Trajectory versus probability density entropy

Mauro Bologna,^{1,*} Paolo Grigolini,^{1,2,3,†} Markos Karagiorgis,¹ and Angelo Rosa³

¹Center for Nonlinear Science, University of North Texas, P.O. Box 311427, Denton, Texas 76203-1427

²Istituto di Biofisica del Consiglio Nazionale delle Ricerche, Area della Ricerca di Pisa, Via Alfieri 1, San Cataldo, 56010,

Ghezzano-Pisa, Italy

³Dipartimento di Fisica dell'Università di Pisa and INFM Piazza Torricelli 2, 56127 Pisa, Italy (Received 3 March 2000; revised manuscript received 5 April 2001; published 27 June 2001)

We show that the widely accepted conviction that a connection can be established between the probability density entropy and the Kolmogorov-Sinai (KS) entropy is questionable. We adopt the definition of density entropy as a functional of a distribution density whose time evolution is determined by a transport equation, conceived as the only prescription to use for the calculation. Although the transport equation is built up for the purpose of affording a picture equivalent to that stemming from trajectory dynamics, no direct use of trajectory time evolution is allowed, once the transport equation is defined. With this definition in mind we prove that the detection of a time regime of increase of the density entropy with a rate identical to the KS entropy is possible only in a limited number of cases. The proposals made by some authors to establish a connection between the two entropies in general, violate our definition of density entropy and imply the concept of trajectory, which is foreign to that of density entropy.

DOI: 10.1103/PhysRevE.64.016223

PACS number(s): 05.45.-a, 03.65.Sq, 05.20.-y

I. INTRODUCTION

The so called Kolmogorov-Sinai (KS) entropy [1,2], called h_{KS} , is a property of a time sequence of symbols and can be interpreted as the mean entropy increase per unit of time. In the case of a dynamic system the sequence of symbols is generated by a trajectory running through a phase space divided into many cells of finite size and labeled with given symbols. In this case this important form of entropy can be related to the Lyapunov coefficients of the trajectory under study through the well known expression, derived by Pesin [3],

$$h_{KS} = \int d\mathbf{x} \rho_{eq}(\mathbf{x}) \sum_{i, \lambda_i(x) > 0} \lambda_i(x).$$
(1)

Here the symbols λ_i denote the Lyapunov coefficients, and the sum on the right side of this equation refers only to the positive Lyapunov coefficients. The symbol ρ_{eq} denotes the invariant measure. From an intuitive point of view we can say that when the size of the time windows used to determine the KS entropy of the symbolic sequence is so large that the trajectory explores within that time window the whole phase space, the resulting entropy increase reflects the mean of the sum of all positive Lyapunov coefficients.

It seems to be evident, on the basis of this expression, that, if the Gibbs distribution density perspective is adopted, the physical condition corresponding to Eq. (1) is statistical equilibrium, thereby implying that the distribution density entropy is constant. This is the reason why a connection between the two forms of entropy, if it ever exists, can only be obtained by considering initial conditions for the distribution density that are far from equilibrium. From an intuitive forms of entropy is straightforward, especially in the case of systems with only one Lyapunov coefficient (maps) independent of the position x. In fact, the nonequilibrium entropy increase is easily related to the local Lyapunov coefficient, which, due to the Pesin theorem of Eq. (1), coincides in this case with the KS entropy. For a tutorial demonstration the reader can consult, for instance, the book of Hilborn [4]. A much more sophisticated mathematical approach is needed to address the problem in general. This was already done as early as 19 years ago by Goldstein and Penrose [5] and Goldstein [6]. Of special interest is the second paper, where the nonequilibrium entropy introduced by Goldstein and Penrose, defined on nonstationary probability measures, is quantitatively related to the KS entropy of the system.

point of view establishing a connection between the two

The main purpose of the present paper is that of revisiting this important issue from a perspective more familiar to physicists, a significant example of which is given by the recent work of Latora and Baranger [7]. These authors found that the nonequilibrium entropy increase of invertible maps is characterized by three distinct regimes. The first is a *regime of transition to thermodynamics* lasting for a given time t_D . The second is a regime of entropy increase linear in time, lasting from the time t_D to the time $t_S > t_D$. Latora and Baranger [7] proved that the rate of entropy increase of this regime coincides with the KS entropy, and for this reason we call it *Kolmogorov regime*. Finally, the third regime, concerning times $t > t_S$, corresponds to equilibrium, and the distribution density entropy is time independent. We refer to it as *saturation regime*.

To properly discuss these results we have to define the concept of density entropy. Our definition of density entropy is close to the *physical entropy* of Latora and Baranger [7], which, in turn, is nothing but the Gibbs entropy. We use the term *density* rather than *physical* to avoid the impression that we judge the density entropy to be more fundamental than the trajectory entropy. Furthermore, as clearly pointed out by

^{*}Email address: mb0015@unt.edu

[†]Email address: grigo@jove.acs.unt.edu

Lebowitz [8,9], in accordance with Boltzmann's point of view, the relevant entropy for understanding the time evolution of macroscopic systems is the Boltzmann entropy and not the Gibbs entropy.

This is not the issue under discussion in the present paper. We do not take position on whether trajectories are more fundamental than densities, or vice versa, and on whether mixing type of behavior is essential or not for the irreversible behavior of macroscopic systems. We limit ourselves to arguing that our definition of density entropy might be incompatible with the emergence of the KS regime, and this definition, as we shall see in the concluding remarks of Sec. VI, makes it impossible for us to adopt the expedient of Latora and Baranger themselves [7] to deal with the case of nonconstant Lyapunov coefficients. We assume first that a *transport equation* exists. This transport equation can be the Liouville equation

$$\frac{\partial}{\partial t}\rho(\mathbf{x},t) = -iL\rho(\mathbf{x},t),\tag{2}$$

valid in the case of Hamiltonian systems, or the Frobenius-Perron equation,

$$\rho(\mathbf{x},t+1) = \Lambda \rho(\mathbf{x},t), \tag{3}$$

valid in the case of low-dimensional maps [10]. Actually, we shall discuss in this paper only the second type of transport equation. However, our remarks on invertible maps apply also to the case of Hamiltonian systems and thus to the first kind of transport equations.

