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Entropy Production: From Open Volume-Preserving to Dissipative Systems

T. Gilbert[1] **and J. R. Dorfman**[1]

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We generalize Gaspard's method for computing the ε-entropy production rate in Hamiltonian systems to dissipative systems with attractors considered earlier by Tél, Vollmer, and Breymann. This approach leads to a natural definition of a coarse-grained Gibbs entropy which is extensive, and which can be expressed in terms of the SRB measures and volumes of the coarse-graining sets which cover the attractor. One can also study the entropy and entropy production as functions of the degree of resolution of the coarse-graining process, and examine the limit as the coarse-graining size approaches zero. We show that this definition of the Gibbs entropy leads to a positive rate of irreversible entropy production for reversible dissipative systems. We apply the method to the case of a two-dimensional map, based upon a model considered by Vollmer, Tél, and Breymann, that is a deterministic version of a biased-random walk. We treat both volume-preserving and dissipative versions of the basic map, and make a comparison between the two cases. We discuss the ε-entropy production rate as a function of the size of the coarse-graining cells for these biased-random walks and, for an open system with flux boundary conditions, show regions of exponential growth and decay of the rate of entropy production as the size of the cells decreases. This work describes in some detail the relation between the results of Gaspard, those of of Tél, Vollmer, and Breymann, and those of Ruelle, on entropy production in various systems described by Anosov or Anosov-like maps.

KEY WORDS: Entropy production; thermostated systems; nonequilibrium stationary states; SRB measure; deterministic diffusion.

I. INTRODUCTION

Over the past few years, a great deal of attention has been devoted to the issues of entropy production in chaotic, thermostated systems subjected to

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[1] Department of Physics and Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742; e-mail: tmg@ipst.umd.edu, jrd@ipst.umd.edu.

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external fields.$^{(1-5)}$ Such systems are often used in molecular dynamics simulations of irreversible processes in fluids, such as shear flows, or diffusive flows. The external field is used to provide a mechanism to establish a flow in the system, and the thermostat maintains a constant kinetic or total energy in the system, and produces a non-equilibrium, stationary state. The presence of the thermostat is felt in the dynamics of the particles of the system, which becomes, in the usual configuration and momentum variables, at least, a non-Hamiltonian, non-symplectic system.$^{(6)}$ The theoretical analyses of these thermostated systems has led to very interesting and fruitful connections between chaotic dynamics, transport coefficients, and irreversible thermodynamics.$^{(7-16)}$

One of the results of this analysis is a relation between transport coefficients, such as the coefficient of shear viscosity or of diffusion, and the sum of all of the Lyapunov exponents of the system.$^{(3,\,10)}$ This sum, in contrast with that of a Hamiltonian, symplectic system, is not zero but is negative, and is proportional to the square of the external field strength, for small enough external fields. This connection is generally established by means of entropy production arguments, whereby two expressions for the irreversible entropy production in a thermostated system are set equal to each other. One of these expressions is just the usual relation between the irreversible entropy production per unit time, σ, and the fluxes, J_i and forces, X_i, in an irreversible process, given by

$$\sigma = \sum_i J_i X_i = \sum_{i,\,j} L_{ij} X_i X_j \tag{1}$$

Here we assumed that, for thermostated systems in small external fields, the fluxes, J_i, are related to the forces, X_j, through linear laws

$$J_i = \sum_j L_{ij} X_j \tag{2}$$

In Eqs. (1) and (2), the quantities L_{ij} are the Onsager coefficients, which are directly related to the transport coefficients, and are supposed to form a positive definite matrix, so that the entropy production per unit time is positive.$^{(17)}$ The other of these two expressions for the entropy production is rather problematic. Usually one considers the time derivative of the Gibbs entropy, S_G, for the thermostated system, given by

$$\frac{d}{dt} S_G(t) \equiv -\frac{d}{dt} \int d\Gamma\, \rho(\Gamma, t)[\ln \rho(\Gamma, t) - 1] \tag{3}$$

Here $\Gamma = (q_1,..., q_{Nd}, p_1,..., p_{Nd})$ is a point in the phase space of the system, and $\rho(\Gamma, t)$ is the phase space density of the system. Here the q_i, p_i, for $1 \leqslant i \leqslant Nd$, are the configuration and momentum variables of a system of N particles in d space dimensions. Because the system is no longer Hamiltonian, ρ no longer obeys the Liouville equation. However, ρ does obey a conservation equation of the form

$$\frac{\partial}{\partial t}\rho(\Gamma, t) = -\sum_i \left[\frac{\partial}{\partial q_i}(\dot{q}_i\rho(\Gamma, t)) + \frac{\partial}{\partial p_i}(\dot{p}_i\rho(\Gamma, t))\right] \tag{4}$$

with the usual "dot" notation for the time derivative of a dynamical variable. This conservation equation can also be expressed in terms of the total time derivative of $\rho(\Gamma, t)$ as

$$\frac{d\rho}{dt} = -\rho(\Gamma, t)\sum_i \left[\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i}\right] \tag{5}$$

We will use this form below.

As is well known, for a closed, Hamiltonian system, or one with periodic boundary conditions, the Gibbs entropy is constant in time, but for a thermostated system this is no longer true. Instead one finds, after using Eq. (5), and some partial integrations,$^{(3)}$ that

$$\frac{d}{dt}S_G(t) = \int d\Gamma\, \rho(\Gamma, t)\sum_i \left[\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i}\right] \tag{6}$$

Here we have assumed that the phase space distribution function vanishes at all boundaries in configuration and momentum space. For a Hamiltonian system, the right hand side of Eq. (6) vanishes, but for a thermostated system, the divergence of the phase space velocity is not zero. The right hand side of Eq. (6) is easily related to the sum of the Lyapunov exponents of the system, by the following argument. We write the phase space density $\rho(\Gamma, t)$ as

$$\rho(\Gamma, t) = \frac{\mathscr{N}}{\mathscr{V}(t)} \tag{7}$$

where $\mathscr{N}$ is a fixed number of members of the ensemble in a small phase space volume, $\mathscr{V}(t)$. It then follows from the conservation equation, Eq. (5), that

$$\frac{d\rho}{dt} = -\rho\sum_i \left[\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i}\right] = -\rho\,\frac{d\ln \mathscr{V}(t)}{dt} \tag{8}$$

Now the small phase space volume, $\mathscr{V}(t)$, changes with time as

$$\mathscr{V}(t) \simeq \mathscr{V}(0)\exp\left[t\sum_j \lambda_j\right] \tag{9}$$

where λ_j are the local Lyapunov exponents at the point in phase space where ρ is evaluated. It then follows immediately from Eqs. (5)–(9), that the rate of entropy production is given by

$$\frac{dS_G(t)}{dt} = \int d\Gamma\, \rho(\Gamma, t) \sum_j \lambda_j(\Gamma) = \sum_j \langle \lambda_j \rangle \tag{10}$$

and is negative whenever there is an average contraction of phase space volumes! A very similar argument, using the Frobenius–Perron equation, shows that this conclusion is also valid for maps as well as for flows. This circumstance makes it difficult to equate the positive entropy production from irreversible thermodynamics to the negative change in the Gibbs entropy.

This paradoxical situation is usually resolved in the literature,(3, 4, 16) by saying that the negative entropy production inside the system is compensated by a positive entropy production in the thermostat itself, so that the total entropy production per unit time of the [system + thermostat] is positive, or zero. One assumes that a non-equilibrium steady state is produced, eventually, in which the total entropy production in the [system + thermostat] is zero. Then the hypothetical (positive) entropy production in the thermostat is equated to the phenomenological (positive) entropy production, which produces the desired relation between the Lyapunov exponents and the transport coefficients. This procedure is not quite satisfactory for the following reasons:

(1) One expects from phenomenological arguments that the rate of change of the local entropy, $s(\vec{r})$, in a small region about a point $\vec{r}$ can be decomposed into a term that represents the entropy flow into or out of the region plus a term that represents the local irreversible entropy production within the region. For thermostated systems one would like to represent the entropy flow term as the sum of two pieces, one representing the flow of entropy from neighboring regions due to physical currents, and another term representing the flow of entropy to or from the thermostat.(18) This suggests that, for thermostated systems, the local entropy change should be written as

$$\frac{ds}{dt} = \frac{d_{th}s}{dt} + \frac{d_e s}{dt} + \frac{d_i s}{dt} \tag{11}$$

where the first term on the right hand side is identified with the local flow of entropy from the thermostat to the region. The second term, denoted by the subscript e, is the rate of flow of entropy into the region from its local environment, and the third term, denoted by the subscript i, is the local rate of irreversible entropy production in the region. In the analysis described in Eq. (6) for thermostated systems, the thermostat appears in the equations of motion for the particles as a sort of dynamical friction which depends upon the phase point of the particles, and not as a source of a physical current of particles, momentum or energy into or from the system at the boundaries. By using continuous distribution functions as described above, one finds a negative rate of change of the total Gibbs entropy for the system, and one assumes there is a compensating positive entropy flow to the thermostat. The positive rate of change in the thermostat is then identified with the irreversible entropy production required by the Second Law. In this approach however there is no clear indentification of a positive irreversible entropy production within the system. Instead, the total entropy change in the system is due to the. interaction with the thermostat, which lowers the entropy of the system, in effect, by reducing the phase space available to the system to a fractal attractor of lower information dimension than the phase space itself, as discussed below.

(2) This last remark points to fin additional, and perhaps deeper, problem with the analysis given in Eq. (6), especially as it is applied to a system in a non-equilibrium stationary state. If we think of the approach of a thermostated system to a non-equilibrium steady state, then it is not surprising that the Gibbs entropy for the system decreases with time. That is, let us think of a positive entropy production as a loss of information about the system, and a negative entropy production as a gain of information about the system. Since the thermostat has the effect of creating an attractor it phase space, as time goes on the phase point of the system gets closer and closer to the attractor.(7–9) Thus we learn more and more about the location of the phase point of the system as time increases, and this gain of information is reflected in a negative entropy change. However, as emphasized by by Breymann, Tél, and Vollmer(5) and by Gaspard,(19) this use of the Gibbs entropy supposes that we have some way to locate a phase point with arbitrary precision. Further, we have also assumed, in computing the rate of change of the Gibbs entropy, that the distribution function $\rho(\Gamma, t)$ is a differentiable function. While this may be true as the system evolves toward a steady state, it is no longer true in the steady state. Instead, for Anosov systems[2] with phase space contraction, the phase

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[2] As pointed out by Gallavotti and Cohen,(13) the assumption that the system be Anosov can be replaced by Anosov-like, which assumes that the flow be hyperbolic on a subset of the whole phase space that differs from it by a set of measure zero. For the purpose of this paper, the only property that we will require of Anosov-like systems is the existence of a generating partition, namely that the dynamics can be encoded in an unambiguous way by a sequence of symbols taken from a finite alphabet.

space distribution becomes a singular SRB measure on the attractor with a smooth distribution in the unstable directions and a fractal structure in the stable directions. This type of distribution precludes the use of the ordinary calculus of differentiable functions, and requires a more careful analysis of the entropy production in the steady state. Therefore one cannot use differentiable functions to describe the distribution function for the system in a non-equilibrium steady state, and the calculation leading to Eq. (6) is not correct.

Gaspard,(19) in a study of the entropy production in open, Hamiltonian systems, provided a method for analyzing the entropy production in a system with a phase space distribution function that is, properly speaking, a singular measure. He considered a two-dimensional multi-baker map, constructed so as to allow diffusion of non-interacting particles in one space dimension. He then placed a high density reservoir at one end of the multi-baker chain, and a low density reservoir at the other end of the chain. The map then sets up a steady state in which a non-uniform density profile is established along the chain, and the phase space distribution for a particle in the chain, in the infinite system limit, is a nowhere differentiable SRB measure, smooth in the unstable direction, but fractal in the stable direction, see also ref. 20. Since the properties of this SRB measure rule out the use of differentiable distribution functions, Gaspard constructed a so-called ε-entropy, which can be thought of as a kind of coarse grained entropy, appropriate for singular, non-differentiable measures, provided the rate of entropy production is reasonably insensitive to the size of the coarse graining regions. Further, this system has no thermostat, and there is a clear separation of the local ε-entropy change into a local ε-entropy flow and a local irreversible ε-entropy production. The latter is positive, and for large systems, it depends on the density gradient in a way that agrees precisely with the laws of irreversible thermodynamics.

Similarly, Vollmer *et al.*(18) considered a version of the multi-baker map which, though time reversible, is not volume preserving. They argued that their model has the same feature as one sees in thermostated systems, namely the contraction of the distribution function onto an attractor, and they used it to model the entropy production in a thermostated system. They considered the coarse grained entropy production in diffusive processes taking place in this system. Their analysis was based on a coarse graining procedure which uses larger coarse graining regions than that used by Gaspard,(19) but the results were very much the same. A positive production of the entropy was found and the form of this entropy production, in an appropriate macroscopic limit, agrees with the result one expects from nonequilibrium thermodynamics. Moreover, by comparing the results obtained for a volume preserving version of their model with those of the volume non-preserving version, they identified the effect of the thermostat on the rate of entropy production by looking at the difference between the rates of entropy production in the two versions.

