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Entropy Production in Open Volume-Preserving Systems

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We describe a mechanism leading to positive entropy production in volume-preserving systems under nonequilibrium conditions. We consider volume-preserving systems sustaining a diffusion process like the multibaker map or the Lorentz gas. A continuous flux of particles is imposed across the system resulting in a steady gradient of concentration. In the limit where such flux boundary conditions are imposed at arbitrarily separated boundaries for a fixed gradient, the invariant measure becomes singular. For instance, in the multibaker map, the limit invariant measure has a cumulative function given in terms of the non-differentiable Takagi function. Because of this singularity of the invariant measure, the entropy must be defined as a coarse-grained entropy instead of the fined-grained Gibbs entropy, which would require the existence of a regular measure with a density. The coarse-grained entropy production is then shown to be asymptotically positive and, moreover, given by the entropy production expected from irreversible thermodynamics.

KEY WORDS: Entropy production; flux boundary conditions; non-equilibrium steady state; singular measure; multibaker map; Takagi function.

I. INTRODUCTION

The problem of entropy production is one of the oldest open questions in nonequilibrium statistical mechanics. It originates from the confrontation between the thermodynamics of irreversible processes and the classical or quantum mechanics which describe the motion of atoms and molecules in matter. Classical mechanics is reversible and preserves volumes in phase space according to Liouville's theorem. Both of these properties seem to be in contradiction with irreversible thermodynamics.

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Recently, several works have been devoted to the problem of our understanding of the entropy production and of the 2nd law of thermodynamics in the context of the theory of deterministic dynamical systems.[1-8] It is a difficult problem because it is well know that an entropy like the Gibbs entropy

$$S_G(t) = -\int_\Gamma d\mathbf{X}\, f_t(\mathbf{X}) \ln f_t(\mathbf{X}) \tag{1}$$

remains constant during the time evolution of the probability density $f_t(\mathbf{X})$ in closed volume-preserving systems. For a deterministic system, the motion of all the particles is governed by a set of differential equations of first order in time

$$\dot{\mathbf{X}} = \mathbf{F}(\mathbf{X}) \tag{2}$$

where $\mathbf{F}(\mathbf{X})$ is a vector field defined in the phase space Γ of the positions and momenta $\mathbf{X}$. In volume-preserving systems, there exists an absolutely-continuous invariant measure which is the Liouville measure $d\mathbf{X}$. A statistical ensemble of copies of the system is defined by a probability measure ν_t which should be absolutely continuous with respect to the Liouville measure for the corresponding probability density to exist as $f_t(\mathbf{X}) = d\nu_t/d\mathbf{X}$. This probability density evolves in time according to the (generalized) Liouville equation which expresses the local conservation of probability in phase space:

$$\partial_t f_t(\mathbf{X}) + \partial_{\mathbf{X}} \cdot [f_t(\mathbf{X})\, \mathbf{F}(\mathbf{X})] = 0 \tag{3}$$

where $\partial_{\mathbf{X}}$ denotes the gradient with respect to all the phase-space variables $\mathbf{X}$. The time evolution of the probability density induces a time evolution for the Gibbs entropy according to

$$\frac{dS_G}{dt} = -\int_{\partial\Gamma} d\mathbf{A} \cdot \mathbf{J}_{s_G} + \int_\Gamma d\mathbf{X}\, \sigma_{s_G} \tag{4}$$

which is expressed in terms of the Gibbs entropy current and entropy source

$$\mathbf{J}_{s_G} = (-f \ln f)\, \mathbf{F} \tag{5}$$

$$\sigma_{s_G} = f\, \partial_{\mathbf{X}} \cdot \mathbf{F} \tag{6}$$

The first term in Eq. (4) is the flow of entropy at the boundaries of the phase space. The second term is the average value of the divergence of the vector field (2). In a conservative system, this divergence vanishes,

$\partial_{\mathbf{X}} \cdot \mathbf{F} = 0$, and $\sigma_{s_G} = 0$. Hence, the second term vanishes in Eq. (4) so that the time variation of the Gibbs entropy dS_G/dt is only due to the boundary conditions. In a closed system or in a steady state, the entropy current vanishes at the boundaries so that the Gibbs entropy is constant.

These properties of the Gibbs entropy contradict the properties expected for an entropy in the thermodynamics of irreversible processes.[9–12] If we had to identify the Gibbs entropy (1) with the thermodynamic entropy as it is the case in equilibrium statistical mechanics we would face the famous problem that the entropy production should vanish for the class of conservative systems in contradiction with the phenomenology. Over the last few years, several propositions have been discussed in the literature to overcome this famous problem.

Mackey has proposed that a positive entropy production should have its origin in the property of exactness of dynamical systems.[13] Exact dynamical systems are defined as discrete-time systems, $\mathbf{X}_{t+1} = \mathbf{\Phi}(\mathbf{X}_t)$, which are expanding $|\partial_{\mathbf{X}} \mathbf{\Phi}| \geqslant 1$. The expansiveness is compatible with a finite phase space if the mapping $\mathbf{\Phi}$ sends several different points $\mathbf{X}$ onto the same point $\mathbf{\Phi}(\mathbf{X})$. If entropy is conceived as a measure of disorder in phase space we understand that there is a loss of information and thus production of disorder in such systems. In flows, the property of exactness should be expressed by the assumption that $\partial_{\mathbf{X}} \cdot \mathbf{F} \geqslant 0$ which means that the flow is expanding. According to Eqs. (4)–(6), the entropy production would then be positive. However, Hamiltonian systems are not expanding.

Another proposition has been discussed in the context of the recently introduced thermostatted systems.[1–5] In these systems, the trajectories are attracted toward phase-space regions where the flow is contracting on average, $\partial_{\mathbf{X}} \cdot \mathbf{F}$. In such systems, there is a negative entropy production. Indeed, since trajectories converge to a strange attractor which has a fractal dimension lower than the total phase-space dimension the probability distribution $f_t(\mathbf{X})$ is more disordered at the initial time than at following times. As a consequence, the Gibbs entropy—which is a measure of disorder—decreases. To avoid this difficulty, a hypothetical mechanism of entropy conservation between the system and the thermostat has been assumed:[4] $S_{G,\,\text{total}} = S_{G,\,\text{system}} + S_{G,\,\text{thermostat}} = \text{constant}$. If we now consider the so-defined entropy of the thermostat there is a change of sign in its time variation and the entropy production of the thermostat should thus be positive. Although interesting and useful for the computation of some thermodynamic quantities, this reasoning is unsatisfactory as an explanation of the origin of a positive entropy production.

This discussion shows that the propositions based on the assumption $\partial_{\mathbf{X}} \cdot \mathbf{F} \neq 0$ present shortcomings to explain the increase of entropy in consistency with the known laws of microscopic motion.

