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Entropy balance in the presence of drift and diffusion currents: An elementary chaotic map approach

Jürgen Vollmer,[1] Tamás Tél,[2] and Wolfgang Breymann[3]
[1]*Fachbereich Physik, Universität-GH Essen, D-45117 Essen, Germany*
[2]*Institute for Theoretical Physics, Eötvös University, H-1088 Budapest, Puskin utca 5-7, Hungary*
[3]*Olsen & Associates, Seefeldstrasse 233, OH-8008 Zürich, Switzerland and Institute of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland*

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We study the rate of irreversible entropy production and the entropy flux generated by low-dimensional dynamical systems modeling transport processes induced by the simultaneous presence of an external field and a density gradient. The key ingredient for understanding entropy balance is the coarse graining of the phase-space density. This mimics the fact that ever refining phase-space structures caused by chaotic dynamics can only be detected by finite resolution. Calculations are carried out for a generalized multibaker map. For the time-reversible dissipative (thermostated) version of the model, results of nonequilibrium thermodynamics are recovered in the large system limit. Independent of the choice of boundary conditions, we obtain the rate of irreversible entropy production per particle as u^2/D, where u is the streaming velocity (current per density) and D is the diffusion coefficient. [S1063-651X(98)09407-0]

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I. INTRODUCTION

Transport models based on dynamical systems with only a *few degrees of freedom* have become a subject of intensive recent studies [1–19]. They illustrate how macroscopic transport coefficients are related to the properties of the microscopic dynamics. It is a remarkable discovery that in chaotic dynamical systems a rate of irreversible entropy production can be defined [2,4,5,7,20–30], which is, in the large system limit, consistent with the results of nonequilibrium thermodynamics. However, the choice of the entropy for which the above statement holds has long been controversial. Recently, a coarse-grained entropy has been proposed [21–23,25,26,29] (for a review on general considerations, cf. [30]). The first attempt to derive a complete entropy balance equation for such an entropy is due to Gaspard [25] for a map modeling pure diffusion. In the most general setting, however, two types of currents are present: a drift current induced by an external field, and a diffusion current due to a density gradient. The aim of the present paper is to show that (i) an entropy defined with respect to coarse-grained phase-space densities is the appropriate analog of the thermodynamic entropy also in this case, and (ii) the microscopic dynamics has to have a *reversible* [31] dissipation mechanism in order to have a macroscopic limit consistent with thermodynamics. The deviation from phase-space conservation should model the effect of a thermostat [2,1,7].

It is essential for the definition of a thermodynamically relevant entropy that it is independent of time in a macroscopically stationary state. A coarse-grained entropy fulfills this requirement. This choice is physically motivated by the finite resolution of any observation. The use of coarse-grained entropies also avoids the well-known objection against the validity of statistical averages due to Poincaré recurrences because for strongly chaotic systems recurrences can only occur for initial distributions with arbitrarily fine phase-space structure. Such initial conditions cannot be realized in a coarse-grained approach.

In order to be able to carry out explicit calculations, we consider a multibaker map introduced recently [29]. It consists of a chain of N rectangular cells of size $\Gamma = a \times b$ such that the phase space is a rectangle of size $Na \times b$ in the (x,y) plane. The average phase-space density, ϱ_m, in cell $m(1 \leqslant m \leqslant N)$ is called the *cell density*, and the sum $\Gamma \Sigma_{m=1}^{N} \varrho_m$ amounts to the total number of particles in the system [32]. Coarse graining is carried out in *every cell* after each time step. The central object of our investigation is the *coarse-grained entropy* S_m of cell m defined by using the cell density ϱ_m as

$$S_m = -\Gamma \varrho_m \ln \varrho_m . \tag{1}$$

We claim that the proper thermodynamic entropy of a large system consisting of $N \gg 1$ cells is

$$S = \sum_{m=1}^{N} S_m . \tag{2}$$

In these equations the Boltzmann constant k_B has been suppressed for convenience. The expressions we obtain for quantities having a well-defined large system limit are meaningful since they turn out to be independent of the particular choice of the coarse graining (cf. Sec. VIII).

A change of S_m can only be due to a temporal variation of the cell density. This entropy change can be decomposed into an *entropy flux* through the boundaries of cell m and another contribution, which will be called the *irreversible entropy production*. Even when the system is in a steady state there can be an entropy flux flowing through the boundaries. This contribution to the change of entropy must then be counterbalanced by the irreversible entropy production. The latter is caused by averaging over the inhomogeneities generated by the dynamics in the phase-space density $\varrho_m(x,y)$ of cell m. The two contributions to the full entropy change will be computed based on the *Gibbs entropy*

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$$S_m^{(G)} = -\int_{\text{cell } m} \varrho_m(x,y) \ln \varrho_m(x,y)\, dx\, dy \tag{3}$$

of cell m.

For a steady state this entropy eventually has a negative time derivative in a dynamical system, which has been argued to be related to the irreversible entropy production [2,4,20,29]. The Gibbs entropy, however, does not fulfill the thermodynamic requirements for a well-defined entropy since, in nonequilibrium systems, it is not bounded from below. In a steady state of an externally driven thermostated system [2] or in open systems [21,25] it decreases at a constant rate. This is due to the presence of an attractor or a saddle in the phase space. A proper modeling of transport by means of dynamical systems requires, in our view, the *mixing* property [33] of the dynamics. Since this implies chaoticity, the above mentioned attractor or saddle is a strange invariant set and generates fractal structures in the phase-space density on ever-refining scales during time evolution.

Our goal will be to compare the difference between the Gibbs entropy, $S_m^{(G)}$, and the thermodynamically well-behaved coarse-grained entropy, S_m, for the multibaker map. This allows us to identify the entropy flux and the irreversible entropy production of arbitrary steady and non-steady-states. To make contact with nonequilibrium thermodynamics, we consider the macroscopic limit where the cell size a is much smaller than the linear size $L = Na$ of the system $(N \gg 1)$ and the time unit τ of the dynamics is much shorter than that of the macroscopic relaxations. In this limit both a and τ tend to zero,

$$a \to 0, \quad \tau \to 0, \tag{4}$$

while the transport parameters are kept finite. The results are expected to be independent of the order of the limits. Later calculations will often be performed in two steps; first, we carry out the limit $\tau \to 0$, and subsequently $a \to 0$. This is convenient for technical reasons, and is appealing since in the limit $\tau \to 0$ the transport process is described by a Master equation (see [34] for a general discussion of these limits).

In the double limit (4) the transport process becomes compatible with an advection-diffusion (Fokker-Planck) equation [17] describing the time evolution of the distribution of mass density $\rho(x)$ along the x axis [i.e., of the projection of the phase-space density ϱ on the direction of transport] as

$$\partial_t \rho(x,t) = -v\, \partial_x \rho(x,t) + D \partial_x^2 \rho(x,t) \equiv -\partial_x j(x,t). \tag{5}$$

Here v, the drift coefficient (bias), and D, the diffusion coefficient, are the two parameters characterizing macroscopic transport, and

$$j(x,t) = v\rho(x,t) - D\partial_x \rho(x,t) \tag{6}$$

denotes the current density. The mass and charge of particles are set to unity so that mass, number, and charge densities are the same throughout this paper. Note, however, the different symbols ρ and ϱ used for the mass and phase-space densities, respectively.

The expressions we shall obtain for the irreversible entropy production and for the entropy fluxes into external reservoirs go over into expressions well known from nonequilibrium thermodynamics. The model we present provides thus a low-dimensional example from which laws can be derived [29] that are commonly believed [35] to be consequences of large phase-space dimensions.

