properties of such systems (they may easily be corroborated by numerical simulations) can be summarized as follows: Depending on whether the nonhyperbolic points are responsible for transport or for the absence of transport, and depending on the magnitude of the intermittency exponent $\bar{z}$, the diffusion may be anomalous of superlinear or sublinear types.

For the investigation of a system with the help of the thermodynamic formalism, a suitable symbolic representation has to be introduced. This is done by restricting the map via shift and modulo-operation to a unit box. In this way, the so-called reduced map of a unit interval to itself is obtained, as shown in Fig. 2 for the sublinear variant [note that the end points of a unit box have been identified with (0,1)]. For the investigation of generic properties, the behavior around the fixed point of the reduced maps is relevant, and any reduced map with the right fixed point behavior can be used. This means that the reduced map of Fig. 2 can serve for the investigation of both cases, if sufficient care is applied (to derive only generic properties). For the reduced map, a complete ternary symbolic description exists. Using the natural symbols a to denote the left branch, b for the middle branch, and c for the right branch, a typical orbit may be described by symbol sequences such as $a^k b^n c^i$, where k, b, and i are non-negative integers. However, for the problem of diffusion another symbolic description is more advantageous. For sublinear behavior we have to count the number of times the element a (c) which indicates a transport event is visited, as a function of the iteration number n. In the superlinear case we want to count how many iterations are needed to reach symbol a (c). By using a biinfinity of symbols to label the elements of the partition as shown in Fig. 2, this procedure can be simplified. Any sequence of iterations with 1 as the last symbol index can be then be decomposed into a sequence of blocks $\{A_i, A_{i-1}, \ldots, A_1\}$ and $\{C_i, C_{i-1}, \ldots, C_1\}$. In this way, each block is linked to exactly one transport event (in the positive or, respectively, negative direction of the x axis) for the sublinear map. To achieve these events, exactly i iterations are needed. For the superlinear case, each block is related exactly with $i-1$ transport events into the same direction. Note that each A_i is mapped onto A_{i-1} $(i \geq 2)$, and that the twofoldedness of the symbols is a consequence of the two directions in which the diffusion may proceed.

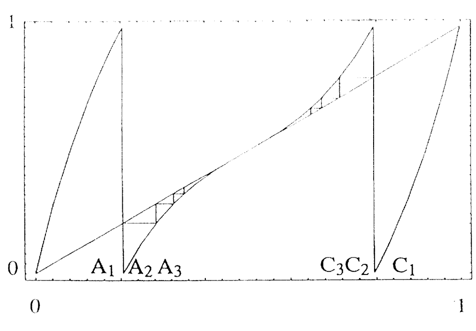

FIG. 2. Reduced map of Eq. (1). In a piecewise linearized approach, the width w_k of the part of the x axis which leads to symbol A_k (or C_k), is equal to the dynamical weight of a block of symbols $\{A_k, A_{k-1}, \ldots, A_1\}$ (or $\{C_k, C_{k-1}, \ldots, C_1\}$) for $\varepsilon \to 0$. Same parameters as in Fig. 1.

III. FROBENIUS-PERRON APPROACH

In what follows we apply a bivariate Frobenius-Perron approach [8–12,23,24] for the characterization of diffusion [25–27]. As a starting point we use the fundamental relation between the partition function based on lengths scales and the associated free energy $F(\beta)$:

$$\sum_j e^{-\lambda_j(n)\beta} \sim e^{nF(\beta)} , \tag{2}$$

where $\lambda_j(n)$ is the stability exponent of a symbolic chain of length n which we label by j. The sum extends over all allowed symbolic sequences of length n. Note that $\lambda_j(n)$ associates with each chain j of length n a typical length scale l_j through the relation $l_j(n) = e^{-\lambda_j(n)}$. Consider now the grand-canonical partition sum

$$\sum_j z^n e^{-\lambda_j(n)\beta} \sim 1 . \tag{3}$$

In view of Eq. (2), $z(\beta) = e^{-F(\beta)}$ then follows. Formally, we may associate a generalized Frobenius-Perron operator with our problem:

$$L_\beta \Psi(x) = \sum_{f(y)=x} \frac{\Psi(y)}{|f'(y)|^\beta} . \tag{4}$$

This operator acts in the space of functions of bounded variation. For the largest eigenvalue μ_{L_β} of L_β, the relation $\mu_{L_\beta} = e^{F_\beta}$ holds. In view of the chosen alphabet of Sec. II, we consider the grand-canonical transfer operator