The purpose of the present paper is to reconsider the problem of entropy production in the light of new results demonstrating that the invariant measure of open *volume-preserving* systems may become singular if nonequilibrium conditions are imposed at arbitrarily large distances.[14,15] These new results have been obtained by a study of deterministic diffusion in strictly volume-preserving systems of large spatial extension such as the Lorentz gas[16] and the multibaker map.[17] This study has yielded to the explicit construction not only of the hydrodynamic modes of diffusion but also of the nonequilibrium steady states corresponding to gradients of concentration under flux boundary conditions. These nonequilibrium steady states are defined on the *complementary* set of the fractal repeller of the chaotic-scattering approach[17-22] and, therefore, have the plain phase space for support. In finite systems, such nonequilibrium steady states are given by invariant measures which are different from the equilibrium Liouville invariant measure but which are absolutely continuous with respect to the Liouville measure. In the limit of large systems where the concentration gradient is maintained to a fixed value, the nonequilibrium invariant measure becomes singular with respect to the Liouville measure.[14,15] For instance, in the multibaker map, Tasaki and Gaspard have shown that the invariant measure corresponding to a nonvanishing gradient of concentration is given in terms of the nondifferentiable Takagi function in the limit where the gradient is imposed at boundaries which are more and more separated while keeping constant the gradient.[14] The convergence of the invariant measure—which remains absolutely continuous as long as the boundaries are finitely separated—to the singular measure is very rapid in the large-system limit because it is determined by the Lyapunov exponential instability. In this way, the absolute continuity disappears exponentially fast below tiny scales in phase space. This result is of crucial importance for the following arguments.

Indeed, if the invariant measure becomes singular in some limit, we are no longer allowed to use the Gibbs entropy because this entropy is defined with the probability density which only exists if the associated measure ν is absolutely continuous with respect to the Liouville measure $f(\mathbf{X}) = d\nu/d\mathbf{X}$. The fine-grained Gibbs entropy is thus no longer appropriate if the probability density f does not exist. Under such circumstances, it is required to consider a coarse-grained entropy and the constancy of this coarse-grained entropy is in question.

From this remark, we develop in detail the calculation of the production of the coarse-grained entropy in the case of the multibaker model. We show that the singular character of the nonequilibrium invariant measure implies that the coarse-grained entropy production reaches the well-known positive value given by irreversible thermodynamics if the large-system

scaling limit is carried out before the fine-graining limit. We explain that the result should be expected to hold in general chaotic volume-preserving systems of large spatial extension. By this reasoning, irreversible thermodynamics turns out to be compatible with the volume-preserving property $\partial_{\mathbf{X}} \cdot \mathbf{F} = 0$ and there is no need to assume $\partial_{\mathbf{X}} \cdot \mathbf{F} \neq 0$.

The plan of the paper is as follows. In Section II, we describe the problem of entropy production by going back to the original definition of entropy production in the thermodynamics of irreversible processes. In Section III, we introduce the open volume-preserving systems and we discuss the choice of appropriate boundary conditions. A probability measure is defined in such open systems with infinitely many particles in terms of a Poisson suspension over the dynamical system. The time evolution of this probability measure is then formulated. In Section IV, we define the coarse-grained entropy we use in the following and we show that the definition is consistent with the standard equilibrium entropy per unit volume. The time evolution of this coarse-grained entropy and the corresponding entropy production are then defined. In Section V, we apply our definitions to diffusion in the multibaker map. We show that the coarse-grained entropy production is determined by the nondifferentiable Takagi function in the large-system limit and that it gives precisely the entropy production expected from irreversible thermodynamics. Conclusions are drawn in Section VI.

II. ENTROPY PRODUCTION IN IRREVERSIBLE THERMODYNAMICS

The concept of entropy production is introduced in the thermodynamics of irreversible processes.[9-12] In order to identify in deterministic dynamical systems a quantity like the entropy production, we shall first present the phenomenological entropy production and discuss its properties which should be recovered in the deterministic approach. We restrict ourselves to the case of diffusion because we intend to discuss the comparison with deterministic models of diffusion such as the Lorentz gas and the multibaker map.

A first remark is that the thermodynamics of irreversible processes is a macroscopic theory where the quantities are defined as averages over volumes of size larger than the mean free path of the fluid particles. In the case of the diffusion of tracer particles in a fluid, the density evolves in time according to the phenomenological equation

$$\partial_t \rho = D \nabla^2 \rho \tag{7}$$

where $\nabla = \partial_{\mathbf{r}}$ denotes the gradient with respect to the positions $\mathbf{r} = (x, y, z)$ of the physical space and where D is the diffusion coefficient which is here supposed to be constant in space. This phenomenological equation is obtained from the conservation law of tracer particles, $\partial_t \rho + \nabla \cdot \mathbf{j} = 0$, where the tracer current is given by Fick's law, $\mathbf{j} = -D \nabla \rho$. If the tracer concentration is not too high we may suppose that the tracer particles and the fluid form an ideal solution so that the entropy S is given as the integral of the entropy per unit volume or entropy density s:

$$S = \int_V \rho \ln \frac{\rho_0}{\rho} d\mathbf{r} \tag{8}$$

ρ_0 being a constant reference density for which $S(\rho_0) = 0$. The time evolution of the entropy (8) can be derived from the diffusion equation (7) as

$$\frac{dS}{dt} = -\int_{\partial V} d\mathbf{A} \cdot \mathbf{J}_s + \int_V \sigma_s \, d\mathbf{r} = \frac{d_e S}{dt} + \frac{d_i S}{dt} \tag{9}$$

in terms of the entropy current and entropy source

$$\mathbf{J}_s = \mathbf{j} \ln \frac{\rho_0}{e\rho} = (-D \nabla \rho) \ln \frac{\rho_0}{e\rho} \tag{10}$$

$$\sigma_s = D \frac{(\nabla \rho)^2}{\rho} \geqslant 0 \tag{11}$$

In Eq. (9), $d_e S/dt$ is the flow of entropy at the boundaries ∂V of the system and $d_i S/dt$ is the so-called *entropy production* inside the system due to the irreversible process of diffusion. This entropy production is always non-negative according to the 2nd law of thermodynamics:

$$\frac{d_i S}{dt} = \int_V \sigma_s \, d\mathbf{r} \geqslant 0 \tag{12}$$

The entropy production vanishes at equilibrium and is positive away from equilibrium. In contrast, the flow of entropy may take positive or negative values depending on the gradient of concentration imposed at boundaries.

In the following, we consider the underlying deterministic motion of atoms or molecules in the fluid in order to understand how the 2nd law of irreversible thermodynamics can emerge at the macroscopic level from the properties of the microscopic motion.

III. OPEN VOLUME-PRESERVING SYSTEMS

A. The Choice of the Boundary Conditions

We suppose that the system of microscopic particles is volume-preserving and open. The openness of the system is very important if we want to conceive a process of the kind of those described by irreversible thermodynamics. As an example, let us consider an open Lorentz gas composed of a finite number of fixed disks forming a lattice of size L. As $L \to \infty$, the lattice occupies the whole plane and becomes periodic. A point particle undergoes elastic collisions on the disks. This mechanical system has two degrees of freedom, is volume preserving, and conserves energy. If the lattice has a finite horizon (the horizon is the largest possible free flight for the point particle) the Lorentz gas is known to have a positive and finite diffusion coefficient.[16] This open Lorentz gas is a typical scattering system as studied in collision theory.[18-20]

A statistical ensemble of copies of the system is introduced which corresponds to filling the phase space with a gas of infinitely many particles which are independent of each other. The time evolution of the statistical ensemble is governed by the Liouville equation (3) with extra conditions to describe the elastic collisions on the disks. Alternatively, the time evolution of the ensemble can be described by a Frobenius–Perron operator as shown elsewhere.[15] Different boundary conditions can be considered to solve the Liouvillian dynamics in such systems:

(1) *Absorbing boundary conditions.*[17-22] For such a condition, the particle density is supposed to vanish at the boundaries of the finite lattice for all times. This condition is equivalent to the escape of trajectories in free flight to infinity outside the scatterer. In this case, the number N_t of particles inside the scatterer decreases exponentially to zero:

$$N_t \simeq N_0 \exp(-\gamma t) \tag{13}$$

in the double limit where the initial number of particles and the time become infinite: $N_0 \to \infty$ and $t \to \infty$. Eq. (13) defines the so-called escape rate γ. From the viewpoint of thermodynamics, the preceding situation translates as follows. At the level of the phenomenological equation (7), the density at boundaries should be zero for all times: $\rho_t|_{\partial V} = 0$. The diffusion equation is solved with this boundary condition to get

$$\rho_t \simeq \varphi \exp(-\gamma t) \qquad (t \to \infty) \tag{14}$$

where φ is the eigenfunction of

$$D\nabla^2\varphi = -\gamma\varphi \tag{15}$$

associated with the smallest eigenvalue $\gamma \geqslant 0$ and satisfying: $\varphi|_{\partial V} = 0$. If we replace this solution into the phenomenological entropy source (11) we get

$$\sigma_s = D\frac{(\nabla\rho)^2}{\rho} \simeq \exp(-\gamma t)\, D\frac{(\nabla\varphi)^2}{\varphi} \to 0 \tag{16}$$

which vanishes when $t \to \infty$. As a consequence, this situation does not allow us to identify the thermodynamic entropy production as a stationary property because the entropy source vanishes together with the density itself due to the escape of all the particles. This argument indicates that the escape rate may not be identified with the thermodynamic entropy production (at least in the absence of an external field) (cf. refs. 5 and 6).

In order to properly identify the thermodynamic entropy production, we consider the following boundary conditions:

(2) *Flux boundary conditions.*[14, 17] We suppose that the Lorentz-type scatterer is submitted to a continuous flux of particles (see Fig. 1). For instance, a flux of density ρ_- of incoming particles reaches the left-hand side of the scatterer while a flux of density $\rho_+ > \rho_-$ reaches the right-hand side. The particles evolve according to the laws of mechanics. If the flux is continuous in time an invariant measure will establish itself after some time at the level of the statistical ensemble. In such open and infinite systems, we have thus to define a measure ν_t at time t which gives the local density of particles in phase space such that $\nu_t(B)$ is the number of particles in the phase-space region B at time t. We notice that this measure is no longer normalizable because there is an infinity of particles in the whole system: $\nu_t(\Gamma) = \infty$. Thanks to the flux boundary conditions, a steady gradient of concentration can be maintained in these open systems, which is a favorable situation for a possible identification of an entropy production. Indeed, the phenomenological entropy source (11) and, thus, the entropy production (12) are now positive and stationary since

$$\sigma_s = D\frac{(\nabla\rho)^2}{\rho} = D\frac{\left(\dfrac{\rho_+ - \rho_-}{L}\right)^2}{\rho_- + \dfrac{\rho_+ - \rho_-}{L}x} \sim \frac{1}{x+c} \tag{17}$$

where c is a constant.

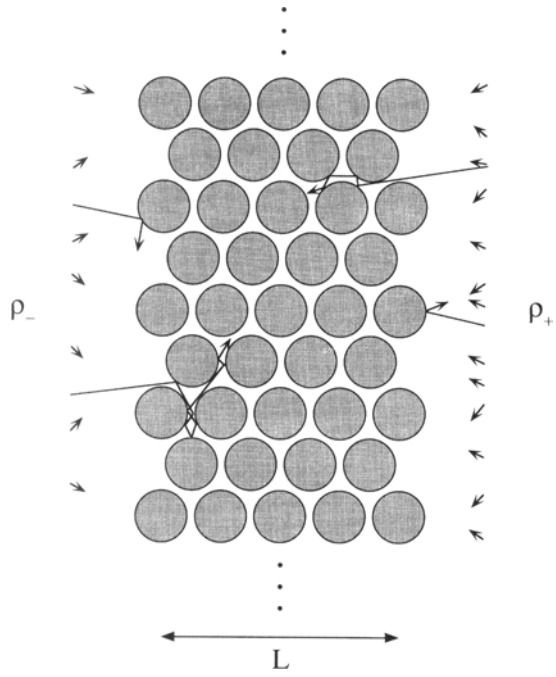

Fig. 1. Schematic representation of a finite Lorentz gas under flux boundary conditions. The finite Lorentz gas is composed of a slab of width L cut out of the infinite Lorentz gas. This slab of disks forms a scatterer for a gas of independent particles arriving at the left-hand boundary with a density ρ_- and at the right-hand wall with a density ρ_+, creating a gradient $\nabla\rho = (1/L)(\rho_+ - \rho_-)\,\mathbf{e}_x$ of concentration.

B. A Probability Measure for Infinite Open Systems

We proceed with the construction of a probability measure μ_t for the Poisson suspension over the dynamical system of measure ν_t.[23] This Poisson suspension is a dynamical system on a phase space which is a direct product of infinitely many copies of the original phase space Γ: $\mathcal{M} = \bigotimes_{i=1}^{\infty} \Gamma_i$. A point in this phase space $\mathcal{M}$ defines an ensemble of copies of the system: $Y = \{\mathbf{X}_i\}_{i=1}^{\infty} \in \mathcal{M}$. We can define subsets of the phase space such that the number of copies $\{\mathbf{X}_i\}$ inside the region B is fixed to the integer k

$$C_{Bk} = \{ Y \in \mathcal{M} : \text{Number}(Y \cap B) = k \} \tag{18}$$

The probability measure of the Poisson suspension corresponding to the measure ν is defined by ref. 23

$$\mu(C_{Bk}) = \frac{[\nu(B)]^k}{k!} \exp[-\nu(B)]$$

and

$$\mu(C_{B_1k_1} \cap C_{B_2k_2}) = \mu(C_{B_1k_1})\,\mu(C_{B_2k_2}) \qquad \text{if} \quad B_1 \cap B_2 = \varnothing \tag{19}$$

To show that this measure is a probability, we consider a partition $\{B_i\}$ of some subset A of the phase space: $A = \bigcup_i B_i \subset \Gamma$ with $B_i \cap B_j = \varnothing$ for $i \neq j$. Each cell B_i of the partition contains a certain number of points of Y given by Number$(Y \cap B_i) = k_i \in \{0, 1, 2, 3, \ldots\}$. The partition induced by $\{B_i\}$ in the phase space $\mathscr{M}$ is constructed as

$$\bigcup_{\{k_i\}} C_{\{B_ik_i\}} \qquad \text{with} \quad C_{\{B_ik_i\}} = C_{B_1k_1} \cap C_{B_2k_2} \cap C_{B_3k_3} \cap \cdots \cap C_{B_mk_m} \tag{20}$$

where $\{k_i\}$ denotes a configuration in which the number of particles in each cell B_i is equal to a given integer k_i. The measure of one element of the induced partition, i.e., the measure of some configuration is obtained by applying the definition (19). Summing over all the configurations $\{k_i\}$, we get

$$\sum_{\{k_i\}} \mu(C_{\{B_ik_i\}}) = \prod_{i=1}^{m} \sum_{k=0}^{\infty} \frac{[\nu(B_i)]^k}{k!} \exp[-\nu(B_i)] = 1 \tag{21}$$

so that the measure μ is normalized to unity at all times t and is thus a probability measure in this sense.

The time evolution under a specific dynamical system (with discrete or continuous time) is defined by the mapping between the initial condition $\mathbf{X}_0$ and the current point $\mathbf{X}_t$ of the trajectory as

$$\mathbf{X}_t = \mathbf{\Phi}^t \mathbf{X}_0 \tag{22}$$

Whereupon, the measure ν_t evolves in time according to

$$\nu_{t+1}(B) = \nu_t(\mathbf{\Phi}^{-1} B) \tag{23}$$

which induces a corresponding evolution for the probability measure μ_t of the Poisson suspension. Let us remark here that the flux boundary conditions break the time-reversal invariance of the steady-state measure ν_∞ under nonequilibrium conditions, in contrast to the Liouville equilibrium measure which is time-reversal invariant.