The paper is organized as follows. In Sec. II we give a brief summary of the classical nonequilibrium thermodynamics treatment of transport due to both drift and diffusion. Then the multibaker map is defined (Sec. III), and the dynamics of the cell densities (Sec. IV) and the entropy balance equation (Sec. V) are derived. The rate of irreversible entropy production is computed in Sec. VI with a special emphasis on the macroscopic limit. The expressions for the entropy flux are discussed in Sec. VII. In particular, we show how it can be split into flows into particle reservoirs and into a heat bath. The independence of the results from the choice of the partition used for coarse graining is demonstrated in Sec. VIII. Finally, the physical picture emerging from these findings is discussed in the concluding Sec. IX.

II. NONEQUILIBRIUM THERMODYNAMICS

In this section we recall the thermodynamic description of transport in the case when drift and diffusion currents are simultaneously present [35]. The temperature T of the system will be kept spatially constant throughout the system (i.e., systems with temperature gradients will not be considered), and we use the laws of nonequilibrium thermodynamics and linear response. We stress, however, that in spite of these assumptions for the derivation, the macroscopic expressions can very well be of more general validity. This is indeed the case for some of them, as will become clear by comparison with the results found for the multibaker map.

A. Mass conservation

The conductivity σ is the transport coefficient that quantifies the amount of a current density j in response to an applied thermodynamic force X. In the presence of a gradient of the chemical potential (μ) and an external force (E) this leads to [35]

$$j = \sigma T X = \sigma(E - \partial_x \mu). \tag{7}$$

In the present paper we restrict ourselves to cases where the external field and the density gradient are both parallel to the x axes so that σ is a scalar.

Next, we rewrite the current in a convenient form. Substituting the thermodynamic expression for the diffusion coefficient

$$D = \sigma \left.\frac{\partial \mu}{\partial \rho}\right|_T \tag{8}$$

into Eq. (7) we find that $j = \sigma E - D\partial_x \rho$. Consequently, the total current j is the sum of the *diffusion current* $-D\partial_x \rho$ and the *drift current* σE. By introducing the drift velocity

$$v \equiv \mu_0 E \equiv \sigma E/\rho, \tag{9}$$

where μ_0 is the mobility of the particles, we find that the streaming velocity

$$u \equiv \frac{j}{\rho} \tag{10}$$

takes the form

$$u = v - D\frac{\partial_x \rho}{\rho}. \tag{11}$$

This expresses a competition between drift and diffusion. In equilibrium we have a stationary state with $u=0$. In that case the field exactly compensates the density gradient, and a profile of the mass density sets in that corresponds to the barometric formula.

With these substitutions the conservation of particles leads to a continuity equation $\partial_t \rho = -\partial_x j$, which for one-dimensional transport corresponds to the advection-diffusion (Fokker-Planck) equation (5).

B. Entropy balance

In every fixed volume V a global entropy balance equation

$$\frac{dS}{dt} = \frac{d_e S}{dt} + \frac{d_i S}{dt} \tag{12}$$

holds [35], expressing that the total change of the thermodynamic entropy S is the sum of a flow of entropy $d_e S/dt$ across the borders into the volume, and the rate of irreversible entropy production $d_i S/dt \geqslant 0$. In a nonequilibrium steady state $dS/dt = 0$, and the flow balances the irreversible entropy production.

The entropy balance per unit volume is obtained by dividing Eq. (12) by V,

$$\frac{d}{dt}\left(\frac{S}{V}\right) = \Phi + \sigma^{(\mathrm{irr})}, \tag{13}$$

where Φ denotes the entropy flux entering the system, and $\sigma^{(\mathrm{irr})}$ the rate of irreversible entropy production per unit volume. (The latter will always be denoted by $\sigma^{(\mathrm{irr})}$ to avoid confusion in the notation with the conductivity σ.)

C. Entropy flux

The entropy flux can be split [35] into a convective contribution

$$\Phi^{(\mathrm{conv})} = \partial_x [j\ (c + \ln \rho)], \tag{14}$$

where c is a constant, characterizing the entropy carried by the flow of particles, and a term $\Phi^{(\mathrm{heat})}$ accounting for a heat flux. For a system at a constant temperature T, subjected to an external field, the latter contribution to the entropy flow corresponds to the heat flow, which dissipates the work done by the external field into a thermostat (Joule's heat). We write this entropy flux as

$$\Phi^{(\mathrm{heat})} = -\frac{Ej}{T} = -\frac{v}{D} j, \tag{15}$$

where we used the definition of the drift (9) and Einstein's relation $\rho D = \sigma T$ to arrive at the last equality.

D. Irreversible entropy production

In the regime of linear response, the rate of irreversible entropy production $\sigma^{(\mathrm{irr})}$ is the product of the current density j and the thermodynamic driving force X [35],

$$\sigma^{(\mathrm{irr})} = jX. \tag{16}$$

In view of Eq. (7), this leads to

$$\sigma^{(\mathrm{irr})} = \frac{j^2}{\sigma T} = \frac{j^2}{\rho D}, \tag{17}$$

where, again, we have used Einstein's relation.

We shall also be interested in the rate of entropy production $P^{(\mathrm{irr})}$ per particle. This can be written as

$$P^{(\mathrm{irr})} = \frac{\sigma^{(\mathrm{irr})}}{\rho} = \frac{u^2}{D}. \tag{18}$$

Besides the diffusion coefficient, it only depends on the streaming velocity u [Eq. (11)]. Expression (18) does not contain the temperature. Therefore, this form is particularly suited for the use in dynamical systems. $P^{(\mathrm{irr})}$ has been argued [29] to be well-defined also for large systems with absorbing boundaries (where no steady states exist), and is thus a good quantity for the comparison of irreversible entropy production in systems subjected to different boundary conditions.

III. THE MULTIBAKER MAP

Baker maps are known to be prototypes of strongly chaotic systems [33]. Multibaker maps are a generalization tailored to model transport processes [14,15,17,29].

The system consists of a chain of identical cells [Fig. 1(a)]. The action of the map on a cell m $(0 < m < N+1)$ is pictorially defined in Fig. 1(b). Every time the square is divided into $k+2$ vertical columns. The rightmost (leftmost) column of width $s_R (s_L)$ is mapped onto a strip of width a and height $\widetilde{s_R}$ $(\widetilde{s_L})$ in the square to the right (left). These columns are responsible for transport in one time step τ. The middle columns of width $s_1, \ldots, s_k$ stay inside the same cell. They are transformed into strips of width a and respective height $\widetilde{s_1}, \ldots, \widetilde{s_k}$, and model the chaotic motion *not* contributing to transport during a single iteration. We will only consider maps with global phase-space conservation, which requires

$$\sum_{i=1}^{k} s_i + s_L + s_R = a, \tag{19a}$$

$$\sum_{i=1}^{k} \widetilde{s_i} + \widetilde{s_L} + \widetilde{s_R} = b. \tag{19b}$$

The local phase-space contraction rates are

$$\sigma_i = -\frac{1}{\tau} \ln \frac{a\widetilde{s_i}}{b s_i}, \quad i = 1, \ldots, k, \tag{20a}$$