We define the density entropy as the time dependent entropy given by

$$S(t) = -\int_{\mathbf{X}} \rho(\mathbf{x}, t) \ln[\rho(\mathbf{x}, t)] d\mathbf{x}$$
(4)

with the request that the time evolution of the distribution density $\rho(\mathbf{x}, t)$ be given by the transport equation and *only* by the transport equation. We shall show that if this definition of density entropy is adopted, then the emergence of the Kolmogorov regime is not guaranteed in general, but only in the case of Lyapunov coefficients independent of the coordinate **x**.

From a rigorous point of view, the adoption of this definition of density entropy would prevent us from adopting the heuristic arguments of Sec. II, which are based on a widely accepted conviction that the time evolution of the distribution density coincides with the result that one would obtain evaluating the time evolution of many trajectories with initial conditions fitting the initial distribution density. This widely accepted perspective has been recently criticized by Petrosky and Prigogine [11,12]. These authors pointed out that there exists a sort equivalence between the case of Hamiltonian systems with infinitely many degrees of freedom and lowdimensional chaotic systems. In both cases the operator driving the transport equation, expanded on a suitable basis set, becomes a matrix of infinite size. In both cases the diagonalization of this matrix of infinite size has to be done using sophisticated methods, implying the use of analytical continuation. The remarks of these authors [11,12] imply that the asserted equivalence between a statistical picture based on trajectories and one based on distribution density must be used with caution.

It is not clear to us if the conclusions of the present paper might be related to the breakdown of the concept of trajectory, claimed by these authors [11,12]. This is still a controversial issue that we do not want to address here. We refer to Refs. [10-12] only as examples of a perspective that would be in line with our definition of density entropy, not involving at any extent the concept of trajectory. It is immediately evident that the definition of density entropy here adopted does not allow us to apply the method of Latora and Baranger [7]. These authors, in the case of the standard map, evaluated the time evolution of S(t) with different initial conditions, and then determined the time evolution of an average entropy S(t), a prescription conflicting with our definition of density entropy. It is not clear to us if this definition also conflicts with the prescription adopted by Goldstein [6]. We think it does since Goldstein's prescription is based on a partition into cells depending upon trajectory dynamics.

II. HEURISTIC ARGUMENTS

The purpose of this section is that of providing a simple explanation for the three regimes detected by Latora and Baranger [7]. We want also to convince the reader about the physical significance of the definition of density entropy given in Sec. I. To give further support to that definition we establish a connection between the work of Latora and Baranger [7] and the work of other authors [13–19]. These authors deal with quantum rather than classical processes; in the case of quantum processes, there are no trajectories available and one is forced to adopt a definition of density entropy coincident with that of Sec. I. Nevertheless, the adoption of heuristic arguments based on the classical trajectories is legitimate, provided that they do not conflict with the prescriptions of Sec. I to evaluate the time evolution of density entropy

Note that the cases studied by Latora and Baranger [7] are two dimensional, and our discussion here refers to a twodimensional case, too. The baker's transformation reads

$$x_{t+1} = 2x_t$$

$$y_{t+1} = y_t/2,$$
(5)

for $0 \leq x_t \leq 1/2$, and

$$x_{t+1} = 2x_t - 1$$

$$y_{t+1} = (y_t + 1)/2,$$
(6)

for $1/2 \leq x_t \leq 1$.

We adopt here the same heuristic arguments as those used by the authors of Ref. [20]. We divide the phase space **X** into W_{max} cells of equal size. We consider *N* distinct trajectories corresponding to different initial conditions, and mimicking a distribution density concentrated in a small portion of the whole phase space. We make the assumption that at all times in any cell there is the same number of trajectories. This means that the probability of finding a trajectory in a given cell is 1/W(t), where W(t) is the number of cells containing trajectories. As a consequence of these assumptions, we obtain

$$S(t) = \ln W(t). \tag{7}$$

We denote by $\boldsymbol{\lambda}$ the positive Lyapunov coefficient, and we set

$$W(t) = W(0)\exp(\lambda t).$$
(8)

By plugging Eq. (8) into Eq. (7) we get

$$S(t) = \lambda t - \ln W(0), \qquad (9)$$

which corresponds to the Kolmogorov regime of Latora and Baranger [7]. In fact, the slope of this linear function of time is the Lyapunov coefficient λ , which is related to the KS entropy through Eq. (1). A more rigorous approach to the coarse-graining procedure necessary to establish a connection between the Gibbs entropy and the KS entropy can be found in Ref. [5]. For all this to hold true, it is necessary that the positive Lyapunov coefficient is independent of **x**. This condition is fulfilled by the baker's transformation, for which it is well known [21] that

$$\lambda = \ln 2. \tag{10}$$

In conclusion, we establish the following attractive connection between the density entropy S(t) and the KS entropy

$$\frac{dS}{dt} = \lambda = \ln 2 = h_{KS}.$$
(11)

We have used arguments based on the trajectory instabilities. However, the conclusion is not incompatible with our definition of density entropy, as confirmed by the calculations of Sec. III that do not rest on the existence of trajectories.