IV. THE COARSE-GRAINED ENTROPY

A. Definition

Thanks to the probability measure of the Poisson suspension, we are now able to define a coarse-grained entropy for open systems with an infinite number of particles.

The entropy of the measure μ corresponding to the partition $\{B_i\}$ of A in the original phase space Γ is defined in terms of the probabilities of the elements of the induced partition in $\mathscr{M}$. As a consequence, this coarse-grained entropy characterizes the disorder of the probability measure μ in the sense of Boltzmann. When all the cells B_i have the same given size ε we denote the coarse-grained entropy as S_ε. Our definition is thus

$$S_\varepsilon = S(\{B_i\}) = -\sum_{\{k_i\}} \mu(C_{\{B_i k_i\}}) \ln \mu(C_{\{B_i k_i\}}) \tag{24}$$

We notice that more systematic definitions of coarse-grained entropy are possible such

$$S_\varepsilon = \inf_{\text{diam } B_i \leqslant \varepsilon} S(\{B_i\}) \quad \text{or} \quad S_\varepsilon = \sup_{\text{diam } B_i \geqslant \varepsilon} S(\{B_i\}) \tag{25}$$

for instance but, for simplicity, we shall use the definition (24) where all the cells are identical. We also mention that a connection exists between the coarse-grained entropy and the so-called ε-entropy, as discussed elsewhere.[24]

Using the definitions (19) and (20), Eq. (24) becomes

$$S_\varepsilon = -\sum_i \sum_{k=0}^{\infty} \mu(C_{B_i k}) \ln \mu(C_{B_i k}) \tag{26}$$

and

$$S_\varepsilon = \sum_i \nu(B_i) \ln \frac{e}{\nu(B_i)} + \mathscr{R}(\varepsilon) \tag{27}$$

where the rest $\mathscr{R}(\varepsilon) = \sum_i \mathcal{O}[\nu(B_i)^2]$ is important only if $\nu(B_i) \gg 1$ but vanishes for $\varepsilon \to 0$ even if the measure is singular. This rest plays no role in the following argument and may be considered negligible but we shall keep it for rigor.

In the case where the measure ν is absolutely continuous with respect to the Liouville measure, the associated density exists: $f(\mathbf{X}) = d\nu/d\mathbf{X}$. The measures of the cells are given by $\nu(B_i) = f(\mathbf{X}_i)\, \Delta\mathbf{X}$ where $\mathbf{X}_i$ is a point

inside B_i according to the mean theorem of Riemann integration theory and where $\Delta\mathbf{X}$ is the Liouville measure of the cells B_i. In this case, the coarse-grained entropy is given by

$$S_\varepsilon = \left(\ln \frac{e}{\Delta\mathbf{X}}\right) \int_A f(\mathbf{X})\, d\mathbf{X} - \int_A d\mathbf{X}\, f(\mathbf{X}) \ln f(\mathbf{X}) + \mathcal{O}(\Delta\mathbf{X}) + \mathcal{R}(\Delta\mathbf{X}) \quad (28)$$

The second term is nothing else than the Gibbs entropy (1). The first term diverges for $\Delta\mathbf{X} \to 0$. Since $\int_\Gamma f\, d\mathbf{X} = 1$ for a closed system with a normalized measure the first term remains constant in time and may be disregarded. This term fixes the famous constant of entropy in respect of the third law of thermodynamics. This term is very important to establish the correspondence with the entropy of quantum statistical mechanics where ε should be fixed according to $\Delta\mathbf{X} = \Delta^f q\, \Delta^f p = (2\pi\hbar)^f$. Thanks to the previous definition (24), we recover the usual expression of the equilibrium entropy per unit volume for instance in an ideal gas where

$$S_\varepsilon^{(\mathrm{vol})} = \rho \ln \frac{e^{5/2}(2\pi m k_B T)^{3/2}}{\rho\, \Delta^3 q\, \Delta^3 p} + \mathcal{O}(\Delta^3 q\, \Delta^3 p) \quad (29)$$

The previous definition is therefore entirely consistent with standard equilibrium statistical mechanics.[25]

B. The Time Variation of the Coarse-Grained Entropy

The coarse-grained entropy (27) of a domain A evolves in time and we are interested in its time variation, i.e., in the difference between its values at two successive instants of time separated for instance by a unit time:

$$\begin{aligned} \Delta S_\varepsilon &= S_\varepsilon(t+1; A) - S_\varepsilon(t; A) \\ &= \sum_{B_i \subset A} \left[\nu_t(\mathbf{\Phi}^{-1} B_i) \ln \frac{e}{\nu_t(\mathbf{\Phi}^{-1} B_i)} - \nu_t(B_i) \ln \frac{e}{\nu_t(B_i)} \right] + \mathcal{R}(\varepsilon) \end{aligned} \quad (30)$$

If the measure ν_t is absolutely continuous with respect to the Liouville measure we obtain

$$\begin{aligned} \Delta S_\varepsilon &= \int_{\mathbf{\Phi}^{-1} A} d\mathbf{X}\, f_t(\mathbf{X}) \ln \left| \frac{\partial \mathbf{\Phi}}{\partial \mathbf{X}} \right| \\ &\quad + \left(\int_{A_{\mathrm{in}}} - \int_{A_{\mathrm{out}}} \right) d\mathbf{X}\, f_t(\mathbf{X}) \ln \frac{e}{f_t(\mathbf{X})\, \Delta\mathbf{X}} + \mathcal{O}(\Delta\mathbf{X}) + \mathcal{R}(\Delta\mathbf{X}) \end{aligned} \quad (31)$$

where we used the identity

$$\int_{\Phi^{-1}A} - \int_A = \int_{A_{\text{in}}} - \int_{A_{\text{out}}} \tag{32}$$

that the difference between the integrals over the preimage of A and over A itself is equal to the difference between the integrals over the domain A_{in} which enters A and the domain A_{out} which exits A.

In a volume-preserving system, the Jacobian of the mapping Φ is equal to unity so that there is no term in (31) which could be identified with the entropy production. However, this holds as long as the density exists so that the terms $\mathcal{O}(\Delta \mathbf{X})$ may be neglected. This is no longer the case for singular measures, which is the cornerstone of our argument.

Let us proceed with the separation of the variation of the entropy into an entropy flow and an entropy production in analogy with Eq. (9). The entropy flow can be naturally defined as the difference between the coarse-grained entropies of the domains ingoing and outgoing A

$$\Delta_e S_\varepsilon = S_\varepsilon(t; A_{\text{in}}) - S_\varepsilon(t; A_{\text{out}}) = S_\varepsilon(t; \Phi^{-1}A) - S_\varepsilon(t; A) \tag{33}$$

where the last identity follows from Eq. (32).

The entropy production can now be defined as

$$\Delta_i S_\varepsilon = \Delta S_\varepsilon - \Delta_e S_\varepsilon \tag{34}$$

In the next section, we shall apply the previous definitions to a simple model of diffusion.