What is perhaps most novel in tile work of Gaspard and of Vollmer *et al.* is the fact that one now has a firm physical and mathematical reason for the coarse graining, namely the existence of underlying singular measures in phase space. Fractal structures in phase space also appear as the support for physical measures for Hamiltonian systems as well. The proper treatment of these phase space measures requires.the use of coarse graining methods in more general cases than those considered here, of course. Moreover, in the proper description of many-particle systems, the use of coarse graining methods arise naturally when one goes from the Gibbs Γ-space description of the system, with a zero fine grained rate of entropy production, to the Boltzmann μ-space description involving reduced distribution functions.(21, 22) However it requires an understanding of the hyperbolic nature of the many-particle system, and the structures in phase space along stable and unstable directions to understand why the reduced distribution functions, themselves, approach their equilibrium values in time, with a positive generation of entropy in the process.(16)

To summarize: For both volume preserving systems driven out of equilibrium and volume non-preserving systems whose microscopic dynamics are described by Anosov-like systems, one should use a coarse grained entropy and entropy production to properly describe the system in a non-equilibrium steady state, since the distribution function is not smooth on any scale, no matter how fine. The use of a coarse grained entropy automatically involves a loss of information about the system since there is always a level of detail about the system which is inaccessible to the coarse grained description. This loss of information can then be identified with a positive irreversible entropy production. In the examples studied so far, this positive entropy production agrees, in the proper limit, with the predictions of irreversible thermodynamics. This agreement is ultimately the chief requirement of any microscopic definition of entropy production. Once one has a good microscopic definition of the rate of entropy production in a thermostated system, one can then try to identify the various terms In Eq. (11) with their microscopic counterparts. We are then provided with a means to identify the role of the thermostat in the production of entropy of the system.

The purpose of this paper is to present a unified view of positive entropy production in both reversible, volume preserving find in reversible, volume "contracting" maps, which are time-discretized-versions of thermostated dynamical systems. This paper can be considered to be a commentary upon and elaboration of work by Gaspard(19) and by Vollmer, Tél and Breymann.$^{(18)}$ What is new here is the observation that Gaspard's ε-entropy procedure, when generalized appropriately, can be usefully applied to both Hamiltonian and thermostated systems, and that for the latter systems, there is much to be gained by a study of the effects of coarse graining on arbitrarily fine scales. In particular, we are able to relate the rate of irreversible entropy production to the difference of the entropies at two levels of resolution of the phase space, (see Eq. (30)), and for simple models we can explicitly evaluate the entropy production as a function of the level of resolution of the coarse graining procedure. Moreover, by carefully studying the effects of different levels of resolution, we can review and refine the relations described above between entropy production, Lyapunov exponents, and transport coefficients. This will allow us to make contact with recent work of Chernov *et al.*$^{(3)}$ and Ruelle,$^{(4)}$ establishing rigorous results on the rate of entropy production in thermostated systems. Vollmer, Tél, and Breymann$^{(23)}$ have recently done related and complementary work on the effects of coarse graining in multi-baker models and on the relation of their work with that of Gaspard, Chernov *et al.*, and Ruelle. However, they do not look at the effects of making the coarse graining cells arbitrarily small, as we do here. We should also mention that while our work here does shed some further light on the nature of irreversible entropy production in simple thermostated systems, it does not answer a host of questions about the nature of entropy production in the more general setting of a many particle system with a large number of degrees of freedom. For such systems our results may be relevant for examining the rate of entropy production when the phase space distribution is projected onto a subspace of a few relevant variables.

In the next section, we define a coarse grained, local entropy which is extensive and depends upon both the measure and the volume of each of the coarse graining regions in phase space. In Section III we describe the rate of change of this coarse grained entropy in a nonequilibrium stationary state. We show that the rate of change of this local entropy is in fact zero in the steady state, but that it can be further decomposed in a way that is consistent with Eq. (11) for dynamical systems with generating partitions, such as a Markov partition. In particular, this applies to those systems that satisfy Gallavotti and Cohen's chaotic hypothesis.$^{(13)}$ For systems where there is no flow of particles through the boundaries, and the distribution function vanishes at the boundaries, we derive, in Section IV, a positive irreversible entropy production rate which is equal to the phase space contraction rate, in agreement with Chernov *et al.*$^{(3)}$ and Ruelle.$^{(4)}$

The general method discussed here is then applied to both volume preserving and volume contracting multi-baker chains, which represent deterministic models of biased random walks on a line. We show, in particular, that our definition of the entropy production leads to results consistent with those of Gaspard,(19) and with Vollmer *et al.*,(18) which we generalize to arbitrary resolution parameters. In particular, we show that, in its leading order, the entropy production rate for these maps increases exponentially as a function of the resolution parameter for a range of resolution parameters, and then, as the finite size effects start to interfere, falls exponentially to zero as the resolution gets finer and finer. We conclude with a discussion of a number of points raised by this work.

II. GIBBS ENTROPY FOR CONTRACTING SYSTEMS

We begin by considering a dynamical system defined by a map Φ on a phase space X with invariant measure μ. As discussed above, the Gibbs entropy for this system, if it were to be well-defined, would be given by Eq. (3), as

$$S_G = -\int_X d\Gamma\, \rho(\Gamma)[\ln(\rho(\Gamma)) - 1] \tag{12}$$

where the phase space density, $\rho(\Gamma)$, at a point Γ, would be the derivative of the measure of a small region about Γ,

$$\rho(\Gamma) = \frac{d\mu(\Gamma)}{d\Gamma} \tag{13}$$

That is, ρ would be the density of μ, formally the Radon–Nikodym derivative of μ with respect to the Liouville measure in phase space. However, as noted above, we must be cautious here, since the existence of a phase space density is only guaranteed for measures that are absolutely continuous with respect to the Liouville measure. In particular, reversible systems in nonequilibrium steady states do not usually satisfy this requirement, especially, but not exclusively, if the system is dissipative with a contraction of phase space volumes. Therefore we cannot define the Gibbs entropy as in Eq. (12). Rather, we should define it as

$$S_G = -\int_X \mu(d\Gamma) \left[\ln \frac{\mu(d\Gamma)}{d\Gamma} - 1 \right] \tag{14}$$

To give this expression a clear meaning, we assume that our dynamical system admits a *generating partition* $\mathscr{A}$ (see for instance ref. 24) and define the (l, k)-partition $\mathscr{A}_{l,k}$ as

$$\mathscr{A}_{l,k} = \Phi^{-l}(\mathscr{A}) \vee \Phi^{-l+1}(\mathscr{A}) \vee \cdots \vee \Phi^{-1}(\mathscr{A}) \vee \mathscr{A} \vee \Phi(\mathscr{A}) \vee \cdots \vee \Phi^{k-2}(\mathscr{A}) \vee \Phi^{k-1}(\mathscr{A})$$

That is, we suppose that there is some partition, $\mathscr{A}$ of the phase space into small, disjoint sets. We then consider forward iterations of these sets, which we denote by $\Phi^{j}(\mathscr{A})$, and backward iterations, which we denote by $\Phi^{-j}(\mathscr{A})$. The collection of very many sets denoted by $\mathscr{A}_{l,k}$ above is obtained by taking all possible intersections of the sets generated by iterating $\mathscr{A}$ forward in time over $k-1$ steps and backwards in time by l steps. Here we use the standard $\vee$ notation for indicating a partitioning of sets into the collection of all the possible intersections of all the indicated sets. For an element A of $\mathscr{A}_{l,k}$, we further define the corresponding volume

$$v(A) = \int_X d\Gamma\, \chi_A(\Gamma) \tag{15}$$

where

$$\chi_A(\Gamma) = \begin{cases} 1, & \Gamma \in A \\ 0 & \text{otherwise} \end{cases}$$

is the characteristic function of A.

We now define the (l, k)-entropy of the triplet (X, Φ, μ), with respect to the measures and volumes of the elements of this partition, by

$$S_{l,k}(X) = -\sum_{A \in \mathscr{A}_{l,k}} \mu(A) \left[\log \frac{\mu(A)}{v(A)} - 1 \right] \tag{16}$$

where $\mu(A)$ is the steady state SRB measure of the set A. With our assumption that the partition $\mathscr{A}$ be generating; the elements of $\mathscr{A}_{l,k}$ shrink to points in the limit when both $l, k \to \infty$. Hence

$$\lim_{l,k \to \infty} S_{l,k} = S_G \tag{17}$$

as defined in Eq. (14). That is, we construct an *extensive* entropy for a particular refinement of our generating partition, and then define the Gibbs entropy to be the limit of the entropy, as the sets of the partition become more and more refined. From a physical point of view, it is expected that the limit in Eq. (17) be independent of the choice of the partition, and this will indeed be the case for the case of a generating partition. In many cases, including those discussed here, the limit in Eq. (17) is negative infinity, since the measure of a set typically decreases more slowly than its volume as the coarse graining cells become small. This occurs whenever the SRB measure is not absolutely continuous with respect to the Lebesgue measure, and the information dimension of the sets are smaller than their phase space dimension.[3] However, we will see subsequently that the rate of entropy production remains well defined as the coarse graining size approaches zero.

There is a subtle limiting procedure being carried out here, that we wish to explain in more detail. If we allow the system to reach a non-equilibrium steady state, we can imagine that the measure μ is an SRB measure which does not have a well defined density. However the measure and the volume of the elements of the partition are well defined, as is the entropy function $S_{l,k}$, for all $l, k > 0$. However, in the conventional approach to the Gibbs entropy for phase space distributions, one always assumes that the phase space density is well defined, in effect, assuming that the limit of an infinitesimally fine partition can be taken *before* the limit $t \to \infty$, and that any non-equilibrium quantity based on that will be well defined in the non-equilibrium stationary state. The exchange of limiting processes is an essential feature of the correct treatment of entropy production in non-equilibrium steady states.

Consider, now, a region B of X whose borders coincide with the borders of some elements of $\mathscr{A}_{l'k'}$, for some l' and k'. For all $l > l'$ and $k > k'$, we *define* the (l, k)-entropy of $B \subset X$ with respect to μ by

$$S_{l,k}(B) = -\sum_{A \in \mathscr{A}_{l,k} \cap B} \mu(A) \left[\log \frac{\mu(A)}{\nu(A)} - 1 \right] \tag{18}$$

In the next section, we derive the (l, k)-entropy change in a time dependent picture and compare it to Eq. (11) in order to identify the various terms in the rate of change of the local entropy.

III. COARSE GRAINED ENTROPY CHANGE

In a time dependent picture, the evolution of the density ρ_t is given by the action of the Frobenius–Perron operator, $\mathscr{P}$. For an invertible map Φ, we have

$$\rho_{t+1}(\Gamma) = \mathscr{P}\rho_t(\Gamma) = \left| \frac{d}{d\Gamma} \Phi^{-1}(\Gamma) \right| \rho_t(\Phi^{-1}(\Gamma)) \tag{19}$$

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[3] We are indebted to P. Gaspard for this observation.

where the derivative in the third term indicates the Jacobian of $\Phi^{-1}(\Gamma)$ with respect to Γ. Since the quantity ρ_t is well defined for finite t, we will use it to construct the measures needed for the computation of the entropy, $S_{l,k}(B)$, and entropy changes. The idea is to express the quantity $\mu(A)/\nu(A)$ appearing in the logarithm on the right hand side of Eq. (18) as a coarse grained density by means of the relation

$$\frac{\mu_t(A)}{\nu(A)} = \bar{\rho}_t(A) \equiv \frac{1}{\nu(A)} \int_A \rho_t(\Gamma)\, d\Gamma \tag{20}$$

Let us now apply the Frobenius–Perron equation to the evolution of a coarse grained density $\bar{\rho}_t(A)$ of some set A. Using Eq. (19), we have

$$\begin{aligned}\bar{\rho}_{t+1}(A) &\equiv \frac{1}{\nu(A)} \int_A \rho_{t+1}(\Gamma)\, d\Gamma \\ &= \frac{1}{\nu(A)} \int_A \left| \frac{d}{d\Gamma} \Phi^{-1}(\Gamma) \right| \rho_t(\Phi^{-1}(\Gamma))\, d\Gamma \\ &= \frac{1}{\nu(A)} \int_{\Phi^{-1}(A)} \rho_t(\Gamma)\, d\Gamma \\ &= \frac{1}{\nu(A)} \mu_t(\Phi^{-1}(A))\end{aligned} \tag{21}$$

Note that the definition of the measure $\mu_t(A)$, together with the Frobenius–Perron equation implies that

$$\mu_{t+1}(A) = \mu_t(\Phi^{-1}(A)) \tag{22}$$

Now consider a region B such as discussed earlier. The change of the (l, k)-entropy of B at time t is given by

$$\widetilde{\Delta S}_{l,k}(B, t) = S_{l,k}(B, t+1) - S_{l,k}(B, t) \tag{23}$$

That is, $\widetilde{\Delta S}_{l,k}(B, t)$ is the entropy change of B with respect to the (l, k)-partition. Then making use of Eqs. (20) and (21), we find

$$\begin{aligned}\widetilde{\Delta S}_{l,k}(B, t) &= \sum_{A \in \mathscr{A}_{l,k} \cap B} \left[-\mu_{t+1}(A) \log \bar{\rho}_{t+1}(A) + \mu_t(A) \log \bar{\rho}_t(A) \right] \\ &= \sum_{A \in \mathscr{A}_{l,k} \cap B} \left[-\mu_t(\Phi^{-1}(A)) \log \frac{\mu_t(\Phi^{-1}(A))}{\nu(A)} + \mu_t(A) \log \frac{\mu_t(A)}{\nu(A)} \right]\end{aligned} \tag{24}$$

We now have an expression for the time dependent change in the coarse grained entropy of some set B in phase space. Suppose we keep the (l, k)-partition fixed but consider the limit $t \to \infty$. If the system reaches a nonequilibrium steady state, then we can expect that the limit

$$\lim_{t \to \infty} \mu_t(A) = \mu(A) \tag{25}$$

will exist for all sets, A, of the partition, and that the measure will be invariant in the stationary state where $\mu(A) = \mu(\Phi^{-1}(A))$, as implied by Eq. (22). But in this case, the entropy change defined above is zero for an invariant measure, i.e.,

$$\widetilde{\Delta S}_{l,k}(B) = 0 \tag{26}$$

Thus we have defined a coarse grained entropy which has a zero rate of change in the nonequilibrium steady state. We now have to decompose it into the three contributions required by Eq. (11). We first consider the time dependent case and then specialize to the case of a steady state with an invariant measure.