The Kolmogorov regime is not infinitely extended. It has an upper bound, given by the fact that when equilibrium is reached, even in the merely sense of a coarse-grained equilibrium, then the entropy stops increasing. An estimate of this time is obviously given by the solution of the following equation

$$\ln W_{max} = \lambda t - \ln W(0), \qquad (12)$$

which yields the following saturation time,

$$t_{S} = \frac{1}{\lambda} \ln \left(\frac{W_{max}}{W(0)} \right). \tag{13}$$

We have now to find the lower bound of validity of the Kolmogorov regime t_D . This depends on the fact that the initial distribution might include a large number of cells. Let us assume that the size of this distribution along the coordinate y is L, and that the size of the cells is ϵ with $\epsilon < L$. Then it is evident that, in spite of the coarse graining, the total

number of cells occupied remains the same for a while. This time is easily estimated using the equation

$$L\exp(-\lambda t) = \epsilon, \qquad (14)$$

which in fact defines the time at which the distribution volume, and consequently, the system entropy starts increasing. This time is denoted by the symbol t_D and reads

$$t_D = \frac{1}{\lambda} \ln \left(\frac{L}{\epsilon} \right). \tag{15}$$

Now we are in a position to evaluate the time duration of the Kolmogorov regime, and to assess under which conditions it can become infinitely extended in time. We denote by U(t) the volume of the distribution density at time *t* and by *V* the volume of the phase space, thereby implying that $U(t) \leq V$. We note that

$$\frac{W_{max}}{W(0)} = \frac{V}{U(0)},$$
 (16)

where V is the total volume of the phase space and U(0) is the initial volume of the distribution density. Thus the Kolmogorov regime shows up in the following time interval,

$$t_D = \frac{1}{\lambda} \ln\left(\frac{L}{\epsilon}\right) < t < t_S = \frac{1}{\lambda} \ln\left(\frac{V}{U(0)}\right).$$
(17)

The time duration of the regime of validity of the Kolmogorov regime can be made infinitely extended by making the cell size infinitely small. This means that the conflict between the KS entropy prescription and the time independence of S(t) can be bypassed by focusing our attention on the intermediate region, whose time duration tends to infinity with $\epsilon \rightarrow 0$. We note that a choice can be made such that $V/U(0) = (L/\epsilon)^{\chi}$, with $\chi > 1$. This means that the onset of the saturation regime can be made χ times larger than the onset of the Kolmogorov regime. For $\epsilon \rightarrow 0$ both time durations become infinite, thereby showing that a Kolmogorov regime of infinite time duration can be obtained at the price, however, of waiting an infinitely long time for the entropy to increase. The infinite waiting time before the regime of entropy increase fits the observation [22,23] that the Gibbs entropy of an invertible map is constant. The linear entropy increase showing up "after this infinite waiting time" allows the emergence of the KS entropy from within the probability density perspective.

In conclusion, if we adopt the perspective of the density entropy defined in Sec. I, and the coarse-graining procedure implicit in the partition adopted by Latora and Baranger [7] as well, we cannot establish a connection with the arguments of Hilborn [4] and Goldstein [6]. This is so because the Kolmogorov regime of density entropy is an intermediate regime occurring after a transition to thermodynamics. With reducing the cell size the time duration of transition to thermodynamics becomes larger and infinitely extended with a vanishing cell size, thereby postponing the physical manifestation of KS entropy. In Sec. III we shall see that this transition regime can be eliminated by adopting the tracing method.

The constraints posed by the adoption of the density entropy are fulfilled also by the authors of Refs. [13–19]. This is so because all these papers, to different extents, share the perspective established by Zurek and Paz [13]. According to this theoretical approach the time evolution of a quantum system, which would be chaotic in the classical limit, can be safely described by using a classical transport equation. This transport equation is the Liouville equation of Eq. (2) with a diffusionlike correction term. This diffusionlike correction corresponds to the influence of a weak stochastic force. The stochastic force has a twofold role. First, it prevents the fragmentation of the Liouville density from becoming so intense as to activate the quantum corrections to the transport equation. Second, it realizes a kind of coarse graining whose effects are essentially indistinguishable from those resulting from the partition of the phase space into cells of finite size.

Let us prove this important aspect, using first of all the inverted stochastic oscillator of Zurek and Paz [13], namely,

$$\frac{d^2x}{dt^2} = \lambda^2 x(t) + \gamma \frac{dx}{dt} + f(t), \qquad (18)$$

where the friction γ and the stochastic force f(t) are related to one another by the standard fluctuation-dissipation relation

$$\langle ff(t) \rangle = 2\gamma \left\langle \left(\frac{dx}{dt} \right)^2 \right\rangle_{eq} \delta(t) \equiv 2D \,\delta(t).$$
 (19)

It is interesting to remark that the proper formulation of the second principle implies that the entropy of a system can only increase or remain constant under the condition of no energy exchange between the system and its environment. In the case of Eq. (19) the energy exchange between system and environment is negligible for any observation made in the time scale

$$t \ll 1/\gamma. \tag{20}$$

To ensure that the system entropy increase takes place with no energy exchange between system and its environment Zurek and Paz [13] set the condition of Eq. (20) and this, in turn, allows them to neglect the friction term in Eq. (18). Then, these authors adopted the modes

$$u \equiv \frac{dx}{dt} + \lambda x \tag{21}$$

and

$$w \equiv \frac{dx}{dt} - \lambda x, \qquad (22)$$

which make it possible for them to split Eq. (18) into

$$\frac{du}{dt} = \lambda u(t) + f(t) \tag{23}$$

$$\frac{dw}{dt} = -\lambda w(t) + f(t).$$
(24)