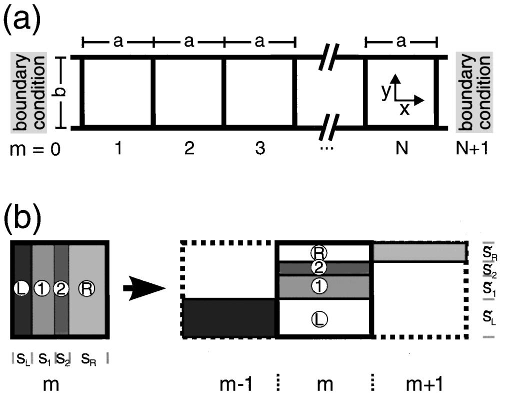

FIG. 1. Graphical illustration of the action of the multibaker map with two internal strips ($k=2$). (a) The mapping is defined on a domain of N identical rectangular cells of size $a\times b$, with boundary condition imposed on the density of two additional cells 0 and $N+1$. (b) Action of the map on any of the cells $m=1,\ldots,N$. Four columns are squeezed and stretched to obtain vertical strips of width a. The two columns of widths s_1 and s_2 are transformed to strips of heights $\widetilde{s_1}$ and $\widetilde{s_2}$, respectively, which stay inside the same cell; the other two columns of width s_R and s_L are transformed to strips of heights $\widetilde{s_R}$ and $\widetilde{s_L}$ and leave the square to the right and the left, respectively. Note the corresponding free spaces to which columns from the neighboring boxes are mapped. We only consider maps where $\widetilde{s_L}+\widetilde{s_1}+\widetilde{s_2}+\widetilde{s_R}=b$ so that phase-space volume is preserved globally (locally, however, contraction or expansion will occur).

$$\sigma_L=-\frac{1}{\tau}\ln\frac{a\widetilde{s_L}}{bs_L}, \tag{20b}$$

$$\sigma_R=-\frac{1}{\tau}\ln\frac{a\widetilde{s_R}}{bs_R}. \tag{20c}$$

The multibaker map possesses a phase-space density $\varrho_m(x,y)$ that can be assumed to take, in each cell, constant values along the x direction. For such a distribution, a point (x,y) of cell m is mapped, in one step of iteration, to cell $m-1$ or $m+1$ with the respective transition probabilities $r=s_R/a$ and $l=s_L/a$. The difference $r-l$ between these transition probabilities gives rise to a drift current, while a diffusion current can be induced by density differences among cells.

The cell-to-cell dynamics of the model is equivalent to a random walk with fixed step length a and transition probabilities r and l. Such random walks are characterized by well-defined drift and diffusion coefficients (v and D), which can be expressed in terms of r and l as [36]

$$r-l=\frac{\tau}{a}v, \tag{21a}$$

$$r+l=\frac{2\tau}{a^2}D+\frac{\tau^2}{a^2}v^2, \tag{21b}$$

or

$$r=\frac{\tau D}{a^2}\left(1+\frac{av}{2D}+\frac{\tau v^2}{2D}\right), \tag{22a}$$

$$l=\frac{\tau D}{a^2}\left(1-\frac{av}{2D}+\frac{\tau v^2}{2D}\right). \tag{22b}$$

These general relations connect the transition probabilities r and l of the microscopic dynamics with the macroscopic transport parameters v and D. However, they do not yet imply the existence of a macroscopic transport equation. It is only in the macroscopic limit (4) where the dynamics of the random walk model is governed by such an equation, namely by the Fokker-Planck equation (5).

To carry out the macroscopic limit it is convenient to express the heights $\widetilde{s_R}\equiv b\tilde{r}$ and $\widetilde{s_L}\equiv b\tilde{l}$ in a way analogous to Eq. (22) by introducing the parameters J and ϵ,

$$\tilde{r}=J\frac{\tau D}{a^2}\left(1+\epsilon\frac{av}{2D}+\frac{\tau v^2}{2D}\right), \tag{23a}$$

$$\tilde{l}=J\frac{\tau D}{a^2}\left(1-\epsilon\frac{av}{2D}+\frac{\tau v^2}{2D}\right). \tag{23b}$$

Here, $J\equiv(\tilde{r}+\tilde{l})/(r+l)$ is the average Jacobian on the union of strip R and L. In view of Eq. (19b), $J\neq 1$ implies that the dynamics cannot be phase-space preserving on the inner strips $i=1,\ldots,k$. The parameter

$$\epsilon\equiv\frac{1}{J}\frac{\tilde{r}-\tilde{l}}{r-l} \tag{24}$$

measures the deviation from uniform phase-space contraction on the strips R and L. For $\epsilon=1$ the Jacobians of these strips are identical, for $\epsilon=-1$ they are reciprocals of one another.

Depending on the choice of the contraction rates, different transport dynamics can be modeled as follows.

(i) Phase-space preserving (Hamiltonian) dynamics:

$$\sigma_L=\sigma_R=\sigma_i=0, \quad i=1,\ldots,k \tag{25a}$$

$(J=1,\ \tilde{r}=r, \tilde{l}=l, \epsilon=1)$.

(ii) Dissipative dynamics with time reversal symmetry:

$$\sigma_R=-\sigma_L=\frac{1}{\tau}\ln\frac{r}{l}, \quad \sigma_i=0, \quad i=1,\ldots,k \tag{25b}$$

$(J=1,\ \tilde{r}=l, \tilde{l}=r, \epsilon=-1)$. This choice mimics the effect of a thermostat [29]. Indeed, a map modeling driven thermostated systems has to be area-contracting (expanding) if the trajectory moves in the direction of (against) the bias in order to model slowing down (acceleration) of particles moving parallel (antiparallel) to the external field (cf. [2,1,7]), while it has to preserve the volume of phase-space elements not displaced with respect to the field. Consequently, we require $\sigma_i=0$ for $i=1,\ldots,k$. Furthermore, the local contraction rates σ_R and σ_L for making a step to the right or to the left, respectively, should add up to zero, $\sigma_R+\sigma_L=0$, so that the overall dissipation vanishes for a closed trajectory. It is worth noting that the map is then reversible in the sense of Ref. [37], i.e., the time reversed dynamics is identical to the direct one up to a geometrical transformation (in our case it is a reflection at the diagonal of every cell). This is consistent with the behavior of thermostats constructed for continuous time systems [2].

(iii) Phase-space preserving dynamics on the inner strips only:

$$\sigma_L \neq -\sigma_R \neq 0, \quad \sigma_i = 0, \quad i = 1, \ldots, k \tag{25c}$$

$(J=1, \epsilon \neq \pm 1)$. This case has similarities with the thermostating algorithm but does not fulfill time reversibility. We consider it as a model of improper thermostating.

IV. MASS CONSERVATION

In this section, the time evolution of the coarse-grained densities is discussed. We consider a single cell m of the multibaker map with cell density ϱ_m. Moreover, the mass density per unit length of the cell corresponds to $\Gamma \varrho_m / a$, i.e., to the number of particles in cell m divided by its width. Note that ρ_m differs only by a factor b from the cell density: $b\varrho_m = \rho_m$. In general, the cell density ϱ_m' after a single time step will differ from ϱ_m due to the outflow to and the inflow from the neighboring cells. The conservation of probability requires

$$\varrho_m' = \left(\sum_{i=1}^{k} \frac{s_i}{a} \right) \varrho_m + r \varrho_{m-1} + l \varrho_{m+1}. \tag{26}$$

This is the basic dynamical equation for the cell density. In a stationary state $\varrho_m' = \varrho_m$. Note that the parentheses equals $1-(r+l)$ because of Eq. (19a), and the dynamics is completely determined by the transition probabilities r and l.