First, we define the rate of (l, k)-entropy *flow* into the set B at time t, $\Delta_e S_{l,k}(B, t)$, by taking the difference between the (l, k)-entropy of the pre-image of B, which we take to be the entropy of set B after the next time step, and the (l, k)-entropy of B, itself. That is, there is no contribution to the *flow* of entropy into B from the set of points which are in B at both t and $t+1$. Thus, the rate of (l, k)-entropy flow of B is defined to be

$$\Delta_e S_{l,k}(B, t) = S_{l,k}(\Phi^{-1}(B), t) - S_{l,k}(B, t) \tag{27}$$

Next we can define the flow of entropy into the set B due to the presence of the thermostat, $\Delta_{th} S_{l,k}(B, t)$. Since the thermostat is modelled by adding frictional terms to the equations of motion of the points and not by any boundary conditions, we have no means of identifying the action of the thermostat other than by the change in the volume of sets in the course of their time evolution. This change in volume is produced by the frictional terms added to the equations of motion. A reasonable definition of $\Delta_{th} S_{l,k}(B)$ should satisfy the requirement that this entropy flow vanishes if the transformation Φ is volume preserving. This condition is satisfied by *defining* the flow of entropy into B due to the presence of the thermostat by

$$\begin{aligned} \Delta_{th} S_{l,k}(B, t) &= S_{l,k}(B, t+1) - S_{l+1,k-1}(\Phi^{-1}(B), t) \\ &= -\sum_{A \in \mathscr{A}_{l,k} \cap B} \mu_t(\Phi^{-1}(A)) \log \frac{\nu(\Phi^{-1}(A))}{\nu(A)} \end{aligned} \tag{28}$$

To obtain the second line in Eq. (28), we have used Eq. (22), and the fact that the preimages of sets in $\mathscr{A}_{l,k}$ are sets in $\mathscr{A}_{l+1,k-1}$. We call attention to the fact that the pre-images of the sets in a (l, k)-partition are sets in a $(l+1, k-1)$-partition. We have defined $\Delta_{th} S_{l,k}(B)$ as the difference between the entropy of the set B at time $t+1$, and the entropy of the preimage of B at time t, where the entropy of the pre-image sets of B are calculated using the pre-image of the (l, k) partition. This definition of the flow of entropy from the thermostat to the set B satisfies the requirement that it vanishes for a volume preserving transformation. The definition of $\Delta_{th} S_{l,k}(B, t)$ given above suffers from the lack of a clear derivation based upon a physical picture of a thermostat, as one would expect for a thermostat which acts only at the boundary of the system. Here the thermostat is an "internal" device which has the effect of modifying the equations of motion and produces a contraction of phase space volumes. Thus our definition of entropy flow to the system from the thermostat must be based on the change of the volumes of cells in phase space with time, as is done in our definition above.

We now want to follow the phenomenological approach as in Eq. (11) and write

$$\widetilde{\Delta S}_{l,k}(B, t) = \Delta_e S_{l,k}(B, t) + \Delta_{th} S_{l,k}(B, t) + \Delta_i S_{l,k}(B, t) \tag{29}$$

where $\Delta_i S_{l,k}(B, t)$ represents the rate of irreversible entropy production in B. By combining Eqs. (29), with Eqs. (27) and (28), we obtain an expression for the irreversible entropy production in set B as

$$\Delta_i S_{l,k}(B, t) = S_{l+1,k-1}(\Phi^{-1}(B), t) - S_{l,k}(\Phi^{-1}(B), t) \tag{30}$$

Note that this equation represents the irreversible entropy production in any set B as the difference in the entropy of the pre-image sets at two levels of resolution. This is an important result which helps us to understand that irreversible entropy production is a direct result of the loss of information in the coarse graining of a system.

Therefore, we have been able to use the phenomenological approach to entropy production, Eq. (11) and some reasonable definitions of entropy flows to obtain an expression for the local rate of irreversible entropy production.

We can easily connect these definitions to that of Gaspard$^{(19)}$ for the entropy production in a Hamiltonian system, by defining an *intrinsic* local rate of entropy change in the set B, $S_{l,k}(B, t)$, by removing the term due to the thermostat as

$$\begin{aligned} \Delta S_{l,k}(B, t) &= \widetilde{\Delta S}_{l,k}(B, t) - \Delta_{th} S_{l,k}(B, t) \\ &= S_{l+1,k-1}(\Phi^{-1}(B), t) - S_{l,k}(B, t) \end{aligned} \tag{31}$$

That is, we have expressed the intrinsic rate of change of the coarse grained entropy of B as the difference between the $(l+1, k-1)$-entropy of the pre-image of B and the (l, k)-entropy of B itself. This expression is identical with the definition of the change in the coarse grained entropy given by Gaspard.(19) Note that in a non-equilibrium steady state, where $\widetilde{\Delta S}_{l,k}(B)=0$, the rate of change of this intrinsic entropy is equal to the rate of flow of entropy from the system to the thermostat, $-\Delta_{th} S_{l,k}(B)$, which as we will see below is positive if there is an average contaction of the phase space accessible to the system on to an attractor.

IV. (l, k)-ENTROPY CHANGE AND PHASE SPACE CONTRACTION

It is important to note that in the steady state, the measure $\mu(A)$ of a set A is invariant, i.e., $\mu(\Phi^{-1}(A))=\mu(A)$. Now, even though the measure $\mu(A)$ of a set A is invariant, the various terms in the rate of entropy production may not be zero because the phase space volumes of the elements of the partition are not equal to the volumes of their pre-image sets. Thus, using the fact that the pre-images of sets in $\mathscr{A}_{l,k}$ are sets in $\mathscr{A}_{l+1,k-1}$, we find that the intrinsic rate of entropy change, $\Delta S_{l,k}(B)$, Eq. (31), becomes

$$\begin{aligned}\Delta S_{l,k}(B) &= S_{l+1,k-1}(\Phi^{-1}(B)) - S_{l,k}(B)\\ &= -\sum_{A\in\mathscr{A}_{l,k}\cap B}\left[\mu(\Phi^{-1}(A))\ln\frac{\mu(\Phi^{-1}(A))}{\nu(\Phi^{-1}(A))}-\mu(A)\ln\frac{\mu(A)}{\nu(A)}\right]\end{aligned} \tag{32}$$

Using the invariance of the measure, we have

$$\Delta S_{l,k}(B)=\sum_{A\in\mathscr{A}_{l,k}\cap B}\mu(A)\ln\frac{\nu(\Phi^{-1}(A))}{\nu(A)} \tag{33}$$

as noted at the end of the previous section.

We also have an expression for the volume of the pre-image sets in terms of the Jacobian, $J(\Phi^{-1}(\Gamma))\equiv|d\Gamma/d\Phi^{-1}(\Gamma)|$, of the transformation

$$\begin{aligned}\nu(\Phi^{-1}(A)) &= \int_{\Phi^{-1}(A)} d\Gamma\\ &= \int_A \frac{d\Gamma}{J(\Phi^{-1}(\Gamma))}\\ &= \frac{1}{J(\Phi^{-1}(\Gamma_A))}\,\nu(A)\end{aligned} \tag{34}$$

where we the last line then follows from the mean value theorem and Γ_A denotes an appropriate point in A.

Thus

$$\Delta S_{l,k}(B) = \sum_{A \in \mathscr{A}_{l,k} \cap B} \mu(A) \ln \frac{1}{J(\Phi^{-1}(\Gamma_A))} \tag{35}$$

In the limit where $l, k \to \infty$ the sum becomes an integral over phase space and we find

$$\lim_{l,k \to \infty} \Delta S_{l,k}(B) = \int_{\Phi^{-1}(B)} \mu(d\Gamma) \ln \frac{1}{J(\Gamma)} \tag{36}$$

Up to a sign change, this result, or, more precisely, its generalization given below, forms the starting point for Ruelle's analysis of the entropy production for diffeomorphisms.$^{(4)}$ The sign difference is due to Ruelle's starting with the argument that the negative change in the Gibbs entropy of the thermostated system is compensated by a positive entropy production. Here we avoid that procedure and see that it is possible to define a coarse grained entropy which has a positive rate of change for the system itself.

We are now in a position to prove our main result, i.e., that the intrinsic rate of change of the entropy defined by Eq. (31) is positive and equals the phase space contraction rate, for a closed, thermostated system. To do this, we identify the set B with the entire phase space, X, and notice that, because the system is closed, there is no flow of entropy into or out of the system so that $\Delta_e S_{l,k}(X)$ vanishes. We can thus identify the rate of change of the, now well defined, Gibbs entropy as the irreversible entropy production in the system, and it is given as

$$\begin{aligned} \Delta_i S_G = \lim_{l,k \to \infty} \Delta S_{l,k}(X) &= \int_X \mu(d\Gamma) \ln \frac{1}{J(\Gamma)} \\ &= -\sum_i \lambda_i \end{aligned} \tag{37}$$

where the integral in the first line of Eq. (37) defines the sum over all of the Lyapunov exponents of the system. Ruelle has proved that this quantity is positive if the map is a diffeomorphism, and μ an SRB measure on X, singular with respect to the Liouville measure.

This result shows that, for a contracting system for which the sum of the Lyapunov exponents is negative, the stationary state intrinsic entropy change, as defined in Eq. (31), is positive. It is in exact agreement with what one expects for the stationary state entropy production rate in these systems. Moreover, it clarifies the paradox, discussed earlier, that the "fine grained" Gibbs entropy yields negative stationary state entropy change rate.(3, 4, 8, 16)

In the next sections, we will use the construction of the (l, k)-entropy given above to compute the (l, k)-entropy flow and irreversible entropy production for two specific cases and show how our formalism corresponds to the results previously obtained by Gaspard(19) for Hamiltonian-like, volume preserving maps, and those of Vollmer, Tél and Breymann(18) for dissipative, volume contracting maps, for open systems with diffusive flows.

V. A DETERMINISTIC BIASED RANDOM WALK

We consider a one-dimensional random walk on a lattice where a particle hops with probability s (resp. $1-s$) to the right (resp. left). The diffusion coefficient for this process can be computed from the Green–Kubo formula, see for instance ref. 16,

$$D = \lim_{T\to\infty} \frac{\langle (x_T - \langle x_T \rangle)^2 \rangle}{2T} = 2s(1-s) \tag{38}$$

where x_T denotes the displacement of a random walker after T time steps. We can also compute the mean drift velocity of this process,

$$v = 1 - 2s \tag{39}$$

measured positively towards the left direction.

A reversible deterministic model of this process is the generalized multi-baker chain defined on the "phase space"[4] $\mathbf{Z} \times [0, 1]^2$, consisting of a horizontal chain of unit squares. A phase point is labelled by an interger index $n \in \mathbf{Z}$ and by internal coordinates (x, y) within a unit square. The dynamics of this multi-baker map is given by

$$\Phi(n, (x, y)) = \begin{cases} \left(n+1, \left(\dfrac{x}{s}, sy\right)\right), & 0 \leqslant x < s \\ \left(n-1, \left(\dfrac{x-s}{1-s}, s + (1-s)\, y\right)\right), & s \leqslant x < 1 \end{cases} \tag{40}$$

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[4] In practice, and for the sake of definiteness of the measure, we will restrict the map to a finite region $\mathscr{L} \in \mathbf{Z}$ and will specify some boundary conditions.