Let us imagine the initial distribution density as a rectangle of size $\Delta w(0)$ along the direction w and $\Delta u(0)$ along the direction u. We keep denoting by U(t) the distribution volume at a given time t. Thus the volume of the initial distribution is

$$U(0) = \Delta u(0) \Delta w(0). \tag{25}$$

In the absence of the stochastic force f(t), Eq. (23) and Eq. (24) result in an exponential increase and an exponential decrease, with the same rate λ , respectively. Consequently, the Liouville theorem U(t) = U(0) is fulfilled. In the presence of stochastic force, we work as follows. In the former equation, with *u* increasing beyond any limit, the weak stochastic force f(t) can be neglected. This is not the case with the latter equation. In fact, *w* is a contracting variable in the absence of the stochastic force. In the presence of the stochastic force the minimum size of the distribution along *w* is given by

$$\langle w^2 \rangle_{eq}^{1/2} = (D/\lambda)^{1/2}.$$
 (26)

This minimum size is reached in a time determined by the solution of the following equation

$$\Delta w(0) \exp(-\lambda t) = (D/\lambda)^{1/2}$$
(27)

yielding

$$t_D = \frac{1}{\lambda} \ln \left(\frac{\lambda}{D} \right)^{1/2} \Delta w(0).$$
(28)

Due to the fact that deterministic chaos is simulated by Zurek and Paz [13] by means of an inverted parabola, these authors did not consider the entropy saturation effects. However, it is straightforward to evaluate the saturation effect with heuristic arguments concerning the case where the total volume of the phase space has the finite value V. From the time $t=t_D$ on, the distribution volume U(t) increases exponentially in time with the following expression

$$U(t) = \Delta w(0) \Delta u(0) \exp(\lambda t) = (D/\lambda)^{1/2} \Delta u(t_D) \exp(\lambda t).$$
(29)

Thus, the saturation time is now given by

$$t_{S} = \frac{1}{\lambda} \ln \left[\frac{V}{\Delta u(0) \Delta w(0)} \right].$$
(30)

Using Eq. (25) we can write this saturation time as

$$t_{S} = \frac{1}{\lambda} \ln \left[\frac{V}{U(0)} \right], \tag{31}$$

which coincides with Eqs. (17) and (13).

We think that the reader can easily realize at this stage why the Kolmogorov regime shows up in all the papers of Refs. [7,13-19].

and

TRAJECTORY VERSUS PROBABILITY DENSITY ENTROPY

Of remarkable clarity is the paper by Pattanayak [19] which shows indeed a surprising similarity with the three regimes of Latora and Baranger [7]. We invite the reader to keep in mind that we plan to prove that the emergence of this Kolmogorov regime is the consequence of the simplifying condition of the Lyapunov coefficient being independent of the coordinate \mathbf{x} of the phase space.

Before ending this section we want to notice that the kind of transport equations used by the authors of Refs. [13-19]can be derived from a Liouville equation using a projection approach method [24]. This is a kind of contraction over "irrelevant" variables, whose effect is that of making entropy increase. This means that the coarse graining resting on the role of the stochastic force is closely related to the *tracing* mentioned by Mackey [23] as a second source of entropy increase. The main difference is that the adoption of the projection method has the effect of producing a new transport equation, which is the sum of two terms, the former still maintaining the invertible properties of the standard Liouville equations, the latter corresponding to a diffusionlike correction, whose strength determines the time it takes the system to make a transition to thermodynamics.

III. THE BERNOUILLI MAP

This section is devoted to a rigorous treatment based only on the time evolution of distribution density, as resulting from the transport equation, with no use, either direct or indirect of the concept of trajectory. We use the theoretical tools described in Ref. [10]. We focus our attention on the Bernoulli shift map,

$$x_{t+1} = 2x_t \pmod{1}.$$
 (32)

The Frobenius-Perron equation of this map is defined by [10]

$$\rho(x,t+1) = \Lambda \rho(x,t) \equiv \frac{1}{2} \left[\rho\left(\frac{x}{2},t\right) + \rho\left(\frac{x+1}{2},t\right) \right].$$
(33)

It is straightforward to show that the Frobenius-Perron operator of Eq. (33) stems from the contraction over the variable y of the baker's mapping, acting in fact on the unit square of two-dimensional space (\mathbf{x}, \mathbf{y}) (see, for instance Ref. [21]). It is shown [21] that the KS entropy of the baker's transformation is well defined and turns out to be the same as that of the Bernoulli shift map, namely, $h_{KS} = \ln 2$. Intuitively, this suggests that the main role of the tracing is that of making inactive the process of contraction, and with it the negative Lyapunov coefficient. Of course, as earlier remarked (see Sec. II) we do not expect any regime of transition to thermodynamics. We expect that the time evolution of the density entropy will be characterized only by the Kolmogorov and saturation regime.

To address this issue according to the prescription of Ref. [10], we express the distribution density at time t under the form given by Ref. [10] which reads

$$\rho(x,t) = 1 + \sum_{j=1}^{\infty} \exp(-\gamma_j t) \frac{B_j(x)}{j!} [\rho^{(j-1)}(1,0) - \rho^{(j-1)}(0,0)].$$
(34)

Note that $\gamma_j \equiv j \ln 2$, $B_j(x)$ are the Bernoulli polynomials [25] and $\rho^{(n)}(x,t)$ denotes the *n*th order derivative of $\rho(x,t)$ with respect to *x*. Hereby, we shall show how to derive from Eq. (34) an expression more appropriate to our purposes.