$$G_{\beta,z} \tilde{\Psi}(x) = \sum_{g(y)=x} \frac{z^n \tilde{\Psi}(y)}{|g'(y)|^\beta} , \tag{5}$$

where $g(x) = f^n(x)$. The condition that the largest eigenvalue $\mu_{\beta,z}$ of $G_{\beta,z}$ fulfills $\mu_{G_{\beta,z}} = 1$ can then be used to select for each β an appropriate $z(\beta)$, which is connected with the largest eigenvalue of L_β by $z(\beta)=1/\mu_{L_\beta}$. Moreover, a unique relation between the associated eigenfunctions of the two operators exists. For $\beta<0.5$ and $0<z\le 1$, the grand-canonical transfer operator $G_{\beta,z}$ is of trace class [28]. Due to its monotonicity properties in β and z, the operator is one-bounded and has therefore a unique first eigenvector. The associated eigenvalue is simple and well-separated from the rest of the spectrum. Using the properties in β and z, the equation $\mu_{G_{\beta,z}}=1$ is always solvable, which yields for given β the function $z(\beta)$. For $\beta<1$ and $\beta>1$, this function is analytic. At $\beta=1$, a nonanalyticity of $F(\beta)$ appears, which is interpreted as a phase transition, the order of the phase transition depending on the intermittency exponent $\bar{z}$.

In order to include the diffusion in the present setting, we use the bivariate partition

$$\sum_j e^{-\lambda_j(n)\beta+\mu(I(f_j^n))q} \sim e^{nF_d(q,\beta)} , \tag{6}$$

where function $\mu(I(f_j^n))$ counts the number of visits of the elements which are responsible for the transport to neighboring cells. To understand this approach, note that the ability of inducing k consecutive jumps can be attached to the partition elements in a measurelike fashion (in the same way as the probabilities are attached to the partition elements in the usual multifractal approach). Again, the grand-canonical partition

$$\sum_j z^n e^{-\lambda_j(n)\beta+\mu(I(f_j^n))q} \sim 1 \tag{7}$$

selects a β- and q-dependent z which is connected with the diffusion-related free energy by $z(\beta,q)=e^{-F_d(q,\beta)}$. The previous case $z(\beta)$ arises for $q=0$. The corresponding grand-canonical Frobenius-Perron operator then obtains the form

$$G_{q,\beta,z}\tilde{\Psi}(x)=\sum_{g(y)=x} \frac{z^n\tilde{\Psi}(y)}{|g'(y)|^\beta e^{-\mu(I(g(y)))q}} . \tag{8}$$

As there exist different solutions of Eq. (8), upon variation of β and q, crossing of the two largest eigenvalues z can be observed. This yields a nonanalyticity which is interpreted as a phase transition of the associated thermodynamics. As in other cases [10,12] of phase-transition behavior related to a bivariate thermodynamic formalism, a critical line emerges in the q-β plane. For the sublinear and superlinear cases, the critical lines have distinct properties which are investigated in the following sections.

IV. GENERIC ASPECTS

In this section we focus on a model system and discuss what will be called generic aspects of intermittent systems (nongeneric properties will be discussed in Sec. VI). For our purpose, the behavior of the system is determined by the length scales $e^{-\lambda_j(n)}$ (this is standard in the thermodynamic formalism). It is easy to see that for intermittent maps the widths of the partition elements A_k scale asymptotically as $w_k \sim k^{-\bar{z}/(\bar{z}-1)}$ (cf. Fig. 2). For the numerical calculation of the bivariate free energy, care must be taken in order to obtain the correct sum of the intervals and their asymptotically correct relative weights. Therefore, a partition of the generic form $w_k=a[k^{-[1/(\bar{z}-1)]}-(k+1)^{-[1/(\bar{z}-1)]}]$ yields the required properties. If above a partition element the (curved) map is replaced by a straight line, these properties remain, and an exactly solvable model is obtained (analogous to the Gaspard-Wang model, cf. Ref. [29]). Then the role of w_k is twofold: On the one hand we have $w_n=e^{-\lambda_j(n)}$, i.e., w_k determines the dynamical weight needed in the thermodynamic formalism [cf. Eq. (8)]. On the other hand, in the associated Markov-chain approach of the system, w_k can be interpreted as the transition probability to land on element A_k after being reinjected by A_1. In the reduced map there is no escape, therefore a is adjusted to the value $a=0.5$. From the expansion of the system into periodic orbits, it can be seen that the non-fixed-point behavior of the system is determined by the partition function of the laminar orbits in the following form:

$$\begin{aligned}1&=\sum_{k=1}^{\infty} z^k(w(A_k,\ldots,A_1))^\beta e^{\mu(+,k)q}\\&\quad+\sum_{k=1}^{\infty} z^k(w(C_k,\ldots,C_1))^\beta e^{\mu(-,k)q}\\&=\sum_{k=1}^{\infty} z^k w_k^\beta e^{\mu(+,k)q}+\sum_{k=1}^{\infty} z^k w_k^\beta e^{\mu(-,k)q} .\end{aligned} \tag{9}$$

In this formula, $\mu(-,k)$ [$\mu(+,k)$] are the diffusion-related weights contributed to the ensemble by a block of length k for the diffusion in the negative (positive) direction of the axis. For the sublinear behavior we have $\mu(-,k)=-1$ for the motion to the left and $\mu(+,k)=+1$ for the motion to the right, according to the discussion in Sec. II. Note that in Ref. [30] a ζ-function approach has been used to derive an analogous relation. Based on the same partition, for the superlinear diffusion we consider the weights $\mu(-,k)=-(k-1)$ and $\mu(+,k)=+(k-1)$, respectively. [If the present approach is compared with the approach of Ref. [30], we can see that the same generic behavior emerges and that minimal differences are obtained for nongeneric properties (e.g., when calculating the diffusion coefficient [31]).] The solutions of Eq. (9) are to be completed by the solutions generated from the fixed points of the map. Of special interest is the marginal fixed point, which leads to no motion and to ballistic motion, respectively. In principle, this behavior is included in the laminar free energy in the limit $k\to\infty$. For numerical calculations, however, it must be taken into account explicitly. From Eqs. (7)–(9), the diffusion-related free energy can be calculated as a function of the parameters q and β. The resulting free energy is then exposed to competition with the free energies obtained from the fixed points of the map. For both cases of anomalous diffusion, the hyperbolic fixed points are of no influence, due to the size of their stability exponents [$\ln_{10}(1/w_1)$]. The concurrence between the solution provided by the laminar free energy and the solution provided by the marginal fixed point are the origin of the phase transition in the system.

V. DISCUSSION OF THE BIVARIATE FREE ENERGY

We start the discussion by collecting a few facts which will help us to understand the numerical results obtained by using Eq. (9).

First, let us note that restricted to $q=0$, the diffusion-related free energy coincides with the usual free energy of the system, whose properties are well known [28]. The left-hand-side derivative of $F_d(q,\beta)$ taken with respect to β at the point $(q=0,\beta=1)$ yields the Lyapunov exponent of the system, which for $\bar{z}\geq 2$ is zero, because of the non-normalizable measure, irrespective of whether sublinear or superlinear diffusion is considered. For the free energy, in Ref. [29] the following expansion was chosen for $\beta<1$:

$$F_d(q=0,\beta)\sim\lambda(1-\beta)+O((1-\beta)^{1/(\bar{z}-1)}) \quad \text{for } \tfrac{3}{2}<\bar{z}<2 \tag{10}$$

and

$$F_d(q=0,\beta)\sim(1-\beta)^{\bar{z}-1} \quad \text{for } \bar{z}>2\ . \tag{11}$$

The value for $q=0$ on the $\beta=0$ axis indicates the topological entropy of the system. Second, let us note that the diffusion coefficient may be obtained analytically from the diffusion-related free energy from the relation

$$D=0.5\frac{\partial^2}{\partial q^2}F_d(q,\beta)|_{q=0,\beta=1}\ , \tag{12}$$

which is expected [26,27] to hold in general contexts (remember that $\beta=1$ selects the natural measure). The diffusion coefficient depends on the diffusion-related free energy for $q\neq 0$; it may therefore be qualitatively different for the sublinear and superlinear cases. Of special interest is the behavior of the free energy at the critical lines, which will help us to understand the diffusional properties of the generic model of Sec. IV.