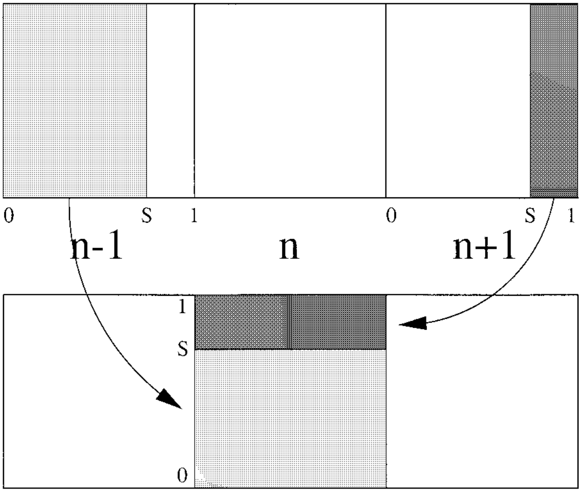

Fig. 1. The volume preserving, deterministic version of the biased random walk, Φ, defined by Eq. (40).

See Fig. 1. This map is volume preserving. If we specifically use periodic boundary conditions and allow no escape of particles from the system, it is easy to show that the two Lyapunov exponents for this map are

$$\lambda_+ = -\lambda_- = -s \ln s - (1-s) \ln(1-s) \tag{41}$$

Notice that for the volume preserving, closed system, the sum of the Lyapunov exponents is zero.

Alternatively, we can think of the bias in the random walk as being driven by the action of some external field and model this driven process by a map that is not area preserving.(18) This would then be a time-discretized model that has features similar to those of a system in an external field with an energy preserving thermostat. That is, as pointed out by Vollmer *et al.*(18) one hopes to capture in this model, the effects of a dynamics that contracts, on the average, volumes in phase space. We thus let

$$\Phi_c(n, (x, y)) = \begin{cases} \left(n+1, \left(\dfrac{x}{s}, (1-s)\, y\right)\right), & 0 \leqslant x < s \\ \left(n-1, \left(\dfrac{x-s}{1-s}, 1-s+sy\right)\right), & s \leqslant x < 1 \end{cases} \tag{42}$$

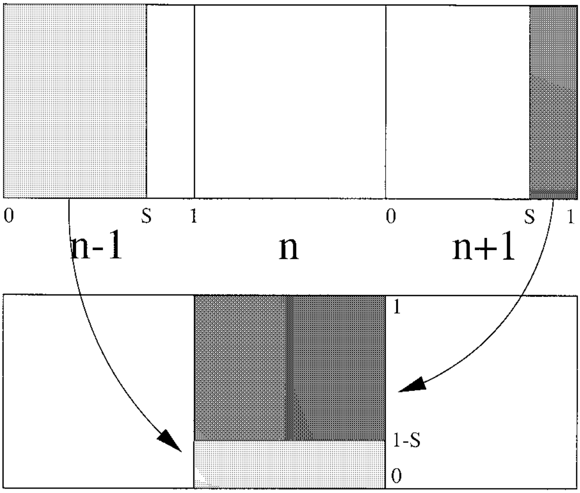

Fig. 2. The dissipative, deterministic version of the biased random walk, Φ_c, defined by Eq. (42).

See Fig. 2. The phase space volumes are not locally preserved and the periodic version of this map has two Lyapunov exponents

$$\begin{aligned}\lambda_+ &= -s \ln s - (1-s)\ln(1-s)\\ \lambda_- &= s\ln(1-s) + (1-s)\ln s\end{aligned} \tag{43}$$

The negative of the sum of the Lyapunov exponents,

$$-(\lambda_+ + \lambda_-) = (2s-1)\ln\frac{s}{1-s} > 0 \tag{44}$$

is the phase space contraction rate. In the following discussions, we consider both of these maps and will make explicit distinctions when appropriate. When we wish to refer to the two maps without distinguishing between them, we will use the notation $\Phi_{(c)}$ for the maps.

For either case, we denote by μ_n the cumulative, or total, measure of the nth unit square. Using the Perron–Frobenius equation or other methods,(19, 20) one can easily see that for either version of the map, $\Phi_{(c)}$, the stationary measure of the chain satisfies the equation

$$\mu_n = s\mu_{n-1} + (1-s)\,\mu_{n+1} \tag{45}$$

The solution of this equation is easily found to be

$$\mu_n = A\alpha^n + B \tag{46}$$

where $\alpha = s/(1-s)$ and A and B are fixed by the boundary conditions.

VI. (l, k)-ENTROPY AND ENTROPY PRODUCTION RATE FOR MULTIBAKERS

We now follow the procedure outlined in Section II, and construct the (l, k)-partitions, and entropies of the maps $\Phi_{(c)}$.

The (l, k)-partition is a collection of 2^{l+k} non intersecting rectangles that cover each of the unit squares in the chain, with an identical covering for each square. Then for each square, the number of elements along a line in the expanding direction is 2^l, and 2^k is the number of those along the contracting direction. To make this more precise, we introduce a symbolic dynamics on the squares. Let us consider one particular square and notice that any (l, k)-partition of that square is generated by images or pre-images of the two sets

$$\Gamma(0) = \{(x, y) \mid 0 \leqslant y < s\}$$

$$\Gamma(1) = \{(x, y) \mid s \leqslant y < 1\}$$

for the case of Φ, (40), and

$$\Gamma_c(0) = \{(x, y) \mid 0 \leqslant y < 1 - s\}$$

$$\Gamma_c(1) = \{(x, y) \mid 1 - s \leqslant y < 1\}$$

for the case of Φ_c, ref. 42.[5]

An (l, k)-set, $\Gamma(\omega_{-l}, ..., \omega_{k-1})$ with $\omega_j \in \{0, 1\}$, $j = -l, ..., k-1$, is the set of points (x, y) such that (regardless of the lattice coordinate)

$$\Phi^{-j}(x, y) \in \Gamma(\omega_j), \; j = -l, ..., k-1$$

---

[5] Following the notations introduced earlier, we have

$$\mathscr{A} = \{\Gamma_{(c)}(n, \omega_n), n \in \mathscr{L}, \omega_n \in \{0, 1\}\}$$

where we indexed the elements of the partition by the square n they belong to. $\mathscr{A}_{l,k}$ can be generated by taking images and pre-images of this partition. However, in order for us not to worry at this point about technicalities involving the boundary conditions, we will find it more convenient to define the (l, k)-partition by iterations of local maps, i.e., dropping the index n for that purpose.

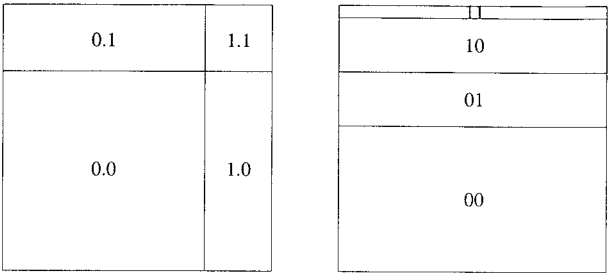

Fig. 3. The (1, 1) and (0, 2)-sets of Φ. The dots indicate the separation between the indices l and k.

Notice also that

$$\Phi^{-1}\Gamma(\omega_{-l},\ldots,\omega_{k-1}) = \Gamma(\omega'_{-l-1},\ldots,\omega'_{k-2}) \tag{47}$$

with $\omega'_j = \omega_{j+1}$,. This expresses the conjugation between Φ and the shift operator on symbolic sequences. We define $\Gamma_c(\omega_{-l},\ldots,\omega_{k-1})$ in a similar way and with the same property. As examples, Figs. 3 and 4 show the (1, 1) and (0, 2)-sets of Φ and Φ_c, respectively.

We will use the notation $\mu_n(\omega_{-l},\ldots,\omega_{k-1})$ to designate the measure of the corresponding (l, k)-set of cell n irrespective of which map is being considered. We will further denote the volume of the corresponding sets by $v(\Gamma(\omega_{-l},\ldots,\omega_{k-1}))$ and $v(\Gamma_c(\omega_{-l},\ldots,\omega_{k-1}))$ and will use the notation $v(\omega_{-l},\ldots,\omega_{k-1})$ when we want to avoid referring to a specific choice of map. We have

$$\begin{aligned} v(\Gamma(\omega_{-l},\ldots,\omega_{k-1})) &= \prod_{j=-l}^{k-1} v(\omega_j) \\ v(\Gamma_c(\omega_{-l},\ldots,\omega_{k-1})) &= \prod_{j=-l}^{-1} v(\omega_j) \prod_{j=0}^{k-1} v^*(\omega_j) \end{aligned} \tag{48}$$

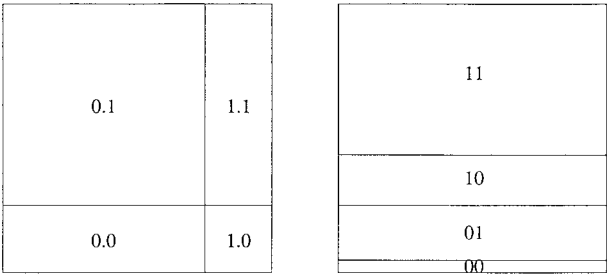

Fig. 4. The (1, 1) and (0, 2)-sets of Φ_c. The dots indicate the separation between the indices l and k.

where

$$\nu(\omega_j) = \begin{cases} s, & \omega_j = 0 \\ 1 - s, & \omega_j = 1 \end{cases} \tag{49}$$

and

$$\nu^*(\omega_j) = \begin{cases} 1 - s, & \omega_j = 0 \\ s, & \omega_j = 1 \end{cases} \tag{50}$$

We now proceed to evaluate the (l, k)-entropy of a site n given by

$$S_{l,k}(n) = -\sum_{\omega_{-l},\dots,\omega_{k-1}} \mu_n(\omega_{-l},\dots,\omega_{k-1}) \left[\ln \frac{\mu_n(\omega_{-l},\dots,\omega_{k-1})}{\nu(\omega_{-l},\dots,\omega_{k-1})} - 1 \right] \tag{51}$$

Notice that this is just the coarse grained version of the Gibbs entropy, defined by Eq. (18) where the set B is now the unit square representing the site n. From now on, we will drop the constant term in the expression (51) of the (l, k)-entropy. As discussed in the Appendix A, the stationary state measure is uniform along the x, or expanding, direction. From this it follows that the entropy is extensive with respect to the x-direction. Thus,

$$S_{l,k}(n) = S_{0,k}(n) \tag{52}$$

and we are allowed to drop the l dependence. When appropriate, we will simply refer to the k-entropy of n and write $S_k(n)$.

To derive the (l, k)-entropy production rate, use Gaspard's method$^{(19)}$ and write the rate of intrisic entropy change as the sum of an entropy flow and an irreversible entropy production, as in Eq. (31).

To compute the rate of change in entropy, we notice from Eq. (47) that the pre-image of an (l, k)-set is an $(l+1, k-1)$-set. Thus as in the more general case discussed earlier,

$$\Delta S_{l,k}(n) = S_{l+1,k-1}(\Phi_{(c)}^{-1}(n)) - S_{l,k}(n) \tag{53}$$

Let us take $l = 0$. The first term on the RHS is then

$$\begin{aligned} S_{1,k-1}(\Phi_{(c)}^{-1}(n)) = -\sum_{\omega_0,\dots,\omega_{k-2}} \Bigg[& \mu_{n-1}(0, \omega_0,\dots,\omega_{k-2}) \ln \frac{\mu_{n-1}(0, \omega_0,\dots,\omega_{k-2})}{\nu(0, \omega_0,\dots,\omega_{k-2})} \\ & + \mu_{n+1}(1, \omega_0,\dots,\omega_{k-2}) \ln \frac{\mu_{n+1}(1, \omega_0,\dots,\omega_{k-2})}{\nu(1, \omega_0,\dots,\omega_{k-2})} \Bigg] \end{aligned} \tag{54}$$

But, from Eq. (48), we know that the measures and volumes appearing in the above equation are given by

$$\begin{aligned}
\mu_{n-1}(0, \omega_0, ..., \omega_{k-2}) &= s\mu_{n-1}(\omega_0, ..., \omega_{k-2})\\
\mu_{n+1}(1, \omega_0, ..., \omega_{k-2}) &= (1-s)\, \mu_{n+1}(\omega_0, ..., \omega_{k-2})\\
\nu(0, \omega_0, ..., \omega_{k-2}) &= s\nu(\omega_0, ..., \omega_{k-2})\\
\nu(1, \omega_0, ..., \omega_{k-2}) &= (1-s)\, \nu(\omega_0, ..., \omega_{k-2})
\end{aligned} \tag{55}$$

We can thus rewrite Eq. (54) as

$$\begin{aligned}
S_{1,k-1}(\Phi_{(c)}^{-1}(n)) = -\sum_{\omega_0, ..., \omega_{k-2}} \Bigg[& s\mu_{n-1}(\omega_0, ..., \omega_{k-2}) \ln \frac{\mu_{n-1}(\omega_0, ..., \omega_{k-2})}{\nu(\omega_0, ..., \omega_{k-2})}\\
& + (1-s)\, \mu_{n+1}(\omega_0, ..., \omega_{k-2}) \ln \frac{\mu_{n+1}(\omega_0, ..., \omega_{k-2})}{\nu(\omega_0, ..., \omega_{k-2})} \Bigg]\\
= {} & sS_{0,k-1}(n-1) + (1-s)\, S_{0,k-1}(n+1)
\end{aligned} \tag{56}$$