In the case of an initial condition close to equilibrium, resulting from the sum of the equilibrium distribution and the first "excited" state, it is easy to prove that the entropy S(t) of Eq. (4) reaches exponentially in time the steady state condition. This suggests that the Kolmogorov regime, where the entropy S(t) is expected to be a linear function of time, must imply an initial condition with infinitely many "excited" states. To deal with a condition of this kind it is convenient to express Eq. (34) in an equivalent form given by

$$\rho(x,t) = 1 + \sum_{j=1}^{\infty} \int_{-\infty}^{+\infty} \frac{B_j(x)}{j!} (-iz\omega)^{j-1} \hat{\rho}(\omega)$$
$$\times [\exp(-i\omega) - 1] \frac{d\omega}{2\pi}, \qquad (35)$$

where $z \equiv \exp[-t(\ln 2)]$ and $\hat{\rho}(\omega)$ is related to the initial condition $\rho(x,0)$ by the Fourier transform

$$\rho(x,0) = \int_{-\infty}^{+\infty} \hat{\rho}(\omega) \exp(-i\omega x) \frac{d\omega}{2\pi}.$$
 (36)

The following equation

$$\sum_{j=0}^{\infty} \frac{B_j(x)}{j!} z^j = z \frac{\exp(zx)}{\exp(z) - 1},$$
(37)

is known [25] to generate Bernoulli polynomials. Using this Bernoulli polynomial generatrix, we arrive, after some algebra, at

$$\rho(x,t) = z \int_{-\infty}^{+\infty} \exp(-i\omega zx) \hat{\rho}(\omega) \frac{\exp(-i\omega) - 1}{\exp(-i\omega z) - 1} \frac{d\omega}{2\pi}.$$
(38)

By expanding the denominator of Eq. (38) into a Taylor series and using Eq. (36), we finally derive the fundamental expression

$$\rho(x,t) = z \sum_{n=0}^{\infty} \left[\rho(zx+zn,0) - \rho(zx+zn+1,0) \right].$$
(39)

This important expression makes it possible for us to discuss analytically the entropy time evolution ensuing the preparation of an initially very sharp distribution. Let us consider in fact

$$\rho(x,0) = \frac{\alpha}{1 - \exp(-\alpha)} \exp(-\alpha x), 0 \le x \le 1.$$
 (40)

For $\alpha \rightarrow \infty$ this initial distribution becomes a very sharp distribution located at x = 0. By plugging this initial distribution density into Eq. (39) we obtain

$$\rho(x,t) = z \alpha \frac{\exp(-\alpha xz)}{1 - \exp(-\alpha z)}.$$
(41)

It is evident that this simple analytical expression for the time evolution of the distribution density is exact, and corresponds to the time evolution dictated by the Frobenius-Perron operator of Eq. (33).

We are now in a position to discuss the central issue of this paper, namely, the time evolution of the density entropy of Eq. (4), which, in the case here under study, reads

$$S(t) = -\int_{X} \rho(x,t) \ln[\rho(x,t)] dx, \qquad (42)$$

with *X* now denoting the interval [0,1]. By plugging Eq. (41) within Eq. (42) we obtain

$$S(t) = 1 - \ln(\alpha z) + \ln[1 - \exp(-\alpha z)] - \frac{\alpha z}{\exp(\alpha z) - 1}.$$
(43)

In the limiting case $\alpha \rightarrow \infty$ this exact prediction is approximated very well by

$$S(t) = -\ln(\alpha) + (\ln 2)t.$$
 (44)

It indicates that a sharp initial distribution makes the Kolmogorov regime emerge immediately with no preliminary regime of transition to thermodynamics, in a full accordance with our expectation. The saturation regime is still present. It is straightforward to show that the saturation time t_s = ln α /ln 2 resulting from Eq. (43) is the same as that of Eq. (13) in the case V=1. In fact using Eq. (16) and V=1 we obtain that $W_{max}/W(0) = 1/U(0)$, where U(0) is the size of the initial distribution. The size of the initial distribution of Eq. (40), for $\alpha \rightarrow \infty$, becomes proportional to $1/\alpha$. Thus, ln $\alpha \approx \ln[W_{max}/W(0)]$ in accordance with Eq. (13).

This is an elegant result, involving a modest amount of algebra. However, it refers to an initial distribution located at x=0. We want to prove that this is a general property, independent of where the initially sharp distribution is located, at the price, as we shall see, of a more complicated mathematical treatment. For this purpose we study the case where the distribution shape is the Lorentzian curve,

$$\rho(x,0) = A \frac{\Gamma}{(x-x_0)^2 + \Gamma^2},$$
(45)

with x_0 being a generic point of the interval [0,1] and x running in the same interval. Setting the normalization condition yields

$$A = \frac{1}{\arctan\left(\frac{x_0}{\Gamma}\right) + \arctan\left(\frac{1-x_0}{\Gamma}\right)}.$$
 (46)

We have to set again the condition that the initial distribution is very sharp. Thus we make the assumption $\Gamma \rightarrow 0$, yielding $A \approx 1/\pi$. We plug this approximated value of A into Eq. (39), thereby obtaining the following density time evolution

$$\rho(x,t) = \frac{z\Gamma}{\pi} \sum_{n=0}^{\infty} \left[\frac{1}{(zx+zn-x_0)^2 + \Gamma^2} - \frac{1}{(zx+zn-x_0+1)^2 + \Gamma^2} \right].$$
 (47)

We are now in a position to study the entropy time evolution again. Plugging Eq. (47) into Eq. (42) we find

$$S(t) = -\int_{X} \rho(x,t) \ln\left(\frac{z}{\pi\Gamma} \sum_{n=0}^{\infty} \left[\frac{1}{\left(\frac{zx+zn-x_{0}}{\Gamma}\right)^{2}+1} -\frac{1}{\left(\frac{zx+zn-x_{0}+1}{\Gamma}\right)^{2}+1}\right]\right) dx$$
$$= -\int_{X} \rho(x,t) \ln\left(\frac{z}{\pi\Gamma}\right) dx$$
$$-\int_{X} \rho(x,t) \ln\left(\sum_{n=0}^{\infty} \left[\frac{1}{\left(\frac{zx+zn-x_{0}}{\Gamma}\right)^{2}+1} -\frac{1}{\left(\frac{zx+zn-x_{0}+1}{\Gamma}\right)^{2}+1}\right]\right) dx.$$
(48)