For the sublinear case, the properties of the operator related to $z(\beta)$ for $q=0$ also hold in the case of $|q|>0$. For $q\neq 0$, the solution $z(\beta,q)$ is analytic as long as $z<1$, by the same line of arguments as indicated in Sec. III. Note that these conclusions are valid in a rather general setting [28]. The free energy increases with β, decreases with $|q|$, and is symmetric in q. These facts are easily deducible from Eq. (9). The behavior of the marginal fixed point becomes important for $\beta\geq 1$, where the corresponding eigenvalue is larger than the eigenvalue from the hyperbolic contribution. Therefore, the critical line coincides with the β axis itself, for $\beta\geq 1$. As can also be concluded directly from Eq. (9), upon increasing $|q|$, the order of the phase transition decreases. This is also indicated by the calculated free energy F_d [see Fig. 3(a)]. In order to gain more insight into the nature of the phase transition at $\beta=1$ (this point is important for the diffusion behavior), we consider the spectrum of Lyapunov exponents $\phi(\lambda)$ (see Figs. 4). For $\bar{z}<2$, the Lyapunov exponent is nonzero, so that a first-order phase transition is obtained. A higher-order phase transition is observed in the case $\bar{z}>2$. For sublinear behavior, the dependence on q can be extracted from the sum in Eq. (9). Expanding the dependence on q around q_0 and estimating the sum as an integral, one obtains $\ln_{10}(z)\sim(q-q_0)^{2/\{1+\beta[1/(\bar{z}-1)]-\beta\}}$. For $\beta=1$, $F_d(q,\beta=1)\sim q^{2/[1/(\bar{z}-1)]}$ determines the dependence of

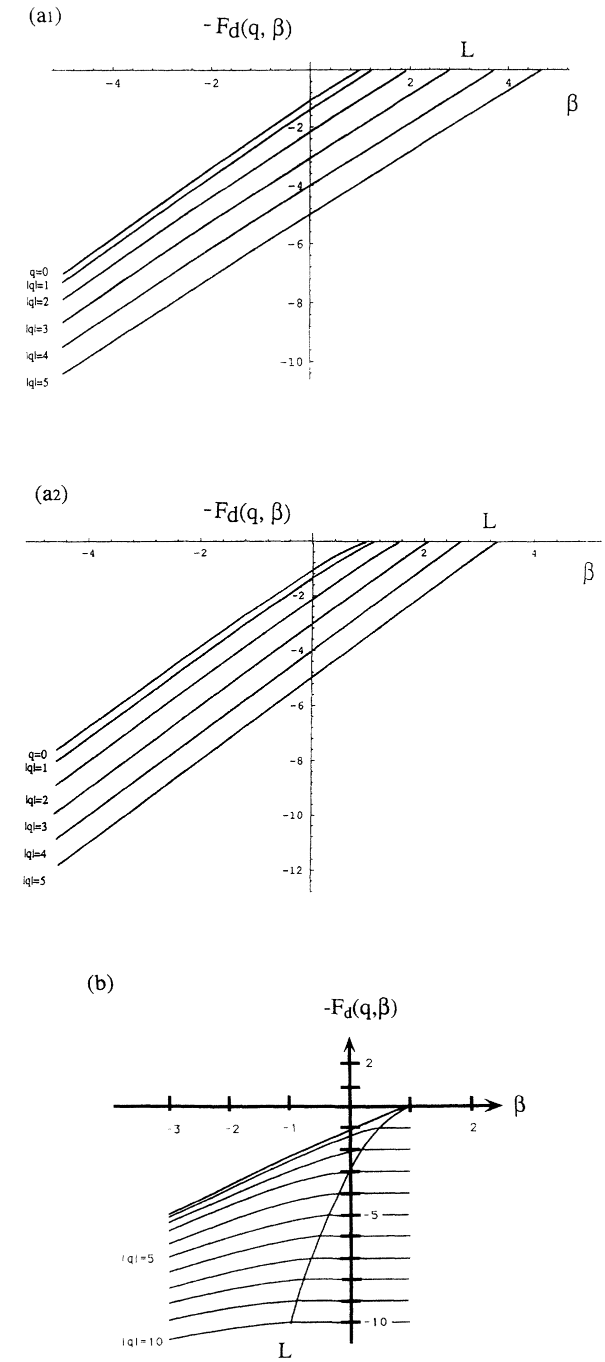

FIG. 3. (a) Diffusion-related free energy for the sublinear case, for (a1) $\bar{z}=1.6$ and (a2) $\bar{z}=2.2$. The critical line coincides with the β axis for $\beta\geq 1$ (see text). (b) Free energy for the superlinear case ($z=2$). The critical line is denoted by L. For the numerical evaluation, maximal values of k between 80 and 120 were chosen.