By making use of Eq. (52), we conclude that the rate of entropy change at site n satisfies the simple difference equation

$$\Delta S_k(n) = sS_{k-1}(n-1) + (1-s)\, S_{k-1}(n+1) - S_k(n) \tag{57}$$

We now consider the contributions to this entropy change from the entropy flow and the irreversible entropy production. The entropy flow rate is given by

$$\Delta_e S_{l,k}(n) = S_{l,k}(\Phi_{(c)}^{-1}(n)) - S_{l,k}(n)$$

By the same argument as above,

$$S_{1,k}(\Phi_{(c)}^{-1}(n)) = sS_{0,k}(n-1) + (1-s)\, S_{0,k}(n+1) \tag{58}$$

So that, using Eq. (52) again, we have

$$\Delta_e S_k(n) = sS_k(n-1) + (1-s)\, S_k(n+1) - S_k(n) \tag{59}$$

With Eqs. (57), and (59), we can derive an expression for the irreversible entropy production rate

$$\begin{aligned}
\Delta_i S_k(n) &= \Delta S_k(n) - \Delta_e S_k(n)\\
&= s[S_{k-1}(n-1) - S_k(n-1)] + (1-s)[S_{k-1}(n+1) - S_k(n+1)]\\
&= S_k(n) - S_{k+1}(n)
\end{aligned} \tag{60}$$

where the last line is a consequence of Eq. (45). Using Eq. (51), we can obtain useful expressions for the irreversible entropy production as

$$\Delta_i S_k(n) = \sum_{\omega_0,\dots,\omega_k} \mu_n(\omega_0,\dots,\omega_k) \ln \frac{\mu_n(\omega_0,\dots,\omega_k)}{\nu(\omega_k)\, \mu_n(\omega_0,\dots,\omega_{k-1})} \tag{61}$$

for the case of the volume preserving map, Φ, and

$$\Delta_i S_k(n) = \sum_{\omega_0,\dots,\omega_k} \mu_n(\omega_0,\dots,\omega_k) \ln \frac{\mu_n(\omega_0,\dots,\omega_k)}{\nu^*(\omega_k)\, \mu_n(\omega_0,\dots,\omega_{k-1})} \tag{62}$$

for the case of the contracting map, Φ_c.

Notice that Eq. (60) contains the important result that

$$\Delta_i S_k(n) = s\, \Delta_i S_{k-1}(n-1) + (1-s)\, \Delta_i S_{k-1}(n+1) \tag{63}$$

This relation enables us to compute the k-entropy production rate recursively from a knowledge of the 0-entropy production rate.

VII. ENTROPY PRODUCTION RATE FOR FLUX BOUNDARY CONDITIONS

In this section, we specify our study to the case of flux boundary conditions. That is, we consider a chain of L sites and impose the boundary conditions:

$$\mu_0 = 1$$

$$\mu_{L+1} = L+2$$

This way, there is an average gradient of density of 1 per unit cell across the system. With these boundary conditions, the constants A and B in Eq. (46) are found to be

$$\begin{aligned} A &= \frac{L+1}{\alpha^{L+1}-1} \\ B &= 1-A \end{aligned} \tag{64}$$

Figure 5 shows μ_n for $L = 100$ and parameter values $s = 0.45, 0.5, 0.55$. Notice that, with the exception of $s = 0.5$ which corresponds to a linear growth, the exponential growth is so steep that the density is almost constant on the larger part of the lattice. In the limit when $L \to \infty$, μ_n becomes a constant and is either $L+2$ or 1 depending on whether $s < 0.5$ or $s > 0.5$ respectively. As we will see shortly, it is precisely the exponential profile of

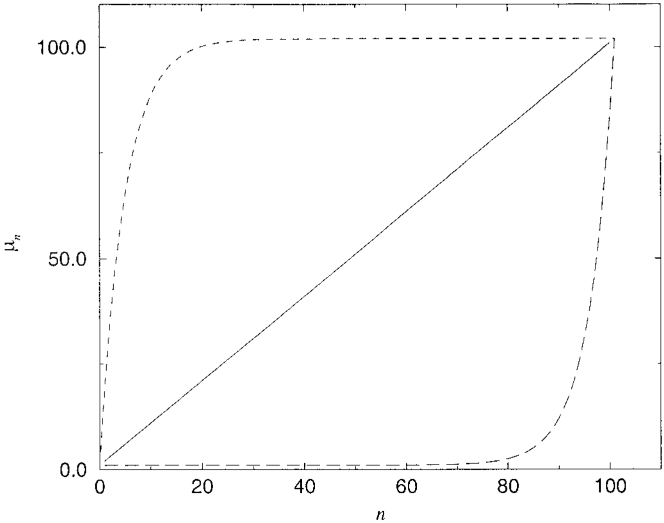

Fig. 5. The stationary state distribution μ_n, solution of Eqs. (46) and (64), on a chain of $L = 100$ sites as a function of the lattice coordinate n ($s = 0.5$ is the solid line, $s = 0.45$ the dadhed lined and $s = 0.55$ the long dashed line).

the density that is responsible for the divergence of the k-entropy production rate, see Eqs. (68) and (69).

A. Volume Preserving Case

Let us now apply the formulae (61, 63) to the system with the specific boundary conditions given by Eqs. (46), and (64). We first compute the 0-entropy production rate.

$$
\begin{aligned}
\Delta_i S_0(n) &= \sum_{\omega_0} \mu_n(\omega_0) \ln \frac{\mu_n(\omega_0)}{v(\omega_0)\,\mu_n} \\
&= s\mu_{n-1} \ln \frac{\mu_{n-1}}{\mu_n} + (1-s)\,\mu_{n+1} \ln \frac{\mu_{n+1}}{\mu_n} \\
&= s(A\alpha^{n-1} + B) \ln \frac{A\alpha^{n-1} + B}{A\alpha^n + B} + (1-s)(A\alpha^{n+1} + B) \ln \frac{A\alpha^{n+1} + B}{A\alpha^n + B} \\
&= s(A\alpha^{n-1} + B) \ln \left[1 + \frac{A\alpha^n}{A\alpha^n + B} (\alpha^{-1} - 1) \right] \\
&\quad + (1-s)(A\alpha^{n+1} + B) \ln \left[1 + \frac{A\alpha^n}{A\alpha^n + B} (\alpha - 1) \right] \qquad (65)
\end{aligned}
$$

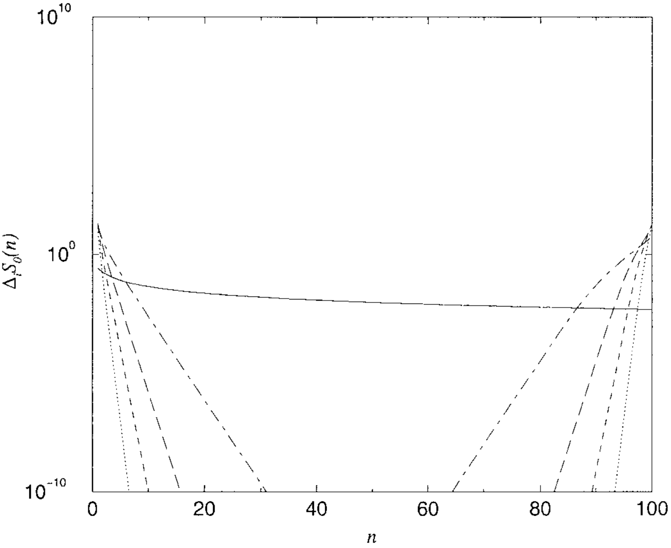

Fig. 6. 0-entropy production, $\Delta_i S_0(n)$, in the volume preserving case, Eq. (65) for a chain of $L = 100$ sites as a function of the lattice coordinate n and for $s = 0.1,..., 0.9$ from left to right (the solid line corresponds to $s = 0.5$).

Figure 6 shows a numerical computation of this quantity. The dependence on n is exponential with slope $2 \ln \alpha$ with the exception of $s = 0.5$ for which the entropy production goes like $1/n$, which is the case considered by Gaspard.(19)

If we now assume $L \gg n \gg 1$, the second terms in the logarithms are very small so that we can expand the logarithms around 1 and keep the leading terms (up to second order). After carefully examining the relative sizes of the various terms, we find that the irreversible entropy production is given by

$$\Delta_i S_0(n) = \frac{(1-2s)^2}{2s(1-s)} \frac{A^2 \alpha^{2n}}{A\alpha^n + B} \tag{66}$$

Now, if we define the discrete gradient of μ_n with respect to n as a symmetrized finite difference, i.e.,

$$\begin{aligned} \nabla \mu_n &= \frac{1}{2} \left[(\mu_{n+1} - \mu_n) + (\mu_n - \mu_{n-1}) \right] \\ &= A\alpha^n \frac{2s-1}{2s(1-s)} \end{aligned}$$

then the 0-entropy rate production (66) becomes

$$\Delta_i S_0(n) = D \frac{(\nabla \mu_n)^2}{\mu_n} \tag{67}$$

where D is the diffusion coefficient (38).

With our recurrence relation (63), we can now carry out the computation of the k-entropy production rate for any k. In Figs. 7 and 8, we show the first ten k's for the same lattice of length $L = 100$ and $s = 0.45$ and $s = 0.55$ respectively. Notice that these curves display some k dependence. In Figs. 9 and 10, we show the k dependence of the entropy production for the middle site, $n = 50$, of a 100 sited chain, for both small and large k. The k-entropy appears to increase exponentially for the lower part of the k range, Fig. 10, and then starts to decay exponentially, Fig. 10.

The exponential growth can be understood directly form Eqs. (63) and (66). Indeed, let us assume

$$\Delta_i S_k(n) = \frac{(1-2s)^2}{2s(1-s)} \frac{A^2 \alpha^{2n}}{A\alpha^n + B} \beta^k \tag{68}$$

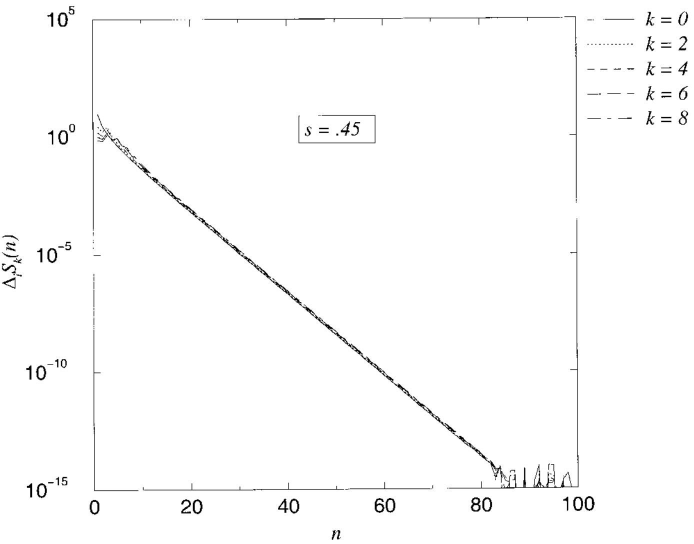

Fig. 7. k-entropy production, $\Delta_i S_k(n)$, in the volume preserving case, for $k = 0, 2, 4, 6, 8$, numerically computed using Eq. (63), $s = 0.45$ and $L = 100$.

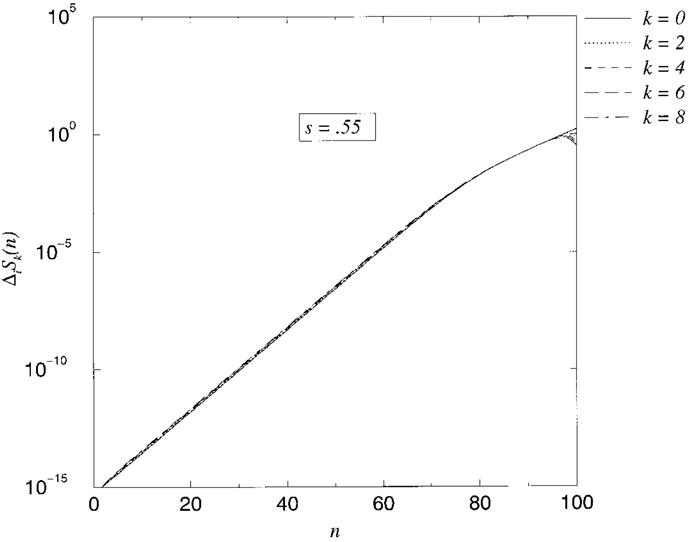

Fig. 8. k-entropy production, $\Delta_i S_k(n)$, in the volume preserving case, for $k = 0, 2, 4, 6, 8$, numerically computed using Eq. (63), $s = 0.55$ and $L = 100$.