In the limiting case of Γ very small, it is possible to derive a more tractable expression as follows. The argument of the logarithm is a series whose terms are the differences between two contributions. These contributions are almost zero, except for $n = -[x] + [x_0/z] = [x_0/z]$ (first contribution), and for $n = -[x] - [(1-x_0)/z] = -[(1-x_0)/z]$ (second contribution). Note that, as usual, we denote by [.] the integer part of the number. The condition making different from zero the second contribution is never realized, since *n* is a positive integer. Thus the whole series is reduced to only one term, which is the first contribution with $n = -[x] + [x_0/z] = [x_0/z]$, thereby making the entropy S(t) read as follows:

$$S(t) \approx \ln \Gamma + (\ln 2)t - \ln \pi - \int_0^{z/\Gamma} \frac{\ln(y^2 + 1)}{y^2 + 1} dy, \quad (49)$$

which, in the limiting case $z/\Gamma \rightarrow \infty$, becomes

$$S(t) \approx -\ln\frac{1}{\Gamma} + (\ln 2)t - \ln \pi - \int_0^\infty \frac{\ln(y^2 + 1)}{y^2 + 1} dy$$

= $-\ln\frac{1}{\Gamma} + (\ln 2)t - \ln \pi - \pi \ln 2$
 $\approx -\ln\frac{1}{\Gamma} + (\ln 2)t.$ (50)

As in the earlier case, the validity of the approximation yielding the linear dependence of S(t) on time, is broken at the time $t \sim (\ln 1/\Gamma)/\ln 2$. In conclusion, the Kolmogorov regime is realized by very sharp initial distributions.

We would be tempted to believe that the tracing is a way of ensuring a correspondence with the asymptotic arguments of Hilborn [4] and Goldstein [6]. In fact, there is no transition to thermodynamics. Thus we can conclude that for $\Gamma \rightarrow 0$ in Eq. (50), or $\alpha \rightarrow \infty$ in Eq. (44), an unlimited Kolmogorov regime emerges, fitting the theoretical prediction of Hilborn [4]. However, this attractive result is limited to the case where the Lyapunov coefficient is independent of the phase space coordinate. In Secs. IV and V we shall show that in general this attractive property is lost.

IV. THE TIME DEPENDENT LYAPUNOV COEFFICIENT

Let us consider the case of the Manneville map [26]

$$x_{t+1} = x_t + x_n^z \pmod{1}$$
 (51)

with z>1. This map is known to be characterized by two regions, a laminar region ranging from x=0 to x=d(z)<1, and a chaotic region ranging from d(z) to 1. The value d is determined by

$$1 = d(z) + d(z)^{z}.$$
 (52)

The laminar region on the left is responsible for only a limited amount of entropy increase, since the trajectories of an initial distribution very sharp and imbedded within the laminar region will depart very slowly from one the other. The Frobenius-Perron operator in this case reads,

$$\rho(x,t+1) = \frac{1}{1+zf(x)^{z-1}}\rho(f(x),t) + \frac{1}{1+zf(x+1)^{z-1}} \times \rho(f(x+1),t).$$
(53)

Here f(x) is the solution of the following equation

$$x = f(x) + f(x)^{z}$$
. (54)

Although Eq. (53) cannot be easily used to determine the time evolution of the distribution density, it can be adopted, however, to determine the rate of increase of the entropy of Eq. (4). First of all we find

$$S(t+1) - S(t) = -\int_{0}^{1} dx \rho(x,t+1) \ln[\rho(x,t+1)] dx + \int_{0}^{1} \rho(x,t) \ln[\rho(x,t)] dx.$$
(55)

We replace Eq. (53) into Eq. (55). In the resulting expression, we make the change of integration variable $x \rightarrow f(x)$. All this, after some algebra, yields:

$$S(t+1) - S(t) = L(t) + R(t),$$
(56)

where

$$L(t) \equiv -\int_{0}^{f(1)} dx \rho(x,t) \ln \left[\frac{1}{1+zx^{z-1}} + \frac{1}{1+z[f(f^{-1}(x)+1)]^{z-1}} \frac{\rho f((f^{-1}(x)+1),t)}{\rho(x,t)} \right]$$
(57)

and

$$R(t) = -\int_{f(1)}^{1} dx \rho(x,t) \ln \left[\frac{1}{1+zx^{z-1}} + \frac{1}{1+z[f(f^{-1}(x)-1)]^{z-1}} \frac{\rho f((f^{-1}(x)-1),t)}{\rho(x,t)} \right].$$
(58)

We note that the function f(x) fits the conditions: f(0) = 0 and f(1) = d(z), where d(z) is given by the solution of Eq. (52). The terms R(t) and S(t), contributing the righthand side of Eq. (56), correspond to the laminar and chaotic region, respectively. Let us consider an initial condition with a sharp distribution density close to x=0 and not overlapping with the chaotic region. It takes several steps for the distribution to broaden so as to overlap with the chaotic region. For this extended period of time [27] R(t) and the second term within the square brackets at the right-hand side of Eq. (57) vanish. As a consequence the rate of entropy increase reads as follows:

$$S(t+1) - S(t) = \int_0^{f(1)} dx \rho(x,t) \ln(1+zx^{z-1}).$$
 (59)

Note that this expression is reminiscent of the expression afforded by Pesin theorem, with f(1) replaced by 1 and $\rho(x,t)$ replaced by the invariant distribution. This expression would provide the KS entropy, namely, the steady entropy increase of a stationary trajectory. However, the invariant distribution is reached moving from an initial out of equilibrium condition as a result of trajectories crossing several times the border between the laminar and the chaotic region. This would provoke the breakdown of the condition ensuring the validity of Eq. (59).