V. ENTROPY PRODUCTION IN THE MULTIBAKER MAP

A. The Model

The multibaker map is a model of deterministic diffusion which can be seen as a caricature of the collision dynamics of the Lorentz gas.[14, 17, 19] Indeed, the dynamics of the elastic collisions of a particle from disk to disk is given by a Birkhoff map which governs the coordinates of the successive impact points and velocity angles at collisions in the Lorentz gas. The Birkhoff map is area-preserving and of hyperbolic character. The Lorentzian dynamics can be simplified while keeping its two aforementioned essential properties. We replace the Birkhoff map of the Lorentz gas by transformations of the baker type between several squares which

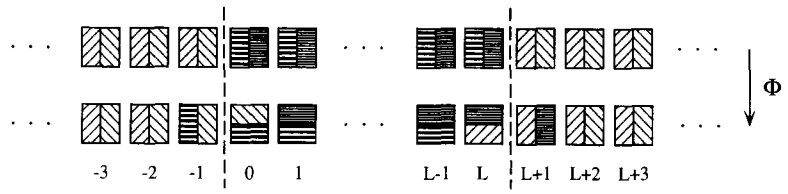

Fig. 2. Representation of the action of the open multibaker map in its phase space which is composed of an infinity of squares. The map acts like a baker transformation on the chain of the squares $0 \leqslant n \leqslant L$ and by left or right translations outside the chain up to infinity.

correspond to the different disks of the Lorentz gas. Points are mapped from square to square like particles undergoing collisions from disk to disk, which results in a deterministic motion of diffusion. The multibaker can also be viewed as a deterministic realization of a symmetric random walk.

Since we consider finite scatterers we suppose that the transformation is of the baker type only on a finite number of squares forming a chain of length $L+1$. At both ends of the chain, particles may exit or enter the chain in free motion with velocities $+1$ or -1. This is realized by a simple composition of translations to the left or the right in the half squares extending from both ends to infinity (see Fig. 2). The phase space is therefore given by (n, x, y) where $0 \leqslant x, y \leqslant 1$ and $-\infty < n < +\infty$ is an integer labeling the square where the particle currently lies. The multibaker map is thus[14]

$$\mathbf{\Phi}(n, x, y) = \begin{cases} \left(n-1, 2x, \dfrac{y}{2}\right), & 0 \leqslant x < 1/2, \quad +1 \leqslant n \leqslant L+1 \\ \left(n+1, 2x-1, \dfrac{y+1}{2}\right), & 1/2 \leqslant x \leqslant 1, \quad -1 \leqslant n \leqslant L-1 \\ (n-1, x, y), & 0 \leqslant x < 1/2, \quad n \leqslant 0 \quad \text{or} \quad L+2 \leqslant n \\ (n+1, x, y), & 1/2 \leqslant x \leqslant 1, \quad n \leqslant -2 \quad \text{or} \quad L \leqslant n \end{cases} \tag{35}$$

B. Flux Boundary Conditions and the Steady-State Measure

A flux of particles is supposed to flow continuously across the chain. The particles in the half squares, $1/2 \leqslant x \leqslant 1$ with $n \leqslant -1$, arriving from infinity on the left-hand end are assumed to be uniformly distributed with the density ρ_-, while those in the half squares, $0 \leqslant x < 1/2$ with $L+1 \leqslant n$, arriving on the right-hand end have a density ρ_+.

As a consequence of the chaotic time evolution inside the chain, there is a fractal repeller in the squares $0 \leqslant n \leqslant L$, which has the partial Hausdorff dimension[14]

$$d_{\mathrm{H}} = 1 + \frac{1}{2 \ln 2} \ln \cos \frac{\pi}{L+2} = 1 - \frac{1}{4 \ln 2} \left(\frac{\pi}{L+2} \right)^2 + \mathcal{O}(L^{-4}) \tag{36}$$

Therefore, there are three types of orbits which exit the scatterer (i.e., for $n \leqslant -1$ and $L+1 \leqslant n$):

(1) The orbits which entered at the left-hand end: The density is ρ_- in their vicinity.

(2) The orbits which entered at the right-hand end: The density is ρ_+ in their vicinity.

(3) The orbits of the unstable manifolds of the repeller. The unstable manifolds are segments of horizontal lines which separate the regions of density ρ_+ from those of density ρ_-.

Since the repeller is fractal, it is also the case for its unstable manifolds so that the measure is very complicated on the half squares which exit the chain. However, the density always exists since it is equal to either ρ_+ or ρ_-, except on the set of the unstable manifolds which is of zero Lebesgue measure.

In the limit $L \to \infty$, the partial Hausdorff dimension (36) of the unstable manifolds tends to the unit value. We understand that, as a consequence, the invariant measure becomes singular because the density alternates between the values $\rho_\pm$ over thiner and thiner regions across the phase space.

Since we expect singular measures in some limit we define the cumulative distribution function associated with the measure ν_t as[14]

$$G_t(n, x, y) = \nu_t(n, [0, x[\otimes [0, y[) \tag{37}$$

which exists as a function even when the density does not exist. With this definition, Tasaki and Gaspard have shown that the invariant measure corresponding to the gradient of concentration

$$\nabla \rho = \frac{\rho_+ - \rho_-}{L+2} \tag{38}$$

is given by the cumulative function:

$$G_\infty(n, x, y) = x[\rho_n y + (\nabla \rho)\, T_n(y)] \equiv x g_n(y) \tag{39}$$

where

$$\rho_n = (\nabla\rho)(n+1) + \rho_- \tag{40}$$

is the average density in the nth square and where $\{T_n(y)\}$ are the incomplete Takagi functions defined by the iterations

$$T_n(y) = \begin{cases} \frac{1}{2}T_{n-1}(2y) + y, & 0 \leqslant y < \frac{1}{2} \\ \frac{1}{2}T_{n-1}(2y-1) + 1 - y, & \frac{1}{2} \leqslant y \leqslant 1 \end{cases} \tag{41}$$

with the boundary conditions, $T_{-1}(y) = T_{L+1}(y) = 0$.[14] The incomplete Takagi functions are differentiable almost everywhere because it is the case for the cumulative function (39) since the corresponding density exists according to the above reasoning. Let us mention here the property that $T_n(0) = T_n(1) = 0$.

However, in the limit where $L \to \infty$ and $(\rho_+ - \rho_-) \to \infty$ keeping constant the gradient (38), the incomplete Takagi functions converge to the Takagi function defined by the following iteration[26]

$$T(y) = \begin{cases} \frac{1}{2}T(2y) + y, & 0 \leqslant y < \frac{1}{2} \\ \frac{1}{2}T(2y-1) + 1 - y, & \frac{1}{2} \leqslant y \leqslant 1 \end{cases} \tag{42}$$

The convergence is exponentially fast like[14]

$$\sup_{0 \leqslant y \leqslant 1} |T_n(y) - T(y)| \leqslant 2(\tfrac{1}{2})^{\min(n,\, L-n)} \tag{43}$$

so that $T_n(y) = T(y) + \mathcal{O}(2^{-L/2})$ in the middle of the chain at $n = [L/2]$.

The Takagi function is nondifferentiable almost everywhere because its derivative with respect to y is formally given by[15]

$$\frac{dT}{dy}(y) = \sum_{\tau=0}^{\infty} \xi[\beta^\tau(y)] \tag{44}$$

where $\beta(y) = 2y \pmod 1$ is the Bernoulli map of the interval and $\xi(y) = \pm 1$ if $y < 1/2$ or $y > 1/2$. The derivative of the Takagi function is thus given by a sum of plus and minus ones corresponding to the jumps of the particle to the right ($\xi = +$) or to the left ($\xi = -$) under the inverse multibaker mapping $\mathbf{\Phi}^{-1}$. Figure 3 shows the first few iterations of (42) where we observe that, at the τth iteration, the function has already converged to its limit values at the points $y = m/2^\tau$ with $m = 0, 1, 2, \ldots, 2^\tau$.