The system will be subjected to flux boundary conditions that model the contact with two particle reservoirs at the ends:

$$\varrho_0 \equiv \varrho_L, \quad \varrho_{N+1} \equiv \varrho_R, \tag{27}$$

where the two densities $\varrho_R \geqslant \varrho_L$ are kept constant. These boundary conditions are convenient since for $\varrho_R \neq \varrho_L$ they allow nonzero density gradients and related diffusion currents in the system, even in steady states. As far as the coarse-grained densities are considered, the special case of $\varrho_R = \varrho_L \neq 0$ is equivalent to periodic boundary conditions. In that case the steady state is characterized by cell densities that do not depend on the spatial position (i.e., the index m). In such steady states there is only a drift current.

In a general non-steady-state one has to distinguish the currents

$$j_m^- = \frac{a}{\tau} (r \rho_{m-1} - l \rho_m) \tag{28a}$$

and

$$j_m^+ = \frac{a}{\tau} (r \rho_m - l \rho_{m+1}) \tag{28b}$$

through the left and right boundaries of cell m, respectively. Note that the currents are defined with respect to the mass density, and, by definition, $j_m^- = j_{m-1}^+$. Taking into account Eq. (19a), one can express the evolution equation of the density (26) as

$$\frac{\rho_m' - \rho_m}{\tau} = -\frac{j_m^+ - j_m^-}{a}, \tag{29}$$

which is a discrete continuity equation. It goes over into the advection-diffusion equation (5) in the macroscopic limit (4), when $b\varrho_m = \rho_m \to \rho(x=ma)$ and $j_m^\pm \to j(x=ma)$. Equation (29) can be rewritten in the form

$$\frac{\varrho_m'}{\varrho_m} = \frac{\rho_m'}{\rho_m} = 1 - \tau \frac{j_m^+ - j_m^-}{a \rho_m} \equiv 1 - \tau \gamma_m. \tag{30}$$

Here, γ_m is a local decay rate characterizing the relaxation of a cell density towards its stationary value. It vanishes in any stationary state. Note that the ratio of two cell densities is the same as the ratio of the corresponding mass densities.

The average local streaming velocity is defined as

$$\overline{u}_m = \frac{j_m^+ + j_m^-}{2 \rho_m}. \tag{31}$$

With these definitions the ratios between densities of neighboring cells can be expressed as

$$\frac{\varrho_{m-1}}{\varrho_m} = \frac{\rho_{m-1}}{\rho_m} = \frac{l}{r} \left(1 + \frac{\tau}{la} \overline{u}_m - \frac{\tau}{2l} \gamma_m \right), \tag{32a}$$

$$\frac{\varrho_{m+1}}{\varrho_m} = \frac{\rho_{m+1}}{\rho_m} = \frac{r}{l} \left(1 - \frac{\tau}{ra} \overline{u}_m - \frac{\tau}{2r} \gamma_m \right). \tag{32b}$$

The above relations can be considerably simplified in a steady state, where the cell densities are independent of time $\varrho_m' = \varrho_m$. Then the current density

$$j = \frac{a}{\tau} (r \rho_{m-1} - l \rho_m) = \frac{a}{\tau} (r \rho_m - l \rho_{m+1}) \equiv u_m \varrho_m \tag{33}$$

is homogeneous in space. Note, however, that the streaming velocity $\overline{u_m} = u_m$ can still depend on m because of a spatial dependence of ρ_m.

For the coarse-grained invariant density (the cell as well as the mass density) of a steady state with flux boundary conditions we obtain a geometrical progression along the chain:

$$\rho_m = \rho_L - c + c \left(\frac{r}{l} \right)^m, \tag{34}$$

where

$$c = \frac{\rho_R - \rho_L}{(r/l)^{N+1} - 1}. \tag{35}$$

This general result contains two well-known limiting cases. In the equilibrium state without current it reduces to a discretized version $\rho_m = \rho_L (r/l)^m$ of the barometric formula.

For a steady state without drift (i.e., in the limit $r \to l$) one recovers Fick's law — a linear density profile.

V. ENTROPY BALANCE

The entropy balance equation is the analog of Eq. (26) for the entropy $-\Gamma \varrho_m \ln \varrho_m$. In this section we assume that coarse graining takes place instantaneously after each iteration. Thus, every iteration of the map starts with a homogeneous phase-space density in each cell. The change of S_m in one time step can have several reasons.

(i) A temporal change of the cell density ϱ_m into ϱ_m' leads to a new coarse-grained entropy

$$S_m' = -\Gamma \varrho_m' \ln \varrho_m' . \tag{36}$$

The difference

$$\Delta S_m \equiv S_m' - S_m \tag{37}$$

is the temporal change of the coarse-grained entropy. It can be used as a proper generalization of the full time derivative of the entropy appearing on the left-hand side of Eq. (12).

(ii) Part of the temporal change of the coarse-grained entropy is due to an entropy flux through the boundaries of the cell. Indeed the columns in cell m are mapped partially onto strips in the neighboring cells [cf. Fig. 1(b)], leading to an entropy flux ΔS_{out}. Correspondingly, regions from the neighboring cells are mapped into cell m, giving rise to a flux ΔS_{in}. The entropy flowing out of cell m is related to the densities of the columns L and R *before* the action of the mapping:

$$\Delta S_{\mathrm{out}} = -\Gamma (\varrho_m r \ln \varrho_m + \varrho_m l \ln \varrho_m). \tag{38a}$$

We define the entropy inflow as the entropy content of the strips R and L coming from cells $m-1$ and $m+1$, respectively, i.e., this contribution of the entropy flux is evaluated *after* application of the mapping [38]. The strips have respective width $\widetilde{s_R}$ and $\widetilde{s_L}$, and carry the densities $\varrho_{m-1} r/\tilde{r}$ and $\varrho_{m+1} l/\tilde{l}$. This leads to

$$\Delta S_{\mathrm{in}} = -\Gamma \left[\varrho_{m-1} r \ln\left(\varrho_{m-1} \frac{r}{\tilde{r}} \right) + \varrho_{m+1} l \ln\left(\varrho_{m+1} \frac{l}{\tilde{l}} \right) \right]. \tag{38b}$$

In a time step the net entropy flow into the cell through the boundaries is thus

$$\Delta_e S_m = \Delta S_{\mathrm{in}} - \Delta S_{\mathrm{out}} . \tag{39}$$

Note that a part of this entropy flow is due to an exchange of particles between neighboring cells. Another part of it describes the entropy flowing into or out of the thermostat to which the cells are coupled. In particular, the factors $r/\tilde{r}$ and $l/\tilde{l}$ in Eq. (38b) arise from such contributions (for further discussions see Sec. VII).

(iii) In addition to the flux, there is a change of entropy in a cell due to coarse graining. In order to see how this can be taken into account, let us first work out the change in the Gibbs entropy. With a uniform initial density, the entropy $S_m^{(G)\prime}$ inside cell m after one time step differs from the initial entropy because different strips inside cell m carry densities different from the initial ϱ_m, namely $\varrho_{m-1} r/\tilde{r}$ on strip R, $\varrho_{m+1} l/\tilde{l}$ on strip L, and $\varrho_m s_i/\widetilde{s_i}$ on strips $i=1, \ldots, k$. Thus, we obtain

$$S_m^{(G)\prime} = -\Gamma \left\{ \varrho_m \sum_i \left[\frac{s_i}{a} \ln\left(\varrho_m \frac{b s_i}{a \widetilde{s_i}} \right) \right] + \varrho_{m-1} r \ln\left(\varrho_{m-1} \frac{r}{\tilde{r}} \right) + \varrho_{m+1} l \ln\left(\varrho_{m+1} \frac{l}{\tilde{l}} \right) \right\}. \tag{40}$$

This expression is markedly different from S_m', and the difference

$$\Delta_i S_m \equiv S_m' - S_m^{(G)\prime} \tag{41}$$

is related to the irreversible entropy production as will be discussed below.