We note that at z=1 the Manneville map becomes identical to the Bernouilli map studied in Sec. III. However, in spite of the fact that Eq. (59) yields the correct expression for the KS entropy in this case, the condition z=1 is incompatible with the existence of a laminar region. As illustrated in Ref. [28], even if z-1 is very small, but nonvanishing, a region close enough to x=0 can be found so that a sharp initial distribution, located in that region, can broaden for several time steps without overlapping with the chaotic region. The case z=1 is a singularity forcing us to use the theory of Sec. III, which cannot be derived from the theoretical approach of this section. All this should make clear that the emergence of the Kolmogorov regime, in accordance with the arguments of Sec. III, rather than being an ordinary condition, is a singularity of a more general condition where the Kolmogorov regime cannot emerge.

It is interesting to notice that the results of this section are reminiscent of those of Refs. [16–19]. In fact these authors did succeed in relating the rate of the density entropy to the Lyapunov coefficient. It has to be remarked, though, that the success of their attempt, even in the case where the ordinary Lyapunov coefficient would depend on the phase space coordinates, is made possible by the adoption of a generalized form of entropy and of Lyapunov coefficient. In the case where we use the ordinary entropic indicator and the ordinary Lyapunov coefficient, this result is only possible when the Lyapunov coefficient is independent of the phase space coordinates.

V. THE CASE OF SPORADIC RANDOMNESS

To make more compelling our arguments on the conflict between the adoption of the trajectories and distribution density perspective, let us consider the following equation of motion for the distribution density $\rho(x,t)$:

$$\frac{\partial}{\partial t}\rho(x,t) = -\frac{\partial}{\partial x} [x^{z}\rho(x,t)] + C(t), \qquad (60)$$

where $0 \le x \le 1$ and

$$C(t) \equiv \rho(1,t). \tag{61}$$

The physical meaning of this equation is clear. It corresponds to the distribution density representation of a dynamics process that in terms of single trajectories corresponds to the following simple picture. A trajectory moves from the initial condition x(0) in the interval 0 < x < 1 driven by the equation of motion

$$dx/dt = x^z. \tag{62}$$

When the trajectory reaches the border x=1 it is abruptly injected back in the interval 0 < x < 1. The probability of getting any value x of this interval is uniform. This is the source of randomness, and the choice of this value could be made by means of the Bernouilli map, so that the Kolmogorov entropy associated to this choice is $\ln 2$. This means that if we adopt as ''time'' the number of times this random number is selected, the entropy of the system increases as follows:

$$S(N) = N \ln 2. \tag{63}$$

However, the physical time t is that involved by Eq. (62), and a more proper picture of the entropy increase as a function of time is given by

$$N(t) = \int_{T}^{t} dt' C(t'), \qquad (64)$$

where *T* is a time of the order of the time it takes a sharp initial distribution to broaden till it touches the border x=1. The function C(t) of Eq. (60) is the number of times the trajectories of a given Gibbs set are injected back into the interval [0,1] per unit of time. This has to do with the entropy increase, as a consequence of the fact that the process of injection back is random. We assume that the probability of injection back is uniform thereby making this process equivalent to the random drawing of a number of the interval [0,1]. This is why the integral of Eq. (64) is identified with the number *N* of Eq. (63).

The solution of Eq. (60) yields, after some algebra, the following result. For z < 2, in the time asymptotic limit of t $\rightarrow \infty$ the function C(t) becomes proportional to 2-z. If z >2, for $t \rightarrow \infty$ the function C(t) tends to zero. These results agree with the earlier findings of Ref. [29]. In spite of the fact that the dynamic system of Eq. (60) is not equivalent to the Manneville map, the essence of sporadic randomness is the same in both systems, and we can use the earlier analytical results to support the main conclusion of this paper. The KS entropy of the Manneville map is evaluated using time windows so large as to correspond to the single trajectory jumping back from the chaotic into the laminar region a number of times. If we adopt the perspective of considering the transport equation as the only theoretical prescription to evaluate the density entropy, this immediately implies that the density entropy corresponding to the KS entropy is time independent.

Equilibrium is the result of a balance between the first and second term on the right-hand side of Eq. (60). The first term corresponds to the trajectories moving from the left to the right, with no entropy production (with no significant entropy production in the case of the Manneville map), whereas the second term corresponds to a significant entropy production that becomes steady at equilibrium. However, we can recognize this process of entropy production only if we use C(t) to count the trajectories jumping back from the chaotic region, namely, if we depart from the distribution density perspective forced upon us by the definition of density entropy of Sec. I. In this specific case, there is no room left for the emergence of the Kolmogorov regime of the density entropy. In fact, an out of equilibrium condition in this case would imply a departure from the steady condition resulting in the KS entropy. The KS entropy corresponds to time windows of so large size as to imply that the distribution density $\rho(x,t)$ coincides with the invariant distribution.

VI. CONCLUDING REMARKS

A simple way to account for our conclusions rests on the observation that when the Gibbs probability distribution is at equilibrium, so that the density entropy is time independent, still the microscopic trajectories keep running and are associated with a steady entropy increase, the KS entropy, if a sufficiently large time window is used to make this observation. The picture afforded by Eq. (60) is illuminating. In fact, at equilibrium, the function C(t), which represents the action of randomness, is constant, thereby implying a steady entropy increase. Yet, in this condition the density entropy is constant. Thus, the KS entropy is a trajectory property that, in general, cannot be recovered from the time evolution of the out of equilibrium density entropy. Different conclusions, namely, an out of equilibrium regime can be always found where the rate of increase of the density entropy coincides with the KS entropy, are seemingly derived from the earlier work of other groups [6,7]. This is due to the fact that these authors depart from our definition of denisty entropy. In the case of Ref. [7], for instance, the authors study the time evolution of the density entropy with different initial conditions, and then evaluate the mean rate of entropy increase, which, of course, cannot be reproduced by the density entropy of Sec. I. We note that the study of quantum dynamic processes would make it impossible to depart from our definition of density entropy.