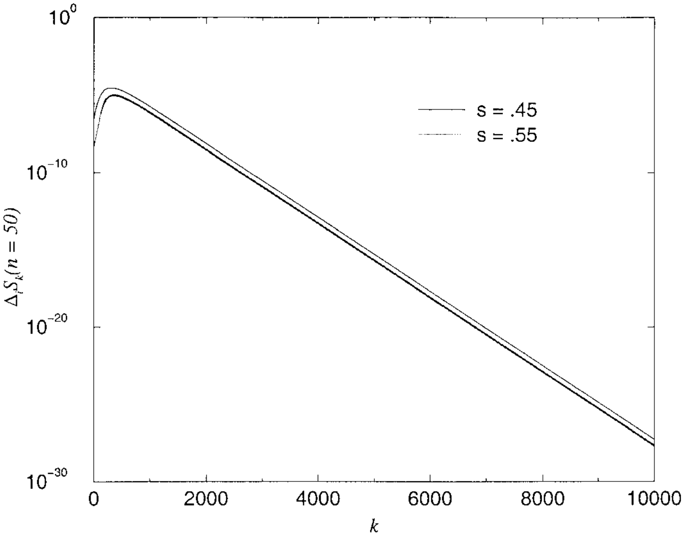

Fig. 9. k-entropy production, $\Delta_i S_k(n = 50)$, in the volume preserving case, as a function of k, numerically computed using Eq. (63), $L = 100$. Both $s = 0.45$ and $s = 0.55$ are displayed. On the long range scale, the entropy production decays exponentially as a function of k as the invariant measure gets mostly smooth on the corresponding scales.

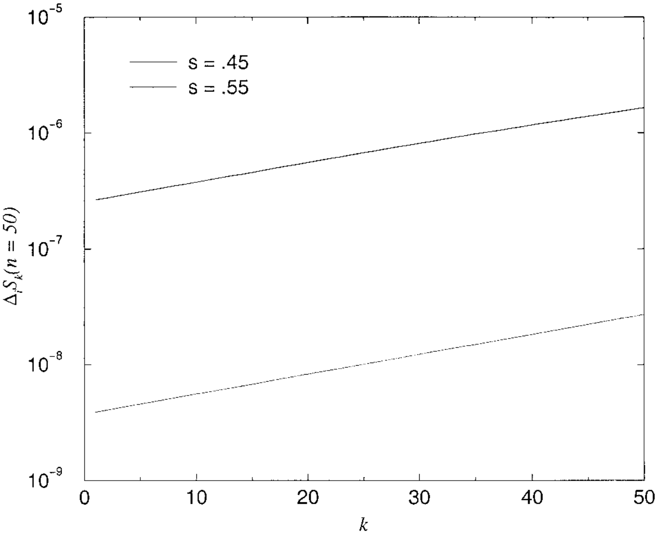

Fig. 10. Blow up of Fig. 10 for $k = 0, \ldots, 50$. The k-entropy diverges exponentially with k. The slope is given by Eq. (A23).

Using Eq. (63), we find

$$\beta = \frac{(1-s)^3 + s^3}{s(1-s)} \tag{69}$$

In Appendix A, we rederive this k dependence from the knowledge of the stationary state and Eq. (62), see Eq. (A23). Notice that this ignores the finite size effects. Of course, this exponential divergence is of unphysical nature and one would expect that the entropy production be independent of k. In their model with a third middle band, Vollmer *et al.*[(18)] introduced a special scaling that allowed them to get rid of this divergence, while keeping the zeroth order term in Eq. (68).

The finite size effects are those responsible for the exponential decay at large values of k. To understand these finite size effects, notice that the value of k gives the number of time steps for which we know where the points located in a specific set will go. The only possibility for these sets to produce entropy is if they remain in the chain for more than k steps. Indeed, among all the sets, those that exit the chain within k steps will propagate freely forever either to the left or to the right so that no further information is gained by increasing the resolution of these sets. Now, as we increase k there are more and more such sets that do not contribute to the entropy production rate. This exponential decay continues for arbitrarily large k because, in the steady state, there are arbitrarily fine variations in the density of points on the chain, as can be seen from the singular nature of the SRB measure.

The relation of this exponential decay to the escape rate is easy to derive. Indeed if, for an open system, the probability density decays like γ (the escape rate), then one easily finds that the entropy should decay like γ. This can be verified numerically. For the case of a system with mean drift velocity v, given in our case by Eq. (39), Tél *et al.*[18] showed that the escape rate formula of Gaspard and Nicolis should be generalized to

$$\gamma = \frac{1}{4} \frac{v^2}{D} + \frac{\pi^2}{L^2} D \tag{70}$$

Figure 11 shows a comparison between that formula and the numerically computed decay rate of the entropy production. The agreement is best around $s = 1/2$. We believe that the small discrepancies for other values of s, which are quadratic in s, may be due to small numerical errors and/or to next order corrections in $1/L$.

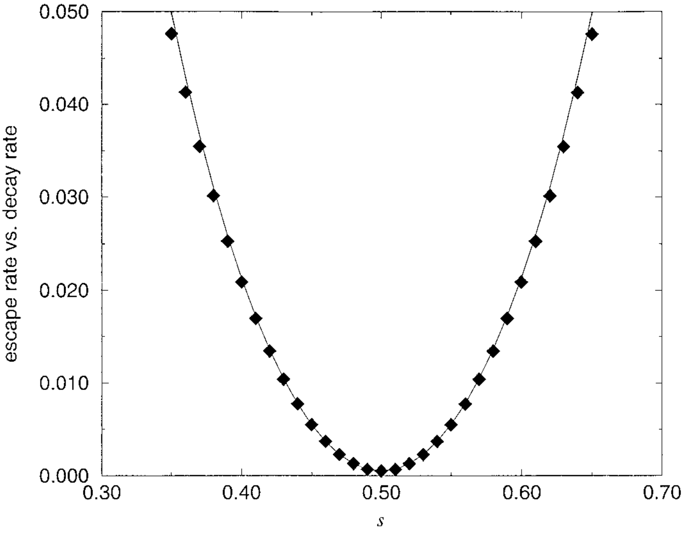

Fig. 11. A comparison between the escape rate given by Eq. (70) (solid line) and the numerically computed decay rate (diamonds) of the entropy production at large values of k as a function of s ($L = 100$ and the decay rate was measured at $k = 8000$).

B. Dissipative Case

We now switch to Φ_c and use formula (62) to compute the 0-entropy production rate.

$$\begin{aligned}
\varDelta_i S_0(n) &= \sum_{\omega_0} \mu_n(\omega_0) \ln \frac{\mu_n(\omega_0)}{\nu^*(\omega_0)\, \mu_n} \\
&= s\mu_{n-1} \ln \frac{s\mu_{n-1}}{(1-s)\,\mu_n} + (1-s)\,\mu_{n+1} \ln \frac{(1-s)\,\mu_{n+1}}{s\mu_n} \\
&= s\mu_{n-1} \ln \frac{\mu_{n-1}}{\mu_n} + (1-s)\,\mu_{n+1} \ln \frac{\mu_{n+1}}{\mu_n} \\
&\qquad + (s\mu_{n-1} - (1-s)\,\mu_{n+1}) \ln \frac{s}{1-s} \\
&\equiv \varDelta_i S_0^{(vp)}(n) + \varDelta_i S_0^{(d)}(n)
\end{aligned} \tag{71}$$

where

$$\varDelta_i S_0^{(vp)}(n) = s\mu_{n-1} \ln \frac{\mu_{n-1}}{\mu_n} + (1-s)\,\mu_{n+1} \ln \frac{\mu_{n+1}}{\mu_n}$$

is the contribution from the volume preserving part, identical to Eq. (65), and

$$\begin{aligned}
\varDelta_i S_0^{(d)}(n) &= (s\mu_{n-1} - (1-s)\,\mu_{n+1}) \ln \frac{s}{1-s} \\
&= (2s-1)(B - A\alpha^n) \ln \frac{s}{1-s}
\end{aligned} \tag{72}$$

reflects the presence of phase space contraction. Figure 12 shows a numerical computation of this last term. It is constant and positive everywhere except in the vicinity of the boundaries, where it may become negative. It is remarkable, though, that the total 0-entropy production rate, Eq. (71), is positive everywhere, as shown in Fig. 13. Also, notice that the contribution due to the dissipative term is generally much larger than the first term which is the only contribution in the volume preserving case.

Note that the dissipative term,

$$(\mu_n - 2A\alpha^n)(2s-1) \ln \frac{s}{1-s}$$

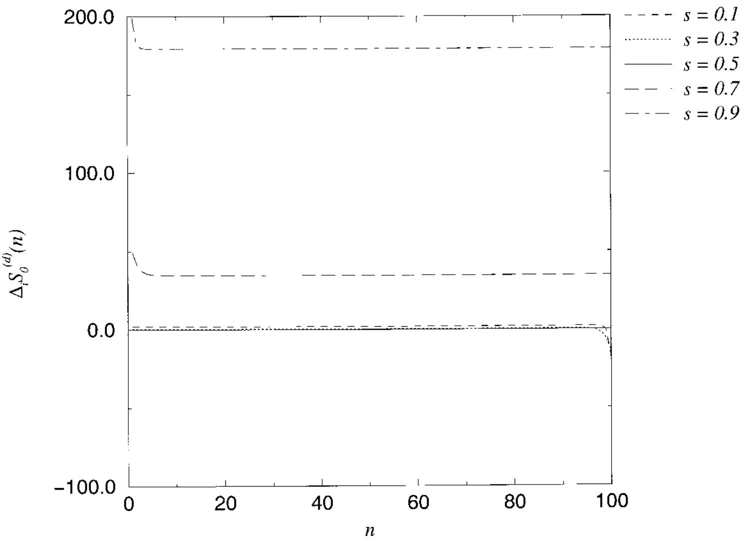

Fig. 12. Dissipative part, $\Delta_i S_0^{(d)}(n)$, of the 0-entropy production, Eq. (72), for a chain of $L = 100$ sites as a function of the lattice coordinate n. $s = 0.1, 0.3, 0.5, 0.7, 0.9$. The s-values increase from top to bottom.

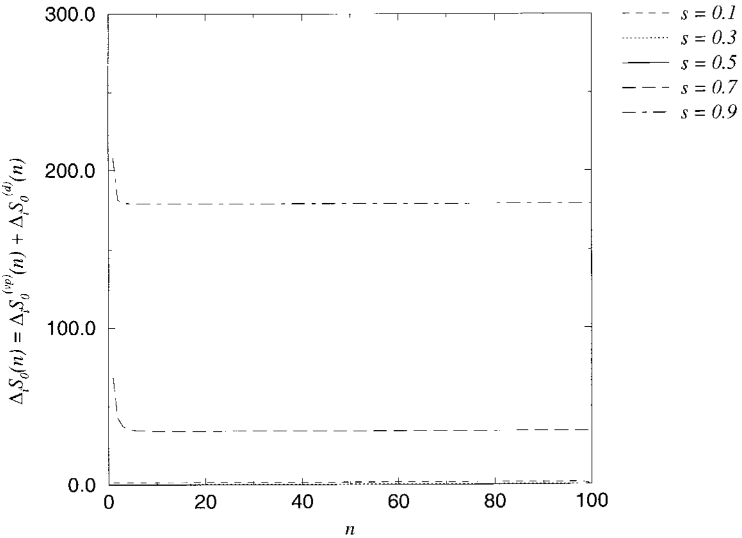

Fig. 13. Total 0-entropy production, Eq. (71), in the dissipative case for a chain of $L = 100$ sites as a function of the lattice coordinate n. $s = 0.1, 0.3, 0.5, 0.7, 0.9$. The s-values increase from top to bottom.

is nothing but the phase space contraction rate (44) multiplied by $\mu_n - 2A\alpha^n$. We have thus shown that

$$\Delta_i S_0(n) = D\,\frac{(\nabla\mu_n)^2}{\mu_n} - (\mu_n - 2A\alpha^n)(\lambda_+ + \lambda_-) \tag{73}$$

In the infinite volume limit B takes on the values 1 or $L+2$, depending upon α, and one can check that the entropy production rate becomes independent of the boundary conditions. Indeed, the squared gradient term is overwhelmed by the second term, which is equal to the phase space contraction rate one gets for periodic boundary conditions, and the third term, involving $A\alpha^n$, is negligible in this limit.

We also note that the thermostated system approach has been applied by Chernov *et al.*(3) to systems in which no density gradient is present. They consider the diffusion of a charged, moving particle in a fixed array of hard scatterers, the periodic Lorentz gas, and use an [electric field + thermostat] to generate an isokinetic electric current in the system. In this case, there is no density gradient and all of the irreversible entropy production comes from the phase space contraction. The entropy production is then determined only by the Lyapunov exponents and for small electric fields, at least, the entropy production is proportional to the square of the electric field with a coefficient that agrees with the predictions of irreversible thermodynamics.

Returning to our model, we can make use of the recursion relation, Eq. (63), to compute the entropy production for different values of k. Although the k dependence will remain in the volume preserving part, we find that the dissipative term does not depend on k so that in this case the largest contribution to the entropy production rate does not depend on the resolution parameter. We remark that this property is specific to piecewise linear maps and should not be expected to be a general feature. Indeed, whereas, for a piecewise linear map, Eq. (35) has a constant Jacobian in every single region of the partition, it will not be so for non piecewise linear maps. As suggested by Eq. (37), we will in general need to take the limit of infinite resolution to retrieve the phase space contraction rate.