the order of the phase transition at $\beta=1$ from $\bar{z}$. From the expansion around q_0 the order of the phase transition at the critical line $\beta>1$ can also be obtained. In a second step we investigate the information contained in the second derivative of the diffusion-related free energy of our generic model. The second left-hand-side derivative of the numerically obtained free energy at $\beta=1$ is plotted in Fig. 5 for different intermittency exponents $\bar{z}$. Upon increasing $\bar{z}$, when the second derivative vanishes, we no longer have normal diffusion. This occurs when the diffusion-related free energy changes from first to second order and then to a higher-order phase transition at the point (1,0). To work out this point further, let us focus on the diffusion coefficient of our model which can be calculated using Eqs. (9) and (12). The result $D\sim(\sum_{k=1}^{\infty}kw_k)^{-1}$ is easily obtained. Obviously, the sum is finite for $\bar{z}<2$ (note also that the denominator can be interpreted as the average escape time). Using the properties of w_k from this expression, the behavior

$$\langle r^2(t)\rangle\sim t^{\alpha}\ , \tag{13}$$

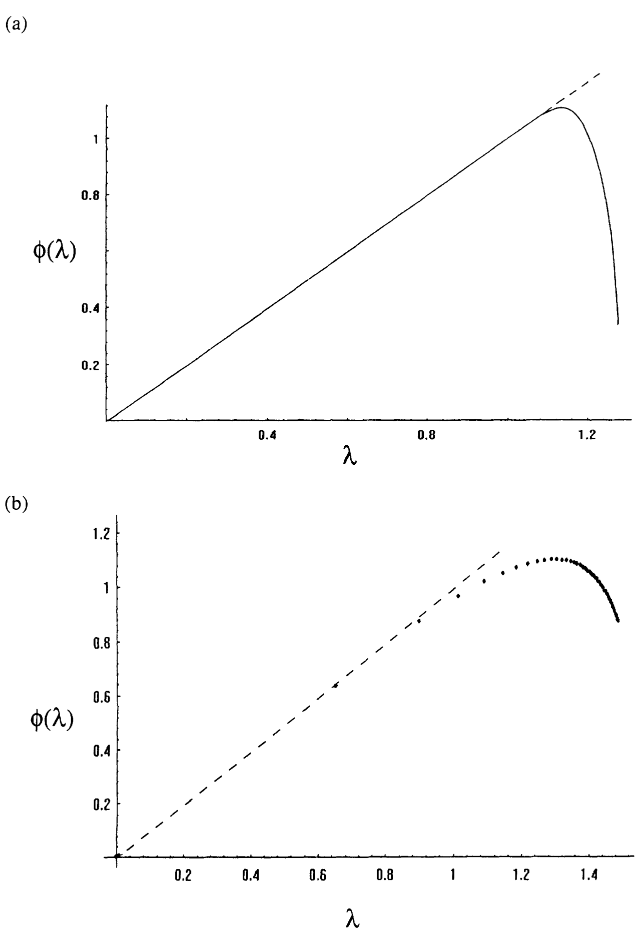

FIG. 4. Dynamical spectrum $\phi(\lambda)$, for (a) $\bar{z}=1.6$ and (b) $\bar{z}=2.2$. For $\bar{z}>2$, only a slow convergence to the asymptotic result with a zero Lyapunov exponent is obtained, as a function of the length n of the orbits considered (a method which can be applied for time series has been used for the evaluation). The dots indicate the result for $n=65$.

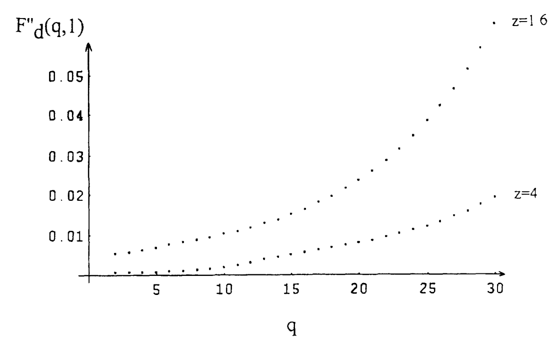

FIG. 5. Second derivative of the diffusion-related free energy at $\beta=1$, for $\bar{z}<2$ and $\bar{z}>2$ (sublinear case).

can be recovered [where $\alpha=1$ for $\bar{z}<2$ and $\alpha=1/(\bar{z}-1)$ for $\bar{z}>2$].