To find a balance equation for the entropy, we notice that by means of Eqs. (39), (40), and (1) the entropies $S_m^{(G)\prime}$, $\Delta_e S_m$, and S_m are related to each other as

$$S_m^{(G)\prime} - \Delta_e S_m = S_m - \Gamma \varrho_m \tau \chi, \tag{42}$$

where

$$\chi = -\frac{1}{\tau} \sum_i \frac{s_i}{a} \ln\left(\frac{a \widetilde{s_i}}{b s_i} \right) \tag{43}$$

denotes the average phase-space contraction rate on the strips $i=1, \ldots, k$. Subtracting Eq. (42) from S_m' we find

$$\Delta S_m = \Delta_e S_m + \Delta_i S_m - \Gamma \varrho_m \tau \chi. \tag{44}$$

Dividing this equation by τ, we see that it is of the same structure as Eq. (12) provided that $\chi=0$. Thus, we can find an analogy with the thermodynamic entropy balance only if the internal dynamics is phase-space preserving (Hamiltonian), i.e., if

$$a \widetilde{s_i} = b s_i . \tag{45}$$

In the following we therefore focus on systems where this condition holds. In combination with Eq. (19) this implies that the average Jacobian on the union of strips R and L has to be unity: $J=1$. In physical terms, condition (45) ensures that the internal dynamics of a cell does not contribute to entropy changes. The mixing of phase-space densities between neighboring cells, i.e., the *transport process* is responsible for all changes in entropy.

With condition (45) we find that

$$\frac{\Delta_i S_m}{\tau} \geqslant 0 \tag{46}$$

is the dynamical-system analog of irreversible entropy production. Its positivity is due to the fact that the Gibbs entropy contains in general more information on the phase-space structures than the coarse-grained entropy.

In particular, in a steady state and with homogeneous initial density, for which $S'_m = S_m = S_m^{(G)} \neq S_m^{(G)\prime}$, the irreversible entropy production

$$\frac{\Delta_i S_m}{\tau} = \frac{S_m^{(G)} - S_m^{(G)\prime}}{\tau} = -\frac{\Delta S_m^{(G)}}{\tau} \tag{47}$$

coincides with the *negative* time derivative of the Gibbs entropy. This is in agreement with a recent result for general dynamical systems [21], and with the observations based on thermostated molecular-dynamics simulations [1,2]. The use of the coarse-grained entropy provides a natural framework to derive this result.

Finally, we note that the particular expressions used for the value of the entropy and its temporal change still depend on our choice of the coarse graining unit as a cell. This dependence seems to be much weaker for the temporal changes than for the entropy itself. In particular, we show in Sec. VIII that in the macroscopic limit (4) the flux and the irreversible entropy production go over into forms independent of the type of coarse graining.

VI. IRREVERSIBLE ENTROPY PRODUCTION

Substituting Eqs. (26) and (40) into the expression (41) for $\Delta_i S_m$ and using Eqs. (45) and (19a) again, we obtain for the rate of specific irreversible entropy production in cell m,

$$P_m^{(\mathrm{irr})} = \frac{\Delta_i S_m}{\tau \Gamma \varrho_m} = \frac{1}{\tau}\left[\frac{\varrho_{m-1}}{\varrho_m} r \ln \frac{r \varrho_{m-1}}{\tilde{r} \varrho_m} + \frac{\varrho_{m+1}}{\varrho_m} l \ln \frac{l \varrho_{m+1}}{\tilde{l} \varrho_m} - \frac{\varrho'_m}{\varrho_m} \ln \frac{\varrho'_m}{\varrho_m}\right]. \tag{48}$$

In this section, we evaluate $P_m^{(\mathrm{irr})}$ in the general setting of the multibaker, and discuss the macroscopic limit (4) for fixed transport parameters v and D.

First, we use Eqs. (22) and (23) to express the microscopic parameters r, l, $\tilde{r}$, $\tilde{l}$ in terms of the discrete units τ and a of time and lengths, respectively, and of v and D. By taking into account also relations (30) and (32a) for the density ratios in terms of the average streaming velocity and the local decay rate, we obtain

$$\begin{aligned} P_m^{(\mathrm{irr})} = \frac{D}{a^2}\Bigg\{ & \left[1 + \frac{a}{2D}\left(2\overline{u}_m - v - a\gamma_m + \frac{\tau v^2}{a}\right)\right] \ln\left[\frac{1 + \frac{a}{2D}\left(2\overline{u}_m - v - a\gamma_m + \frac{\tau v^2}{a}\right)}{1 + \epsilon\frac{va}{2D} + \frac{\tau v^2}{2D}}\right] \\ & + \left[1 - \frac{a}{2D}\left(2\overline{u}_m - v + a\gamma_m - \frac{\tau v^2}{a}\right)\right] \ln\left[\frac{1 - \frac{a}{2D}\left(2\overline{u}_m - v + a\gamma_m - \frac{\tau v^2}{a}\right)}{1 - \epsilon\frac{va}{2D} + \frac{\tau v^2}{2D}}\right]\Bigg\} - \frac{1}{\tau}[1 - \gamma_m \tau] \ln[1 - \gamma_m \tau]. \end{aligned} \tag{49}$$

Note that this expression is an even function of the microscopic length scale a so that the corrections to the macroscopic limit $a, \tau \to 0$ can only contain even powers of a (the reason is that $\overline{u}_m$ and v are odd functions of a). Moreover, by a rearrangement of the logarithms one can show that the terms in braces are at least of order a^2, i.e., even the lowest order corrections in τ scale like τa^2. Consequently, the macroscopic limit does not depend on the order of the limits $a \to 0$ and $\tau \to 0$. We first carry out the limit $\tau \to 0$. All terms containing positive powers of τ can be neglected in this limit. In the last term on the right-hand side of the equation only γ_m survives. Moreover, in the braces the local relaxation rate γ_m only appears as a product with a^2/D, i.e., with the microscopic time scale governing the diffusion process. The latter is small on the macroscopic scale: $\gamma_m a^2/D \ll 1$. Therefore, it is sufficient to evaluate $P_m^{(\mathrm{irr})}$ in leading order in γ_m, which yields

$$\begin{aligned} P_m^{(\mathrm{irr})} = \frac{2\overline{u}_m - v}{2a} & \ln\left[\left(\frac{1 + \frac{a}{2D}(2\overline{u}_m - v)}{1 - \frac{a}{2D}(2\overline{u}_m - v)}\right)\left(\frac{1 - \epsilon\frac{va}{2D}}{1 + \epsilon\frac{va}{2D}}\right)\right] + \frac{D}{a^2}\ln\left[\frac{1 - \left(\frac{a}{2D}(2\overline{u}_m - v)\right)^2}{1 - \left(\frac{\epsilon v a}{2D}\right)^2}\right] \\ & - \frac{\gamma_m}{2}\ln\left[\frac{1 - \left(\frac{a}{2D}(2\overline{u}_m - v)\right)^2}{1 - \left(\frac{\epsilon a v}{2D}\right)^2}\right]. \end{aligned} \tag{50}$$