These points can be assigned to symbolic sequences with symbols $\omega_\tau = 0$ or 1 whether $\xi_\tau = +1$ or -1 according to

$$y_{\omega_1 \cdots \omega_\tau} = \frac{\omega_1}{2} + \frac{\omega_2}{4} + \cdots + \frac{\omega_\tau}{2^\tau} \tag{45}$$

Using the construction of Fig. 3, we deduce the following properties of the Takagi function:

$$2T\left(y_{\omega_1 \cdots \omega_\tau} + \frac{1}{2^{\tau+1}}\right) - T\left(y_{\omega_1 \cdots \omega_\tau} + \frac{1}{2^\tau}\right) - T(y_{\omega_1 \cdots \omega_\tau}) = \frac{1}{2^\tau} \tag{46}$$

and

$$\sum_{\omega_1 \cdots \omega_\tau} \left[T\left(y_{\omega_1 \cdots \omega_\tau} + \frac{1}{2^\tau}\right) - T(y_{\omega_1 \cdots \omega_\tau}) \right]^2 = \frac{\tau}{2^\tau} \tag{47}$$

Both properties will be used in the following. We notice that the Takagi function has no second derivative with respect to y. If it had, the second derivative would decrease like $2^{-2\tau}$ in contradiction with Eq. (46).

In the limit $L \to \infty$, we moreover observe that the invariant measure (39) remains absolutely continuous with respect to the Lebesgue measure in the *unstable* direction x. This is because an initially regular measure is stretched in the unstable direction under the time evolution and, thus, converges to a measure which is absolutely continuous in this direction. The measure is furthermore uniform in the unstable direction because the stretching is uniform in the multibaker map. In contrast, the measure (39) becomes singular in the stable direction because of the difference between the ingoing densities imposed at both ends. Formally, the density in the middle of an arbitrarily long chain is given by

$$f_\infty(n, x, y) = \partial_x \partial_y G_\infty(n, x, y) = \rho_n + (\nabla \rho) \sum_{\tau=0}^{\infty} \xi[\beta^\tau(y)] \tag{48}$$

where the last term is a discrete form of the integral over the velocity of the diffusive particle: $\int_0^{-\infty} v(\mathbf{\Phi}^\tau \mathbf{X})\, d\tau$.[15] In the form (48), we recognize a steady-state measure of the type introduced by Lebowitz and McLennan.[27, 28]

C. The Coarse-Grained Entropy Production

The presence of this singular term is at the origin of a positive entropy production, as shown below.

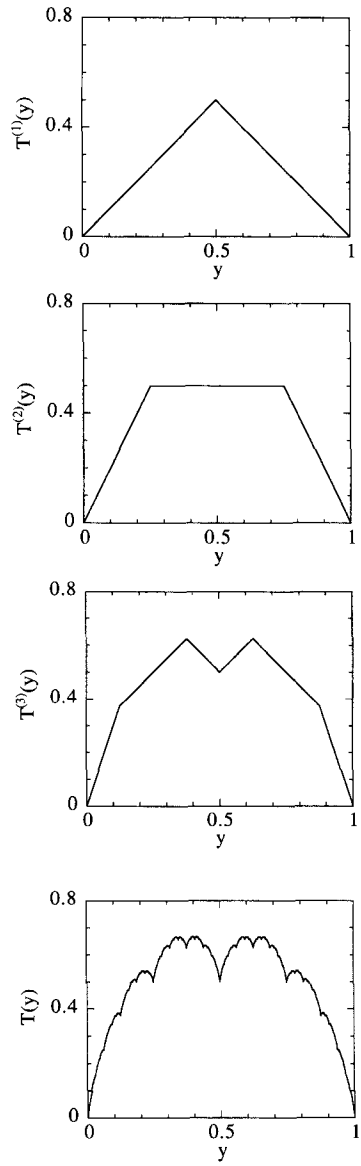

Fig. 3. Construction of the Tagaki function by successive iterations according to Eq. (42): $\lim_{\tau\to\infty} T^{(\tau)}(y) = T(y)$, the seed function being zero.

We consider the coarse-grained entropy production (34) in the nth square of the chain, we denote by A. We take the cells B_i of size Δx in the unstable direction x and of size

$$\Delta y = \frac{1}{2^\tau} \tag{49}$$

in the stable direction y to take advantage of the symbolic decomposition (45). In this case, the role of ε is played by $(\Delta x, \Delta y)$. The number of cells $(\Delta x, \Delta y)$ in the unit square A is equal to $1/\Delta x$ in the unstable direction x and to $1/\Delta y = 2^\tau$ in the stable direction y. From Eq. (39), we infer that the measure of the cell

$$B_i = [x, x + \Delta x[\otimes [y_{\omega_1 \cdots \omega_\tau}, y_{\omega_1 \cdots \omega_\tau} + \Delta y[\ , \tag{50}$$

is

$$\nu(B_i) = \Delta x \, \Delta g_n(\omega_1 \cdots \omega_\tau)$$
$$\text{with} \quad \Delta g_n(\omega_1 \cdots \omega_\tau) = g_n(y_{\omega_1 \cdots \omega_\tau} + \Delta y) - g_n(y_{\omega_1 \cdots \omega_\tau}) \tag{51}$$

with the property that

$$\sum_{\omega_1 \cdots \omega_\tau} \Delta g_n(\omega_1 \cdots \omega_\tau) = g_n(1) - g_n(0) = \rho_n \tag{52}$$

In order to calculate the time variation (30) of the coarse-grained entropy, we must consider the cells B_i of size $(\Delta x, \Delta y)$ in the square $A = (n, [0, 1] \otimes [0, 1])$ as well as their preimages $\Phi^{-1} B_i$ of size $(\Delta x/2, 2\,\Delta y)$ which belong to the half squares $\Phi^{-1} A = (n+1, [0, 1/2[\otimes [0, 1]) \cup (n-1, [1/2, 1] \otimes [0, 1])$ (see Fig. 4). The time variation of the coarse-grained entropy at the steady state is thus given as

$$\Delta S_\varepsilon = \left[\left(\frac{\Delta x}{2}, 2\,\Delta y \right) \text{-entropy of } \Phi^{-1} A \right] - [(\Delta x, \Delta y)\text{-entropy of } A] \tag{53}$$

with the coarse-grained entropy (27).