VIII. DISCUSSION

We have shown that Gaspard's method(19) of defining a coarse grained Gibbs entropy and its rate of change for an Anosov-like, volume preserving dynamical system can be generalized and extended to include non-volume preserving Anosov-like systems which develop a nonequilibrium stationary state SRB measure on an attractor. The rate of entropy production in such a system is positive, and the total rate of entropy production in a closed system is given by the negative of the sum of the Lyapunov exponents of the map. Very close results have previously been obtained by Vollmer, Tél and Breymann.(18) Our contribution is mainly to show that Gaspard's coarse graining method is a natural one to use in this context, and that it reveals quite clearly the relation between the rate of irreversible entropy production and the loss of information about the system's trajectory due to the coarse graining. This method allows one to take a limit where the coarse graining size is taken to zero after the non-equilibrium steady state is reached, and in this limit we recover the formula used by Ruelle(4) to prove that the rate of entropy production is positive in the type of systems treated here.

The biased random walk models discussed here have a number of interesting features. They are relatively simple to analyze, and they exhibit an exponential growth and subsequent decay of the entropy production as the size of the coarse graining regions becomes smaller. However, for all values of s, except $s = 1/2$, the density profile in the non-equilibrium steady state is very unphysical, and the large-system limit yields a trivial result where the density profile is uniform except very close to the boundaries. The exponential divergence of the rate of entropy production as the coarse graining size gets large, at least over a range of k, is a striking difference between the multi-baker chains we consider in this paper and that studied by Gaspard.(19) Indeed, whereas Gaspard showed, for $s = 1/2$, that

$$\lim_{k \to \infty} \lim_{(\nabla\mu_n)/\mu_n \to 0} \lim_{L \to \infty} \frac{\mu_n}{(\nabla\mu_n)^2} \Delta_i S_k = D \tag{74}$$

we find, for $s \neq 1/2$, that

$$\lim_{k \to \infty} \lim_{(\nabla\mu_n)/\mu_n \to 0} \lim_{L \to \infty} \frac{\mu_n}{(\nabla\mu_n)^2} \Delta_i S_k^{(vp)} = D \left(\frac{(1-s)^3 + s^3}{s(1-s)} \right)^k \tag{75}$$

We believe that this point should be seen as a defect of the models we treat and will be addressed with more realistic models in further papers.

Tél, Vollmer and Breymann(5, 18, 23) consider a multi-baker model where the squares are organized in subsets that move to the right, left or stay within the squares. They show that there is a good scaling limit for which the density profile is governed by a well defined Fokker–Planck equation and is linear.

We have chosen an alternative approach to the problem of finding a realistic but analytically tractable model of a system with a thermostat. In a subsequent paper(26) we will discuss a model which can be described as a random walk driven by a thermostated external electric field and which takes the form of a nonlinear baker map. Such models mimic thermostated Lorentz gases which have been the subject of a number of theoretical and computational studies.(3, 12, 14, 27) There we will also find an interesting transition of the dynamics from hyperbolic to non-hyperbolic behavior as a function of the strength of the external field, with dramatic consequences for the diffusive properties of the system.

It has been realized for many years that the resolution of the "Gibbs paradox" in entropy production, for many-particle systems, depends upon using reduced distribution functions which themselves give a very coarse grained description of a many particle system.(16, 21, 22) Then the macroscopic entropy production can be clearly identified, as in Boltzmann's H-theorem, with the loss of information about the system's fine grained phase space distribution with time. We have discussed here a closely related and no less important mechanism for information loss and entropy production, namely the formation of fractal phase space structures in non-equilibrium stationary states as the support for singular measures. The two mechanisms are related by the fact that even for Hamiltionian systems, the support of the fine grained, Gibbs distribution can evolve to a fractal that looks smooth in phase space in some directions but highly singular in others. These fractal structures require the application of coarse graining methods to correctly describe irreversible processes in fluid systems and for an understanding of why the reduced distribution functions approach their. equilibrium values in the course of time.

APPENDIX A: PROPERTIES OF THE SRB MEASURES

In this appendix we briefly summarize the properties of the SRB measures for the multibaker chains discussed in this paper and derive an analytical expression for the *k*-entropy, Eq. (62). For more details we refer to the papers of Gaspard,(19) of Tasaki and Gaspard,(20) and of Tasaki, Gilbert, and Dorfman.(25) We consider here the case of the volume contracting multibaker map, Φ_c, with flux boundary conditions.

The SRB measure for this system is obtained by using the Frobenius–Perron equation to derive an expression for the cumulative measure in each unit square. The Frobenius–Perron equation for the (singular) invariant density associated with this map is

$$\rho(\Gamma) = \int d\Gamma' \, \delta(\Gamma - \Phi_c(\Gamma')) \, \rho(\Gamma') \tag{A1}$$

or

$$\begin{aligned}\rho(n, x, y) &= \frac{s}{1-s}\,\rho\left(n-1, sx, \frac{y}{1-s}\right), & 0 \leqslant y < 1-s \\ &= \frac{1-s}{s}\,\rho\left(n+1, s+(1-s)\,x, \frac{y-1+s}{s}\right), & 1-s \leqslant y \leqslant 1\end{aligned} \tag{A2}$$

The cumulative measure, $G(n, x, y)$ in each square is defined by

$$G(n, x, y) = \int_0^x dx' \int_0^y dy'\, \rho(n, x', y') \tag{A3}$$

The measure of any region in a unit square can then be defined as the difference of two cumulative functions. For example, the region defined by a particular sequence $\{\omega_0,..., \omega_{k-1}\}$ in square n is a horizontal strip extending over the full x interval, and contained between $y(\omega_0,..., \omega_{k-1})$ and $y(\omega_0,..., \omega_{k-1}+1)$, so that

$$\mu_n(\omega_0,..., \omega_{k-1}) = G(n, 1, y(\omega_0,..., \omega_{k-1}+1)) - G(n, 1, y(\omega_0,..., \omega_{k-1})) \tag{A4}$$

where we have introduced the notation

$$\begin{aligned}\omega_{j-1}, \omega_j + 1 &= \omega_{j-1}, 1, & \omega_j = 0 \\ &= \omega_{j-1}+1, 0, & \omega_j = 1\end{aligned} \tag{A5}$$

with the convention that $y(1,..., 1, 1+1) = 1$.

We can also write explicitly

$$y(\omega_0,..., \omega_{k-1}) = \omega_0(1-s) + \sum_{j=1}^{k-1} \omega_j (1-s)\, v^*(\omega_0,..., \omega_{j-1}) \tag{A6}$$

where v^* is as defined by Eq. (50). In particular, we note that

$$y(0, \omega_1,..., \omega_{k-1}) = (1-s)\; y(\omega_1,..., \omega_{k-1}) \tag{A7}$$

$$y(1, \omega_1,..., \omega_{k-1}) = 1 - s(1 - y(\omega_1,..., \omega_{k-1})) \tag{A8}$$

These equations will be used in the sequel.

It follows from the Frobenius–Perron equation (A2) that $G(n, x, y)$ satisfies the equation

$$\begin{aligned} G(n, x, y) &= G\left(n-1, sx, \frac{y}{1-s}\right), \qquad 0 \leqslant y < 1-s \\ &= G(n-1, sx, 1) + G\left(n+1, (1-s)\,x+s, \frac{y-1+s}{s}\right) \\ &\quad - G\left(n+1, s, \frac{y-1+s}{s}\right), \qquad 1-s \leqslant y \leqslant 1 \end{aligned} \tag{A9}$$

Then, the total measure of the n-th square, μ_n, satisfies the equation

$$\mu_n = G(n, 1, 1) = G(n-1, s, 1) + G(n+1, 1, 1) - G(n+1, s, 1) \tag{A10}$$

It is now possible to see that there is a solution of Eq. (A9), for $G(n, x, y)$ which has the form

$$G(n, x, y) = x[\,y(\mu_n - B) + BT_n(y)] \tag{A11}$$

where μ_n is a solution of Eq. (45), B is given by Eq. (64), and $T_n(y)$ satisfies the recursion relation

$$\begin{aligned} T_n(y) &= sT_{n-1}\left(\frac{y}{1-s}\right), \qquad 0 \leqslant y < 1-s \\ &= s + (1-s)\,T_{n+1}\left(1 - \frac{1-y}{s}\right), \qquad 1-s \leqslant y \leqslant 1 \end{aligned} \tag{A12}$$

The boundary conditions on the functions $T_n(y)$ are $T_0(y) = T_{L+1}(y) = y$. These functions will be referred to as incomplete, see Tasaki and Gaspard,$^{(20)}$ as opposed to the function $T(y)$ which appears in the case of periodic boundary conditions, see Tasaki *et al.*,$^{(25)}$

$$\begin{aligned} T(y) &= sT\left(\frac{y}{1-s}\right), \qquad 0 \leqslant y < 1-s \\ &= s + (1-s)\,T\left(1 - \frac{1-y}{s}\right), \qquad 1-s \leqslant y \leqslant 1 \end{aligned} \tag{A13}$$

The solution given by Eq. (A11) leads immediately to the recursion relation, Eq. (45), for the measures μ_n. Furthermore, this expression for $G(n, x, y)$ has the form expected for the cumulative distribution of an SRB measure: it is smooth (actually uniform) in the expanding direction, and singular in the contracting direction. The singularity in the contracting, or

y-direction, can be seen when the recursion relations are solved for the functions $T_n(y)$. In the limit where the boundaries are infinitely far away, $T_n(y)$ is replaced by the limiting function $T(y)$, which is a continuous function that has zero derivatives almost everywhere. It is the singularity of $T(y)$ which prevents the measure from having a well behaved density, and requires the use of the coarse graining procedure described in the body of this paper. Figure 14 shows, for $s = 0.55$, the limiting function $T(y) - y$, singular on every length scale. Figures 15–20 show, for the same value of the parameter s, the incomplete functions $T_n(y) - y$ truncated due to the boundary conditions $T_0(y) = T_{L+1}(y) = y$. For some fixed length scale, these functions quickly become singular (their derivatives have discontinuities inside the corresponding y interval) as we move away from the boundaries. Entropy production is positive in the y intervals where $T_n(y)$ has singularities.

Before we proceed to the derivation of the k-entropy, we make use of Eqs. (A7) and (A8) to derive a useful expression of the $T_n(y)$. Note that

$$\begin{aligned} T_n(y(0, \omega_1,\dots, \omega_{k-1})) &= T_n((1-s)\, y(\omega_1,\dots, \omega_{k-1})) \\ &= sT_{n-1}(y(\omega_1,\dots, \omega_{k-1})) \\ T_n(y(1, \omega_1,\dots, \omega_{k-1})) &= T_n(1-s(1-y(\omega_1,\dots, \omega_{k-1}))) \\ &= s + (1-s)\, T_{n-1}(y(\omega_1,\dots, \omega_{k-1})) \end{aligned}$$

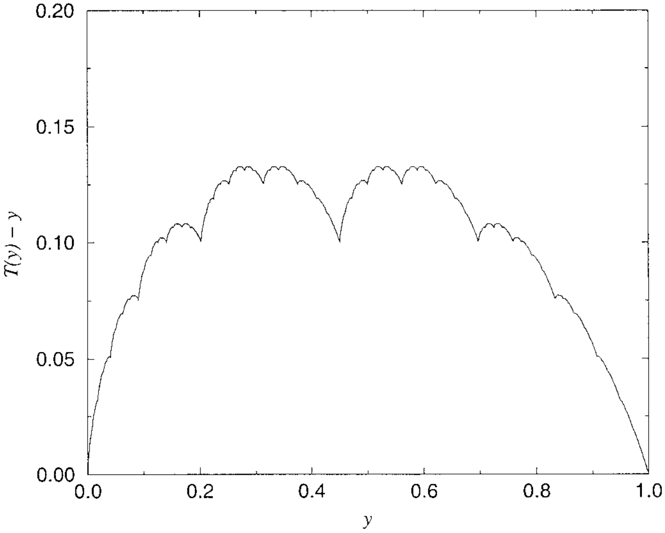

Fig. 14. The limiting function $T(y) - y$, Eq. (A13), $s = 0.55$.

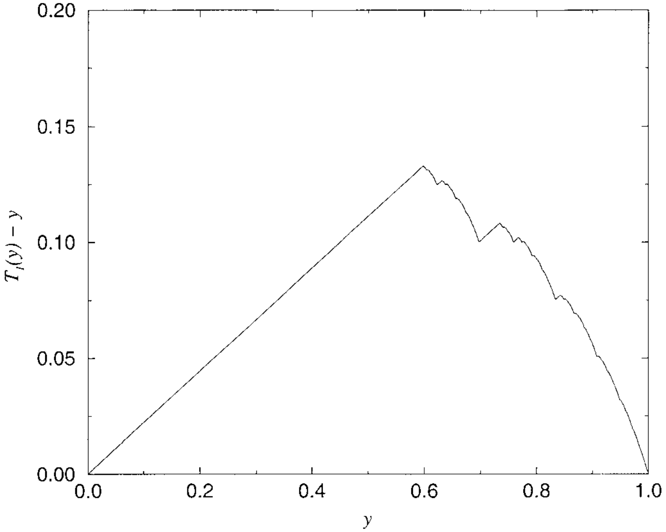

Fig. 15. The incomplete functions $T_n(y) - y$, Eq. (A12), $n = 1$, with the boundary conditions $T_0(y) = T_{101}(y) = y$ and $s = 0.55$.