The superlinear case is investigated in a similar manner. From Eq. (9) it can be concluded immediately that, for $\beta>1$, the diffusion-related free energy does not exist for nonzero q, and that phase transitions may show up for $\beta<1$. These properties are easily observed in Fig. 3(b), where a plot of the numerically obtained diffusion-related free energy is shown. In the figure, the critical line L separates the hyperbolic phase of the system (on the left-hand side of L) from the nonhyperbolic phase of the system (on the right-hand side of L). Whereas the hyperbolic phase is determined by the hyperbolic scaling elements of the partition, the nonhyperbolic phase is determined by the marginally stable fixed point. Again the diffusion coefficient can be evaluated according to Eqs. (9) and (12). We obtain $D\sim(\sum_{k=1}^{\infty}k^2w_k)/(\sum_{k=1}^{\infty}kw_k)$ which explains why, for the superlinear case, anomality sets in at $z=\frac{3}{2}$. In order to investigate the nature of the phase transition at $\beta=1$, one must proceed towards this point within the hyperbolic phase. As has been worked out in a similar context in Ref. [30], one may use Wang's results [29] for the monovariate ($q=0$) free energy to determine the order of the phase transition. To this end, the free energy is expanded for $|q|\ll(1-\beta)$ as $F_d(q,\beta)\sim F_d(q=0,\beta)+(1-\beta)q^2/([q-(1-\beta)^{1/\alpha}][q+(1-\beta)^{1/\alpha}])$ for $\alpha<1$, and as $F_d(q,\beta)\sim F_d(q=0,\beta)+(1-\beta)^{\alpha}q^2/([q-(1-\beta)][q+(1-\beta)])$ for $\alpha>1$, according to the behavior of the free energy $F_d(q=0,\beta)$ in the two cases (the poles are screened by the nonhyperbolic phase). By calculation of derivatives, it is seen that for $\alpha<1$ the diffusion coefficient diverges in the limit $\beta\to 1-$. Higher-order derivatives with respect to β may diverge in the case of $\alpha>1$.

VI. NONGENERIC PROPERTIES

In order to explain generic properties of intermittent systems the use of the model system of Sec. IV was advantageous because we were able to use simple expressions for our analytical and numerical investigations. For experimental intermittent systems, deviations from this generic model have to be expected. In these systems, often not much information is available about the hyperbolic branch, whereas the fixed-point behavior can easily be measured. As far as generic properties are concerned, this is no problem, since these properties are determined by the fixed points of the reduced maps. Whereas the generic properties remain (order of transitions, dependence of the kind of diffusion on $\bar{z}$), properties which depend strongly on the hyperbolic branch of the map are not preserved. For such properties (e.g., the value of the diffusion coefficient), care must be applied to use the proper partition of the map. The generic partition will not be sufficient.

VII. CONCLUSION

In this contribution, the relation between nonhyperbolicity, nonanalyticity, and anomalous diffusion has been worked out. The bivariate thermodynamic formalism proved to be a natural approach for the investigation of these problems. Diffusion-related free energies were calculated for the characterization of the sublinear and the superlinear cases, respectively. As can be expected [12], critical lines emerge in the free energies. The diffusional properties are determined by the behavior of the free energy in the neighborhood of the critical lines. Focusing on the natural measure, a deeper insight into the connection between the system's phase transition in the Lyapunov spectrum and the anomalous diffusion property is obtained. Apart from these generic properties of intermittent systems, the influence of deviations from the generic model was discussed. It is hoped that the present discussion may also help to understand the behavior of experimental intermittent systems better.

Recently, R. Artuso, G. Casati, and R. Lombardi [32] and especially X.-J. Wang and C.-K. Hu [30] arrived at conclusions which are similar to ours. However, no detailed numerical calculations seem to have been performed.

ACKNOWLEDGMENTS

The author would like to thank the members of the Budapest chaos group, and W.-H. Steeb for several illuminating discussions. The support of the Swiss National Science Foundation is gratefully acknowledged.

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