Our conclusion is that setting an out of equilibrium initial condition might not be enough for the density entropy to reveal the underlying KS entropy. A promising direction seems to be that adopted by many authors with thermostating algorithms [30-34], flux boundary conditions [35,36], and escape condition [37,38]. For updated literature on these approaches the interested reader can consult the recent paper of Ref. [39]. For the technical and conceptual difficulties concerning the information content of a chaotic trajectory, the interested reader can consult Sec. 8.11 of the last book of one of the authors of this field of research [40]. Here we limit ourselves to pointing out that the constraints adopted by these authors realize steady out of equilibrium conditions, rather than an out of equilibrium initial condition with a subsequent regression to equilibrium. It might be the subject of future interesting research work to establish if the experimentally observable properties realized by these constraints can be related to the microscopic KS entropy without departing from the definition of density entropy adopted in this paper.

- [1] A.N. Kolmogorov, Dokl. Acad. Sci. USSR 119, 861 (1958).
- [2] Ya.G. Sinai, Dokl. Acad. Sci. USSR 124, 768 (1959).
- [3] Ya.B. Pesin, Adv. Geophys. 32, 55 (1977).
- [4] R. C. Hilborn, Chaos and Nonlinear Dynamics: An Introduction for Scientists and Engineers (Oxford University Press, Oxford, 1994).
- [5] S. Goldstein and O. Penrose, J. Stat. Phys. 24, 325 (1981).
- [6] S. Goldstein, Isr. J. Math. 38, 241 (1981).
- [7] V. Latora and M. Baranger, Phys. Rev. Lett. 82, 520 (1999).
- [8] J.L. Lebowitz, Physica A 263, 516 (1999).
- [9] J.L. Lebowitz, Rev. Mod. Phys. 71, S346 (1999).
- [10] D. J. Driebe, Fully Chaotic Maps and Broken Time Symmetry (Kluwer Academic Publishers, Dordrecht, 1999).
- [11] T. Petrosky and I. Prigogine, Chaos, Solitons Fractals 7, 441 (1996).
- [12] T. Petrosky and I. Prigogine, Chaos, Solitons Fractals 11, 373 (2000).
- [13] W.H. Zurek and J.P. Paz, Phys. Rev. Lett. 72, 2508 (1994).
- [14] P.A. Miller and S. Sarkar, Phys. Rev. E 58, 4217 (1998).
- [15] P.A. Miller and S. Sarkar, Nonlinearity 12, 419 (1999).
- [16] A.K. Pattanayak and P. Brumer, Phys. Rev. Lett. 77, 59 (1996).
- [17] A.K. Pattanayak and P. Brumer, Phys. Rev. E 56, 5174 (1997).
- [18] A.K. Pattanayak and P. Brumer, Phys. Rev. Lett. **79**, 4131 (1997).
- [19] A.K. Pattanayak, Phys. Rev. Lett. 83, 4526 (1999).
- [20] C. Tsallis, A.R. Plastino, and W.-M. Zheng, Chaos, Solitons Fractals 8, 885 (1997).
- [21] J. R. Dorfman, An Introduction to Chaos in Nonequilibrium Statistical Mechanics (Cambridge University Press, Cambridge, 1999).

- [22] A. Lasota, M. C. Mackey, *Chaos, Fractals and Noise, Stochastic Aspects and Dynamics*, 2nd ed. (Springer-Verlag, New York, 1994), p. 13.
- [23] M. C. Mackey, *Time's Arrow: The Origin of Thermodynamic Behavior* (Springer-Verlag, New York, 1992).
- [24] P. Grigolini, Adv. Chem. Phys. 62, 1 (1985).
- [25] M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, Dover, New York, 1972), p. 804.
- [26] P. Manneville, J. Phys. 41, 1235 (1980).
- [27] M. Ignaccolo and P. Grigolini, Phys. Rev. E (to be published), e-print cond-mat/0004155.
- [28] G. Aquino, P. Grigolini, and N. Scafetta, e-print cond-mat/0006245; Chaos, Soliton Fractals (to be published).
- [29] P. Gaspard and X.-J. Wang, Proc. Natl. Acad. Sci. U.S.A. 85, 4591 (1988).
- [30] N.I. Chernov, G.L. Eyink, J.L. Lebowitz, and Ya.G. Sinai, Phys. Rev. Lett. 70, 2209 (1993).
- [31] D.J. Evans, E.G.D. Cohen, and G.P. Morriss, Phys. Rev. Lett. 71, 2401 (1993).
- [32] G. Gallavotti and E.G.D. Cohen, Phys. Rev. Lett. **74**, 2694 (1995).
- [33] L. Rondoni and G.P. Morriss, Phys. Rev. E 53, 2143 (1996).
- [34] W.G. Hoover, O. Kum, and H.A. Posch, Phys. Rev. E 53, 2123 (1996).
- [35] S. Tasaki and P. Gaspard, J. Stat. Phys. 81, 935 (1995).
- [36] P. Gaspard, Physica A 240, 54 (1997).
- [37] P. Gaspard, J. Stat. Phys. 68, 673 (1992).
- [38] P. Gaspard and G. Nicolis, Phys. Rev. Lett. 65, 1693 (1990).
- [39] T. Gilbert and J.R. Dorfman, Physica A 282, 427 (2000).
- [40] W. G. Hoover, *Time Reversibility, Computer Simulation, and Chaos* (World Scientific, Singapore, 1999).