On the other hand, the entropy flow (33) is

$$\Delta_e S_\varepsilon = [(\Delta x, \Delta y)\text{-entropy of } \Phi^{-1} A] - [(\Delta x, \Delta y)\text{-entropy of } A] \tag{54}$$

As a consequence, we obtain the entropy production (34) as

$$\Delta_i S_\varepsilon = \left[\left(\frac{\Delta x}{2}, 2\,\Delta y \right) \text{-entropy of } \Phi^{-1} A \right] - [(\Delta x, \Delta y)\text{-entropy of } \Phi^{-1} A] \tag{55}$$

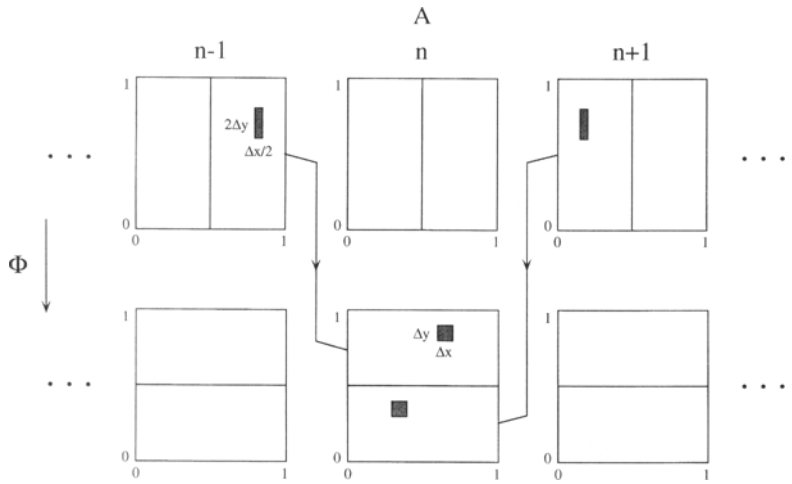

Fig. 4. Action of the multibaker map on three successive squares of the chain and on the cells $\{B_i\}$ of a $(\Delta x, \Delta y)$-partition of the nth square taken as the domain A in Eq. (56).

or, by using the stationarity that implies $\Delta S_\varepsilon = 0$ in Eq. (53), we get

$$\Delta_i S_\varepsilon = [(\Delta x, \Delta y)\text{-entropy of } A] - \left[\left(2\,\Delta x, \frac{\Delta y}{2}\right)\text{-entropy of } A\right] \tag{56}$$

We now calculate the entropy production (56) using the expression (27) for the coarse-grained entropy with the above choice of the cells B_i. According to the uniformity in the x-direction, the sum over all the cells of size Δx in the interval $[0, 1]$ contributes by a factor $1/\Delta x$, which cancels the factor Δx. Besides, we observe that the cell $\omega_1 \cdots \omega_\tau$ is composed of the two cells $\omega_1 \cdots \omega_\tau 0$ and $\omega_1 \cdots \omega_\tau 1$, so that their probability weights add like $\Delta g_n(\omega_1 \cdots \omega_\tau) = \Delta g_n(\omega_1 \cdots \omega_\tau 0) + \Delta g_n(\omega_1 \cdots \omega_\tau 1)$. The property (52) is moreover used to eliminate the factors $e/\Delta x$ in the logarithms. Finally, the coarse-grained entropy production of the multibaker is explicitly obtained as

$$\Delta_i S_\varepsilon = \sum_{\omega_1 \cdots \omega_\tau} \left[\Delta g_n(\omega_1 \cdots \omega_\tau 0) \ln \frac{2\,\Delta g_n(\omega_1 \cdots \omega_\tau 0)}{\Delta g_n(\omega_1 \cdots \omega_\tau 0) + \Delta g_n(\omega_1 \cdots \omega_\tau 1)} \right.$$
$$\left. + \Delta g_n(\omega_1 \cdots \omega_\tau 1) \ln \frac{2\,\Delta g_n(\omega_1 \cdots \omega_\tau 1)}{\Delta g_n(\omega_1 \cdots \omega_\tau 0) + \Delta g_n(\omega_1 \cdots \omega_\tau 1)} \right] \tag{57}$$

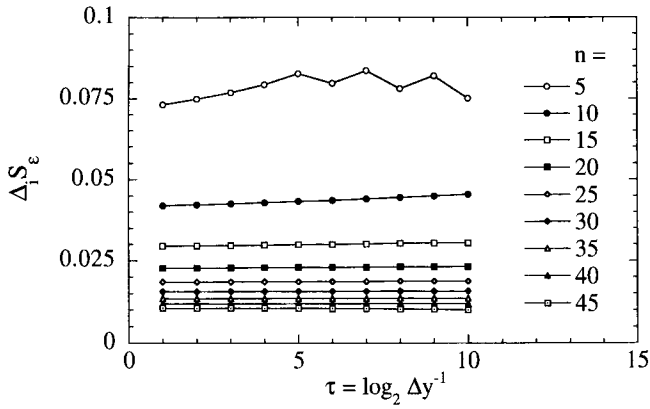

Fig. 5. The coarse-grained entropy production (57) calculated numerically for a multibaker chain of length $L = 50$, a unit gradient $\nabla\rho = 1$, and $\rho_- = 1$. The entropy production is depicted as a function of $\tau = \log_2(1/\Delta y)$, for different positions n along the chain.

where we have taken the limit $\Delta x \to 0$ to eliminate the term of $\mathcal{O}(\Delta x)$ which plays no role in our argument because the measure remains regular in the unstable direction x.

The first remarkable property of this entropy production is its positivity

$$\Delta_i S_\varepsilon = \sum \left(a \ln \frac{2a}{a+b} + b \ln \frac{2b}{a+b} \right) \geqslant 0 \tag{58}$$

which follows from the concavity of the function $z \ln z$ [i.e., $(d/dz)^2(z \ln z) \geqslant 0$].

We have numerically calculated the expression (57) for a multibaker chain of length $L = 50$. Figure 5 shows $\Delta_i S_\varepsilon$ as a function of $\tau = \log_2(1/\Delta y)$. We observe that $\Delta_i S_\varepsilon$ is approximately constant with respect to τ. Therefore, the entropy production as a function of Δy displays a plateau at a positive value which depends on the position n along the chain. In the case of Fig. 5, we have taken $\rho_- = 1$ and $\nabla\rho = 1$ so that the mean density in the nth cell is $\rho_n = n + 2$. Figure 6 shows $\Delta_i S_\varepsilon$ as a function of the position n, for different values of Δy.

We then compare with the behavior expected from the phenomenological entropy production in the nth square of unit length, which is given by

$$\Delta_i S_{\text{phenom}} = D \frac{(\nabla\rho)^2}{\rho_n} = \frac{1}{2(n+2)} \tag{59}$$

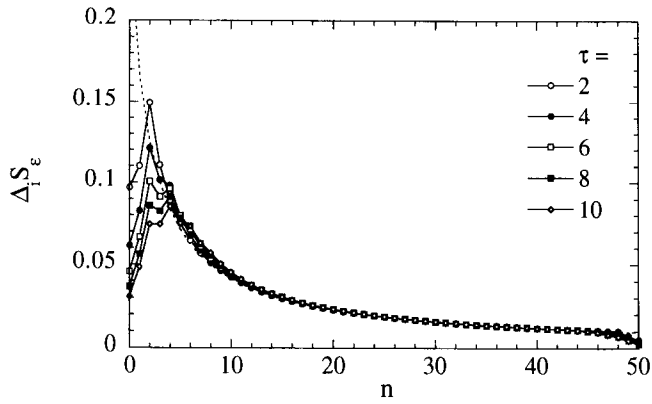

Fig. 6. The same entropy production as in Fig. 5 for a multibaker chain of length $L = 50$ but depicted here as a function of the position n, for different values of Δy. The dashed line represents the phenomenological entropy production (59).

because the diffusion coefficient is $D = 1/2$ in the multibaker. In Fig. 6, we observe a remarkable agreement between both curves except at the ends of the chain. The decrease of the coarse-grained entropy production at the ends is explained by the fact that the density is there constant to the values $\rho_\pm$ over large parts of the square so that $\Delta_i S_\varepsilon$ tends to zero more rapidly at the ends than in the middle of the chain as $\Delta y \to 0$. The critical value of Δy below which $\Delta_i S_\varepsilon$ tends to zero depends on the position n along the chain in a way which is determined by Eq. (43) as

$$\Delta y_c \sim 2^{-\min(n,\, L-n)} \tag{60}$$

Hence, the critical scale decreases exponentially fast as $L, n \to \infty$ due to the Lyapunov instability of the dynamics. For a fixed value of Δy, we should thus observe the vanishing of the coarse-grained entropy production only in some boundary layers of the order of the inverse Lyapunov distance: $n_c \sim (\ln 2)^{-1}$. Away from these small boundary layers, the coarse-grained entropy production reaches a positive value we shall now calculate.