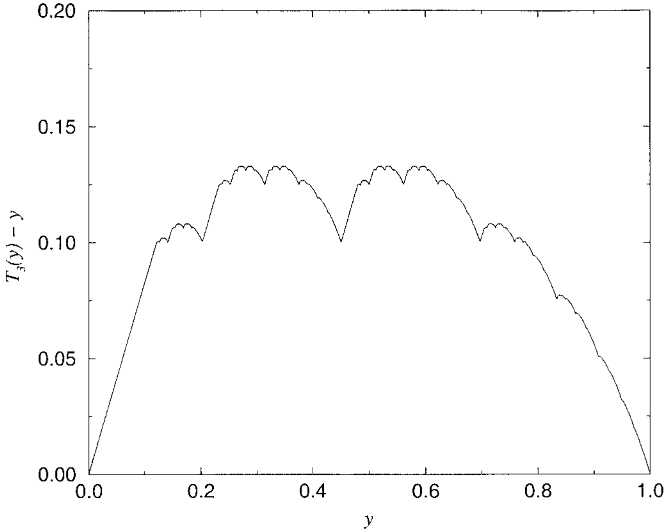

Fig. 16. As in Fig. 15, for $n = 3$.

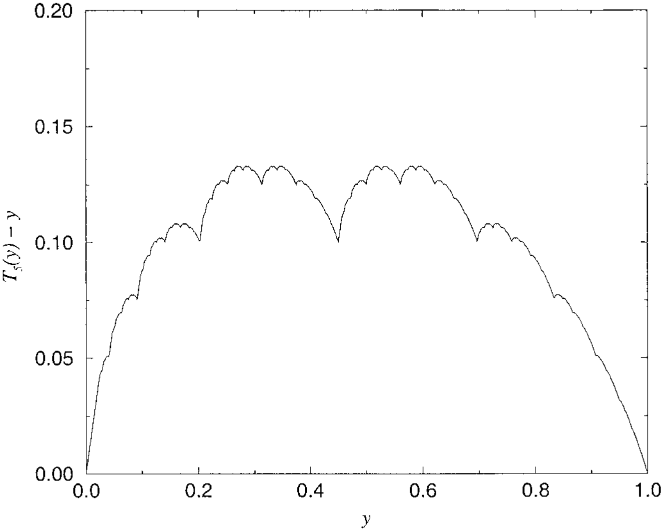

Fig. 17. As in Fig. 15, for $n = 5$.

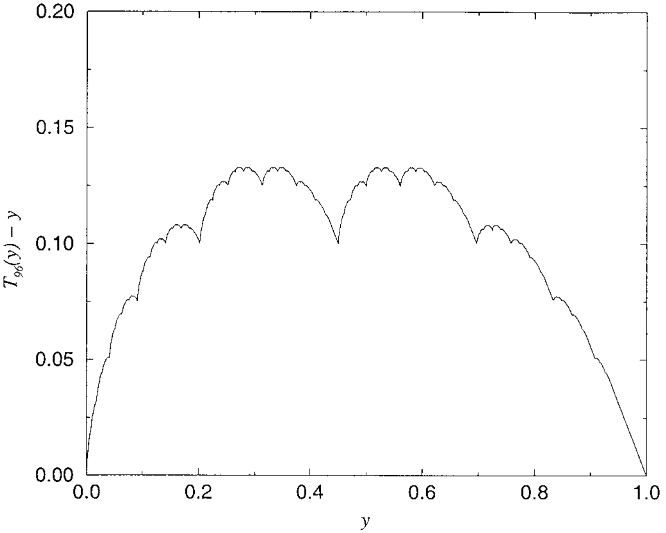

Fig. 18. As in Fig. 15, for $n = 96$.

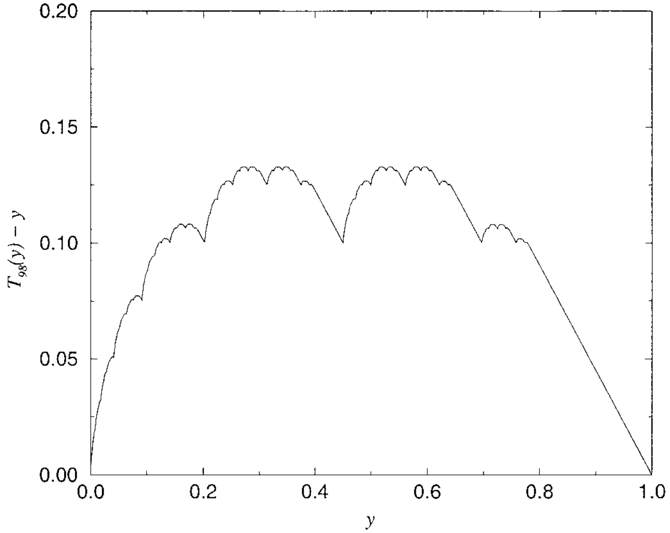

Fig. 19. As in Fig. 15, for $n = 98$.

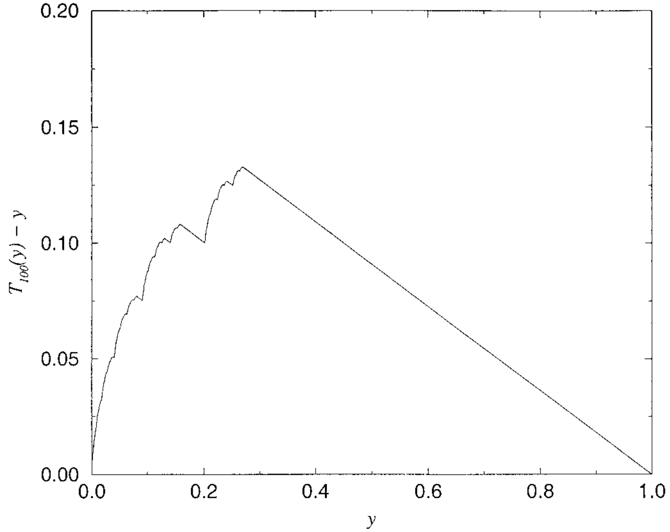

Fig. 20. As in Fig. 15, for $n = 100$.

As long as we are far enough from the boundaries, we can replace the $T_n(y)$ by their limiting values $T(y)$ (this amounts to assuming $1 \ll n \ll L$). In this case, it follows that

$$T(y(\omega_0,..., \omega_{k-1})) = s\omega_0 + \sum_{j=1}^{k-1} s\omega_j v(\omega_0,..., \omega_{j-1}) \tag{A14}$$

where v is as defined by Eq. (49).

With the help of Eq. (A4), we can make use of Eq. (A11) to rewrite the entropy production rate formula, Eq. (62). Ignoring the boundary effects, Eq. (A4) gives

$$\begin{aligned}\mu_n(\omega_0,..., \omega_{k-1}, 0) &= B[T(y(\omega_0,..., \omega_{k-1}, 1)) - T(y(\omega_0,..., \omega_{k-1}))]\\ &\quad + A\alpha^n(1-s)\, v^*(\omega_0,..., \omega_{k-1})\\ \mu_n(\omega_0,..., \omega_{k-1}, 1) &= B[T(y(\omega_0,..., \omega_{k-1}+1)) - T(y(\omega_0,..., \omega_{k-1}, 1))]\\ &\quad + A\alpha^n s v^*(\omega_0,..., \omega_{k-1})\end{aligned}$$

Writing

$$\begin{aligned}\Delta T_a &= T(y(\omega_0,..., \omega_{k-1}, 1)) - T(y(\omega_0,..., \omega_{k-1}))\\ \Delta T_b &= T(y(\omega_0,..., \omega_{k-1}+1)) - T(y(\omega_0,..., \omega_{k-1}, 1))\end{aligned} \tag{A15}$$

$$\varepsilon = A\alpha^n v^*(\omega_0,..., \omega_{k-1}) \tag{A16}$$

the k-entropy production rate becomes

$$\begin{aligned}\Delta_i S_k(n) = \sum_{\omega_0,..., \omega_{k-1}} \bigg[&(B\,\Delta T_a + (1-s)\,\varepsilon) \ln \frac{B\,\Delta T_a/(1-s) + \varepsilon}{B\,\Delta T_a + B\,\Delta T_b + \varepsilon}\\ &+ (B\,\Delta T_b + s\varepsilon) \ln \frac{B\,\Delta T_b/s + \varepsilon}{B\,\Delta T_a + B\,\Delta T_b + \varepsilon} \bigg]\end{aligned} \tag{A17}$$

In the limit $1 \ll n \ll L$, $A\alpha^n \ll 1$ so that we can expand the logarithms. Up to second order, we find

$$\begin{aligned}\Delta_i S_k(n) = \sum_{\omega_0,..., \omega_{k-1}} \bigg[&(B\,\Delta T_a + (1-s)\,\varepsilon) \ln \frac{\Delta T_a/(1-s)}{\Delta T_a + \Delta T_b}\\ &+ (B\,\Delta T_b + s\varepsilon) \ln \frac{B\,\Delta T_b/s}{\Delta T_a + \Delta T_b}\\ &+ \frac{\varepsilon^2}{2B} \left(\frac{(1-s)^2}{\Delta T_a} + \frac{s^2}{\Delta T_b} - \frac{1}{\Delta T_a + \Delta T_b} \right) \bigg]\end{aligned} \tag{A18}$$

The following properties of ΔT_a and ΔT_b follow easily from Eqs. (A14) and (A15):

$$\Delta T_a = s(\Delta T_a + \Delta T_b)$$

$$\Delta T_b = (1-s)(\Delta T_a + \Delta T_b)$$

Equation (A18) thus becomes

$$\Delta_i S_k(n) = \Delta_i S_k^{(vp)}(n) + \Delta_i S_k^{(d)}(n) \tag{A19}$$

where we have set

$$\begin{aligned}\Delta_i S_k^{(vp)}(n) &= \sum_{\omega_0,\ldots,\,\omega_{k-1}} \frac{\varepsilon^2}{2B(\Delta T_a + \Delta T_b)} \left(\frac{(1-s)^2}{s} + \frac{s^2}{1-s} - 1 \right) \\ &= \frac{(1-2s)^2}{2s(1-s)} \frac{A^2 \alpha^{2n}}{B} \sum_{\omega_0,\ldots,\,\omega_{k-1}} \frac{v^*(\omega_0,\ldots,\,\omega_{k-1})^2}{\Delta T_a + \Delta T_b}\end{aligned} \tag{A20}$$

and

$$\begin{aligned}\Delta_i S_k^{(d)}(n) &= (2s-1) \ln \frac{s}{1-s} \sum_{\omega_0,\ldots,\,\omega_{k-1}} [B(\Delta T_a + \Delta T_b) - \varepsilon] \\ &= (2s-1) \ln \frac{s}{1-s} (B - A\alpha^n)\end{aligned} \tag{A21}$$

To derive Eq. (A21) we made use of the property

$$\sum_{\omega_0,\ldots,\,\omega_{k-1}} \Delta T_a + \Delta T_b = 1$$

which follows from the identity

$$\Delta T_a + \Delta T_b = v(\omega_0,\ldots,\,\omega_{k-1}) \tag{A22}$$

that follows itself easily from Eqs. (A14) and (A15).

The comparison between Eqs. (A19)–(A21) and the corresponding 0-entropy production rate, Eqs. (67), (71), and (72) is straightforward. Set $k=0$ in Eq. (A20). Then there is no index over which to sum, v^* is replaced by 1, and

$$\Delta T_a + \Delta T_b = T(1) - T(0) = 1$$

As of Eq. (A21), it is just the same as Eq. (72), thus confirming the k independence of that part of the k-entropy production rate.

Let us now investigate the k dependence of Eq. (A20). To this effect, we rewrite Eq. (A20) using Eq. (A22):

$$\begin{aligned}\Delta_i S_k^{(vp)}(n) &= \frac{(1-2s)^2}{2s(1-s)} \frac{A^2\alpha^{2n}}{B} \sum_{\omega_0,\ldots,\omega_{k-1}} \frac{v^*(\omega_0,\ldots,\omega_{k-1})^2}{v(\omega_0,\ldots,\omega_{k-1})} \\ &= \frac{(1-2s)^2}{2s(1-s)} \frac{A^2\alpha^{2n}}{B} \left(\sum_{\omega} \frac{v^*(\omega)^2}{v(\omega)}\right)^k \\ &= \frac{(1-2s)^2}{2s(1-s)} \frac{A^2\alpha^{2n}}{B} \left(\frac{(1-s)^3+s^3}{s(1-s)}\right)^k \end{aligned} \tag{A23}$$

We thus conclude that the volume preserving part of the k-entropy diverges exponentially with k! This is quite remarkable as it differs dramatically from the expression Gaspard(19) gave for the case $s=0.5$ for which the k divergence is linear and is next order in the small parameter and thus vanishes in the limit (74). In our case, the divergence is of the same order in $A\alpha^n$, which illustrates the breakdown of the k-entropy production for biased random walk models considered here.

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