Here, we have dropped terms that are of order $\gamma_m^2 a^2/D$ at least. Besides the cell size a, this expression depends on the macroscopic length scales $l_v \equiv D/v$ and $l_m \equiv D/u_m$ characterizing the bias and the streaming. In the large system limit $l_v, l_m \gg a$, we obtain, by expanding $P_m^{(\mathrm{irr})}$ in powers of the small dimensionless parameters a/l_v and a/l_m,

$$P_m^{(\mathrm{irr})} = \frac{\left(\overline{u}_m - \frac{1+\epsilon}{2}v\right)^2}{D}\left\{1 + \frac{a^2}{6D^2}\left[\left(\overline{u}_m - \frac{1-\epsilon}{2}v\right)^2 + \frac{\epsilon^2 v^2}{2}\right]\right\} + \gamma_m \frac{a^2}{2D^2}\left[\left(\overline{u}_m - \frac{v}{2}\right)^2 - \frac{\epsilon^2 v^2}{4}\right] + \text{higher-order terms.} \tag{51}$$

Taking the macroscopic limit (4) we see that a cell size independent limit

$$\begin{aligned} P_{m=x/a}^{(\mathrm{irr})} &= \frac{1}{D}\left[u(x,t) - \frac{1+\epsilon}{2}v\right]^2 \\ &= \frac{1}{D}\left[v\,\frac{1-\epsilon}{2} - D\,\frac{1}{\varrho(x,t)}\,\partial_x \varrho(x,t)\right]^2 \end{aligned} \tag{52}$$

exists.

Note that the relaxation rate γ_m only appears in the corrections to expression (52). This implies that in the macroscopic limit [when $\gamma_m \to -\partial_t \ln\varrho(x,t)$] we find identical expressions for the entropy production in steady and nonsteady-states. The only difference between these states is the implication of nonstationarity on the *global* profile of the streaming velocity. Far away from the steady state, however, the term proportional to γ_m can be the most important *correction* to the thermodynamic entropy production.

In the remainder of this section we discuss different special cases of the expression Eq. (51) which also allow us to illustrate the physical content of the equation, and to make contact with previous results.

First, we consider the thermostated case $\epsilon = -1$. For this choice the leading contribution to $P_m^{(\mathrm{irr})}$ coincides with the thermodynamic result (18). It is augmented by a finite size correction that is positive in a steady state, and vanishes only in the equilibrium state $u_m = 0$. Note that Eq. (18) can only be recovered for this particular choice of ϵ. Only proper thermostating can therefore yield results consistent with nonequilibrium thermodynamics.

Another case of interest is $\epsilon = 1$. In this case we find in leading order $P_m^{(\mathrm{irr})} = D(\partial_x \varrho/\varrho)^2$ [cf. Eq. (52)], i.e., only the diffusion current contributes to the entropy production. This implies that transport in driven systems, $v \neq 0$, *cannot* adequately be described in the framework of purely Hamiltonian systems (for more details see the Discussion). For ϵ arbitrary and $v = 0$, on the other hand, Eq. (51) coincides with the expression derived by Gaspard [25] for the unbiased case, including the leading order finite size correction.

Values of ϵ different from ± 1 (improper thermostating) do not have immediate relevance to classical thermodynamics. They represent nevertheless interesting cases in which the current-free steady state $u_m = 0$ can be accompanied by a nonvanishing irreversible entropy production.

There is a special value of the current $j = \varrho_m v(1+\epsilon)/2$, where the irreversible entropy production vanishes in a steady state even though the current might be nonvanishing. This condition on j corresponds to $u_m \equiv v(1+\epsilon)/2$, irrespective of m. Since the current is constant in a steady state, the density must not depend on m, either. As a consequence, there is just one nontrivial stationary state, $\varrho_m = \mathrm{const}$ for all m, $u_m = v$, and $\epsilon = 1$, which does not give rise to entropy production even though there is a nonvanishing current. This situation corresponds to a biased Hamiltonian dynamics with a constant average density in the cells.

VII. ENTROPY FLUX

The entropy flow [Eqs. (39) and (38)] through the boundaries of cell m,

$$\begin{aligned} \Delta_e S_m = \Gamma\Bigg[&(r+l)\varrho_m \ln\varrho_m - r\varrho_{m-1}\ln\left(\varrho_{m-1}\frac{r}{\tilde{r}}\right) \\ &- l\varrho_{m+1}\ln\left(\varrho_{m+1}\frac{l}{\tilde{l}}\right)\Bigg], \end{aligned} \tag{53}$$

can be split into two contributions, one depending on the transition probabilities r, l (and on the densities) only, and another one containing the effect of local phase-space contractions. Correspondingly, the flux can be written as

$$\Phi_m \equiv \frac{\Delta_e S_m}{\tau a} = \Phi_m^{(1)} + \Phi_m^{(2)} \tag{54}$$

with

$$\Phi_m^{(1)} = \frac{j_m^+}{a}\ln\varrho_{m+1} - \frac{j_m^-}{a}\ln\varrho_{m-1} + \frac{\rho_m}{\tau}\left(l\ln\frac{\varrho_m}{\varrho_{m-1}} + r\ln\frac{\varrho_m}{\varrho_{m+1}}\right), \tag{55a}$$

$$\Phi_m^{(2)} = -\frac{\rho_m}{\tau}\left(\frac{\varrho_{m-1}}{\varrho_m} r\ln\frac{r}{\tilde{r}} + \frac{\varrho_{m+1}}{\varrho_m} l\ln\frac{l}{\tilde{l}}\right), \tag{55b}$$

where we used the definition (28) of the currents through the respective boundaries of a cell.

We evaluate the macroscopic limit of both contributions to the entropy flux separately. Substituting Eq. (22) and taking $\tau \to 0$, the former expression can be rewritten as

$$\begin{aligned} \Phi_m^{(1)} = {} & \frac{j_m^+ - j_m^-}{a}(1 + \ln\varrho_m) + \frac{j_m^+}{a}\ln\frac{\rho_{m+1}}{\rho_m} + \frac{j_m^-}{a}\ln\frac{\rho_m}{\rho_{m-1}} \\ & + \frac{D}{a^2}\left[\rho_m \ln\frac{\rho_m^2}{\rho_{m+1}\rho_{m-1}} + (\rho_{m+1} + \rho_{m-1} - 2\rho_m)\right] \\ & - \frac{v}{2a}\left[\rho_m \ln\frac{\rho_{m+1}}{\rho_{m-1}} + (\rho_{m+1} - \rho_{m-1})\right]. \end{aligned} \tag{56}$$

In the large system limit $a \to 0$, when $j_m^{\pm} \to j(x = ma)$ and $b\varrho_m = \rho_m \to \rho(x = ma)$, the first two terms represent the divergence of $j(1 + \ln\varrho)$, and the rest can be combined to obtain the simple expression

$$\Phi^{(1)}(x,t) = \partial_x\{j(x,t)[1 + \ln\varrho(x,t)] - v\rho(x,t)\}, \tag{57}$$

where $x=ma$, and t is the time instant of observation.