We suppose that we are in the middle of the chain at values of Δy above the critical value (60) so that the incomplete Takagi functions in (39) can be replaced by the limiting Takagi function. In Eqs. (57)–(58), we set $a = m + \delta/2$ and $b = m - \delta/2$ and we expand in Taylor series of δ/m to get

$$\Delta_i S_\varepsilon = \sum m \left[\left(\frac{\delta}{2m} \right)^2 + \frac{1}{6} \left(\frac{\delta}{2m} \right)^4 + \mathcal{O}\left(\frac{\delta^6}{m^6} \right) \right] \tag{61}$$

with

$$m = \rho_n \frac{\Delta y}{2} + (\nabla\rho)\frac{\Delta T_a + \Delta T_b}{2} \qquad \text{and} \qquad \delta = (\nabla\rho)(\Delta T_a - \Delta T_b) \quad (62)$$

where

$$\Delta T_a = T\left(y_{\omega_1 \cdots \omega_\tau} + \frac{1}{2^{\tau+1}}\right) - T(y_{\omega_1 \cdots \omega_\tau})$$

$$\Delta T_b = T\left(y_{\omega_1 \cdots \omega_\tau} + \frac{1}{2^\tau}\right) - T\left(y_{\omega_1 \cdots \omega_\tau} + \frac{1}{2^{\tau+1}}\right) \quad (63)$$

We can here use the properties (46) and (47) of the Takagi function which imply that

$$\Delta T_a - \Delta T_b = \frac{1}{2^\tau} = \Delta y \quad (64)$$

$$\sum (\Delta T_a + \Delta T_b)^2 = \frac{\tau}{2^\tau} = \Delta y \log_2 \frac{1}{\Delta y} \quad (65)$$

and, moreover, the property that $\sum (\Delta T_a + \Delta T_b) = T(1) - T(0) = 0$. Expanding in series of $(\nabla\rho)/\rho_n$, we finally obtain

$$\Delta_i S_\varepsilon = \frac{(\nabla\rho)^2}{2\rho_n} + \frac{(\nabla\rho)^4}{2\rho_n^3}\left(\frac{1}{6} + \log_2 \frac{1}{\Delta y}\right) + \mathcal{O}\left[\frac{(\nabla\rho)^6}{\rho_n^5}\right] \quad (66)$$

for $\Delta y > \Delta y_c$. We notice that, if the Takagi function was twice differentiable Eq. (64) would behave like Δy^2 instead of Δy, so that the leading term of Eq. (66) would vanish as $\Delta y \to 0$.

The remarkable result is that the leading term is precisely the positive entropy production expected from irreversible thermodynamics. The next term is a correction which is small like $(\nabla\rho)^4$ and which slowly increases as $\Delta y \to \Delta y_c$. This behavior is observed in Figs. 5 and 6: Near the left-hand end of the chain where ρ_n is small enough, we observe a slow linear increase of $\Delta_i S_\varepsilon$ versus $\log_2(1/\Delta y)$ in Fig. 5. This increase becomes negligible where ρ_n is larger. We emphasize that these results are entirely due to the Tagaki function and to its nondifferentiability, which therefore controls the positive entropy production.

VI. CONCLUSIONS

In this paper, we have revisited the problem of entropy production in volume-preserving system under steady nonequilibrium conditions.

We have supposed that the system sustains a diffusion process and is submitted to flux boundary conditions. With such boundary conditions, the invariant measure is no longer the uniform Liouville measure. Indeed, the invariant measure at a phase-space point $\mathbf{X} \in \Gamma$ has the density of the boundary point $\mathbf{X}_b \in \partial\Gamma$ from which the point $\mathbf{X}$ is issued under time evolution: $\mathbf{X} = \mathbf{\Phi}^t \mathbf{X}_b$. In the limit where fixed nonequilibrium gradients are imposed at arbitrarily large distances, arbitrarily small subsets of phase space contain points coming from almost every point of the boundary $\partial\Gamma$ so that the density varies arbitrarily fast and the measure becomes singular. These asymptotic invariant measures corresponding to nonequilibrium steady states have been known since works by Lebowitz and McLennan.[27,28] They are given as Zubarev local integrals of motion[15,29] (see also ref. 30). In the example of the multibaker map, the cumulative function of these measures is expressed in terms of the nondifferentiable Takagi function.[14] The singular character of these steady-state measures forces us to use a coarse-grained entropy instead of the Gibbs entropy which only applies to regular measures. We have then showed that the coarse-grained entropy production is consistently positive and, above all, has the behavior expected from irreversible thermodynamics for diffusion. Our result can be formulated as

$$\lim_{\varepsilon \to 0} \lim_{(\nabla\rho)/\rho \to 0} \lim_{L \to \infty} \frac{\rho}{(\nabla\rho)^2} \Delta_i S_\varepsilon = D > 0 \tag{67}$$

where the limits are not commutative. Because the limit $L \to \infty$ of a large chain has to be taken before the fine-grained limit $\varepsilon \to 0$ we should understand the entropy production as an emerging property appearing in the scaling limit of large systems. We emphasize that the previous result is independent of the particular coarse graining because the entropy production defined in (67) does not vanish in the fine-grained limit. This is in contrast with the usual coarse-graining considerations which depend on the particular partition used in the coarse graining. The nontrivial fine-grained limit is here due to the singular character of the invariant measure, which is the new result.

We notice that the singular character of the invariant measure under nonequilibrium conditions appears very rapidly in large systems because of the convergence property (43). We can translate this rapid convergence for a fluid of particles of diameter d as follows. From the analogy with a

Lorentz gas, the transition from one square of the multibaker to neighboring squares corresponds to the free flight of a particle from a collision to the next one, i.e., to a mean free path $\ell = 1/(\rho\sigma)$ where ρ is the particle density and $\sigma = \pi d^2$ the collision cross-section. At each collision, a perturbation $\delta\alpha$ on a velocity angle is amplified like $\delta\alpha \to (2\ell/d)\,\delta\alpha$. At a distance $z = m\ell$ of m mean free paths from the wall, about m collisions have occurred so that the critical scale below which the absolute continuity is hidden is $\Delta\alpha_c \sim (d/2\ell)^m$. Expressed in terms of the distance z from the wall, the critical scale would be $\Delta\alpha_c \sim \exp(-z\lambda)$ where $\lambda \sim (1/\ell)\ln(2\ell/d)$ is the Lyapunov exponent per unit distance. The width of the boundary layer where the coarse-grained entropy production should be smaller than its bulk thermodynamic value should thus be $z_c \sim \ell/\ln(\ell/d)$. It is only beyond this boundary layer that we may expect the coarse-grained entropy production to reach its thermodynamic value. We notice that the scale where the absolute continuity of the nonequilibrium invariant measure is hidden becomes exponentially small as $z \gg z_c$ toward the bulk of the fluid because of the Lyapunov dynamical instability. Therefore, the bulk behavior of the nonequilibrium steady state becomes essentially determined by the nondifferentiability of the Tagaki function or, equivalently, by the singularity of the Lebowitz–McLennan steady-state measures. For these reasons, we should expect that the results of the present work are general.

We may conclude that we have here identified the appropriate mechanism at the origin of the thermodynamic entropy production in volume-preserving systems.

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