The second contribution $\Phi_m^{(2)}$ of Eq. (54) reduces, in view of Eqs. (22) and (23), for $\tau\rightarrow 0$ to

$$\Phi_m^{(2)}(x,t)=-\frac{\rho_m D}{a^2}\left\{\left[1+\frac{(2\overline{u}_m-v-a\gamma_m)a}{2D}\right]\ln\frac{1+\dfrac{av}{2D}}{1+\epsilon\dfrac{av}{2D}}\right.$$

$$\left.+\left[1-\frac{(2\overline{u}_m-v+a\gamma_m)a}{2D}\right]\ln\frac{1-\dfrac{av}{2D}}{1-\epsilon\dfrac{av}{2D}}\right\}. \quad (58)$$

If, in addition, $a\rightarrow 0$, it is found to be proportional to $1-\epsilon$:

$$\Phi^{(2)}(x,t)=(1-\epsilon)\left((3+\epsilon)\frac{\rho(x,t)v^2}{4D}-\frac{j(x,t)v}{D}\right). \quad (59)$$

Together, Eqs. (57) and (59) imply in the macroscopic limit

$$\Phi(x,t)=\partial_x\{j(x,t)[1+\ln\varrho(x,t)]\}-\epsilon v\,\partial_x\rho(x,t)$$

$$-\frac{\rho(x,t)v^2}{4D}(1-\epsilon)^2 \quad (60)$$

as the leading order contribution of the entropy flow through the boundaries of cell $m=x/a$.

The first term of Eq. (60),

$$\partial_x\{j(x,t)[1+\ln\varrho(x,t)]\}, \quad (61)$$

is a spatial derivative, and can therefore be interpreted as a convective entropy flux. It agrees with the thermodynamic result (14), where for the multibaker maps we have the explicit expression $c=1-\ln b$ due to the difference between phase-space and configuration-space densities appearing in the respective expressions. In the case of nondriven systems this is the full entropy flux.

For a general value of ϵ, it is natural to identify the heat contribution to the entropy flux with the rest of Eq. (60) as

$$\Phi^{(\mathrm{heat})}(x,t)=-\epsilon v\,\partial_x\rho(x,t)-\frac{v^2}{4D}(1-\epsilon)^2\rho(x,t). \quad (62)$$

In the Hamiltonian case ($\varepsilon=1$) this expression reduces to $\Phi^{(\mathrm{heat})}=-v\,\partial_x\varrho(x,t)$, which vanishes for a constant density, even though there is a finite current $v\varrho$ running through the system. A physical interpretation of this observation will be given in the Discussion (Sec. IX). It is only in the case of a thermostated multibaker map ($\epsilon=-1$) when Eq. (62) goes over into the physical expression

$$\Phi^{(\mathrm{heat})}(x,t)=v\,\partial_x\rho(x,t)-\frac{v^2}{D}\rho(x,t)\equiv-\frac{vj(x,t)}{D} \quad (63)$$

for the heat contribution to the flux. It is related to the density changes of regions mapped between different cells, and requires therefore a spatial variation of the Jacobian of the underlying map. Consequently, the inhomogeneities in the densities along the y direction play an essential role for the determination of the heat flux. It cannot be derived from the dynamics projected to the x axis (i.e., from the Fokker-Planck equation) alone.

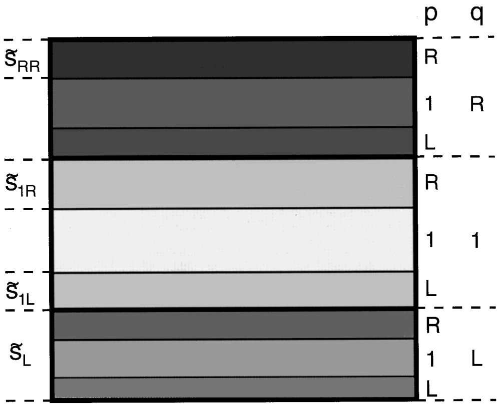

FIG. 2. Notations used to describe the level-2 partitioning of a cell. Every strip is labeled by the two-letter sequence p,q, where $p,q\in\{L,1,\ldots,k,R\}$ label the level-2 strips (p stands for the level-2 strips within level-1 strips selected by the label q). To illustrate the use of these labels, the heights of a few strips are indicated at the left side of the box.

VIII. STRUCTURAL STABILITY OF THE MACROSCOPIC RESULTS

In order to be relevant for a thermodynamic description of transport, the results exposed above must not depend on details of the procedure for coarse graining. To test whether this is indeed the case we consider the entropy balance for entropies calculated with respect to two somewhat more refined descriptions. To this end a finer partitioning consisting of the strips generated by the first iterations of the cells will be taken as the "natural" partitioning. In one case the (coarse-grained) densities are allowed to take different values on the stips of this finer partitioning, and coarse graining is carried out after each time step. In the other case the balance is established by coarse graining on the full cell after every second time step. Although these cases correspond to just the simplest possibilities, they clearly indicate the behavior expected for arbitrary refinements.

A. Preliminaries

We first extend our notations in order to describe densities, entropies, and fluxes defined on the first level of coarse graining. This requires level-2 partitioning (cf. Fig. 2).

In every cell m there are $(k+2)^2$ strips labeled by two symbols (p,q), where $p,q=L,1,\ldots,k,R$. The strips have respective heights $\tilde{s}_{p,q}=\tilde{s}_p\tilde{s}_q/b$, and they carry densities $\varrho_m(p,q)$. In the following we call $\varrho_m(p,q)$, $\varrho_m(q)$, and ϱ_m the level-2, level-1, and level-0 densities, respectively. By construction, the level-0 densities coincide with the cell densities considered in the preceding sections. The quantities defined on different levels are related to each other by the conservation of probability. In our multibaker model these relations read as

$$\varrho_m=\sum_q \frac{\tilde{s}_q}{b}\varrho_m(q)=\sum_{p,q}\frac{\tilde{s}_p\tilde{s}_q}{b^2}\varrho_m(p,q). \tag{64}$$

Owing to the time evolution of the multibaker map there are also relations connecting the densities at different time instants. Let us use prime and double-prime to denote the value of a quantity at time τ and 2τ, respectively. [Equation (64) then holds for primed and double-primed densities, too.] By taking into account the origin of the points of a given region, i.e., the location of their first and second preimages, respectively, we obtain

$$\varrho''_m(p,q)=\frac{b s_q}{a\tilde{s}_q}\varrho'_{m_q}(p)=\frac{b^2 s_p s_q}{a^2\tilde{s}_p\tilde{s}_q}\varrho_{m_{q,p}}, \tag{65}$$

where the subscript

$$m_q=\begin{cases} m+1, & q=L\\ m, & q=1,\dots,k\\ m-1, & q=R\end{cases} \tag{66}$$

[$m_{q,p}\equiv(m_q)_p$] is used as a bookkeeping device to indicate the cell where the points in a given strip come from.

To follow the time evolution we again take the initial densities to be uniform on the full cell, which implies $\varrho_m(p,q)=\varrho_m$ for all (p,q), but now we will allow for other ways of coarse graining. We define the level-i entropy $S_m^{(i)}$ of cell m as the Gibbs entropy taken with respect to the level-i densities. Thus, $S_m^{(0)}\equiv S_m=-\Gamma\varrho_m\ln\varrho_m$,

$$S_m^{(1)}=-\Gamma\sum_p\frac{\tilde{s}_p}{b}\varrho_m(p)\ln\varrho_m(p), \tag{67a}$$

and

$$S_m^{(2)}=-\Gamma\sum_{p,q}\frac{\tilde{s}_p\tilde{s}_q}{b^2}\varrho_m(p,q)\ln\varrho_m(p,q). \tag{67b}$$

For later reference we consider now the level-2 entropy after two time steps, and use Eqs. (65)–(67) to express it in terms of the densities after one time step,

$$S_m^{(2)''}\equiv-\Gamma\sum_{p,q}\frac{\tilde{s}_p\tilde{s}_q}{b^2}\varrho''_m(p,q)\ln\varrho''_m(p,q) \tag{68a}$$

$$=-\Gamma\sum_q\frac{s_q}{a}\varrho'_{m_q}\ln\frac{b s_q}{a\tilde{s}_q}+\sum_q\frac{s_q}{a}S_{m_q}^{(1)'}. \tag{68b}$$

B. Entropy balance on level-1 strips

In order to write down the entropy balance on level-1 strips we relate $S_m^{(2)''}$ to $S_m^{(1)'}$. To this end we use our previous result Eq. (45) stating that the dynamics on the internal strips has to be area preserving: $s_i=\tilde{s}_i$, and carry out the summation over $q=L,1,\dots,k,R$ to see that

$$S_m^{(2)''}=S_m^{(1)'}-\Gamma r\sum_p\frac{\tilde{s}_p}{b}\varrho'_{m-1}(p)\ln\left[\varrho'_{m-1}(p)\frac{r}{\tilde{r}}\right]$$
$$-\Gamma l\sum_p\frac{\tilde{s}_p}{b}\varrho'_{m+1}(p)\ln\left[\varrho'_{m+1}(p)\frac{l}{\tilde{l}}\right]$$
$$+\Gamma(r+l)\sum_p\frac{\tilde{s}_p}{b}\varrho'_m(p)\ln[\varrho'_m(p)]. \tag{69}$$

Notice that the last three terms of Eq. (69) are just the level-1 generalization of the entropy flux [cf. Eqs. (38) and (39)]. As a consequence, we find the generalization of Eq. (42) to be

$$S_m^{(2)''}=S_m^{(1)'}+\Delta_e S_m^{(1)'}. \tag{70}$$

This equation states that the net entropy flux through the boundary of cell m is just the difference between the appropriate Gibbs entropies (in our case the level-2 and level-1 entropies taken one time step later). It is easy to check for the present model that this relation still holds when differences over longer periods of time are considered, and it also applies to individual rectangles of a refining partition. This shows that the difference of the Gibbs entropies taken at the final time with respect to the finest partition and at the initial time taken with respect to the initial partition is the *only* source of the entropy flux. This is reasonable, even in a general context, because this entropy is based on the phase-space densities, which contain the full information about the time evolution of the system.

Based on this observation we can now establish the entropy balance for the level-1 entropies of cell m. Coarse graining is applied on the level-1 strips after every application of the map. It is convenient to start after one time step on level-1 strips and follow the process for another time step. By subtracting $S_m^{(1)'}$ expressed via Eq. (70) from $S_m^{(1)''}$ we obtain

$$S_m^{(1)''}-S_m^{(1)'}\equiv\Delta S_m^{(1)}\equiv\Delta_e S_m^{(1)'}+\Delta_i S_m^{(1)'}, \tag{71}$$

where

$$\Delta_i S_m^{(1)'}\equiv S_m^{(1)''}-S_m^{(2)''}. \tag{72}$$

Note that $S_m^{(1)''}$ is the value of the level-1 entropy (after two time steps) when coarse graining is applied at every time step to the level-1 strips. Thus, Eq. (72) is the immediate generalization of Eq. (41) to entropies that are coarse grained at the first level of refinement. The irreversible change of entropy is again due to the difference between the Gibbs entropy and its coarse-grained counterpart. Note that Eq. (72) holds at any time: in particular it is also valid with one prime less on both sides.

C. Entropy balance over two time steps

We are also interested in the entropy balance for the level-0 entropy when coarse graining is applied only after every second iteration of the map. In other words, we wish to establish the balance equation

$$S_m^{(0)''} - S_m^{(0)} \equiv \Delta^{(2)} S_m^{(0)} \equiv \Delta_e^{(2)} S_m^{(0)} + \Delta_i^{(2)} S_m^{(0)}, \tag{73}$$

where the superscript $^{(2)}$ of $\Delta^{(2)}$ indicates that temporal changes are considered with a time lag of 2τ. The entropy flux $\Delta_e^{(2)} S_m^{(1)}$ through cell m is the sum of the net fluxes during the first and the second time step, yielding

$$\Delta_e^{(2)} S_m^{(0)} = \Delta_e S_m^{(0)} + \Delta_e S_m^{(1)'} = -S_m^{(0)} + S_m^{(2)''}. \tag{74}$$

Here, we used the relation $\Delta_e S_m^{(0)} = S_m^{(1)'} - S_m^{(0)}$ [insert Eqs. (43) and (45) into Eq. (42)] and Eq. (70) to arrive at the final equality. Inserting this expression for the two-step flux into Eq. (73) we find for the irreversible entropy change

$$\Delta_i^{(2)} S_m^{(0)} = S_m^{(0)''} - S_m^{(2)''}. \tag{75}$$

This can also be expressed as

$$\Delta_i^{(2)} S_m^{(0)} = \Delta_i S_m^{(0)'} + \Delta_i S_m^{(1)'}, \tag{76}$$

where $\Delta_i S_m^{(0)} = S_m^{(0)'} - S_m^{(1)'}$ [cf. Eqs. (41) and (72)], showing that the irreversible change can be expressed as the sum of two contributions: the first results from comparing the level-1 entropy with its value obtained for level-0 resolution and the second results from comparing the level-2 entropy with its value obtained for level-1 resolution.

D. Relations among different expressions

Equation (72) relates the rate of irreversible entropy change to the difference between entropies calculated with respect to densities of different resolutions. It is natural to compare it with the irreversible change $\Delta_i S_m^{(0)}$ obtained earlier [Eq. (42)] for the same time period (one unit) by using a coarse graining over the full cell. We define the difference $\delta\Delta_i S_m$ by writing

$$\Delta_i S_m^{(1)'} = \Delta_i S_m^{(0)} + \delta\Delta_i S_m. \tag{77}$$

In the same spirit we also have to compare the entropy production $\Delta_i^{(2)} S_m^{(0)}$, where level-0 coarse graining is done after two time steps, with the value of the same quantity obtained by doing level-0 coarse graining after each time step. The latter is the sum of the single-step entropy productions:

$$[\Delta_i S_m^{(0)}]^{2\ \text{steps}} \equiv \Delta_i S_m^{(0)} + \Delta_i S_m^{(0)'}. \tag{78}$$

In view of Eq. (76) we find

$$\Delta_i^{(2)} S_m^{(0)} = [\Delta_i S_m^{(0)}]^{2\ \text{steps}} + \delta\Delta_i S_m, \tag{79}$$

i.e., the difference is again $\delta\Delta_i S_m$. It is thus sufficient to work out this latter quantity in order to find the difference between different approaches.

E. Evaluation of $\delta\Delta_i S_m$

First we note that

$$\begin{aligned} S_m^{(1)''} &\equiv -\Gamma \sum_q \frac{\tilde{s}_q}{b} \varrho''_m(q) \ln \varrho''_m(q) \\ &= -\Gamma \sum_q \frac{s_q}{a} \varrho'_{m_q} \ln \frac{b s_q}{a \tilde{s}_q} + \sum_q \frac{s_q}{a} S_{m_q}^{(0)'}. \end{aligned} \tag{80}$$

Together with Eq. (68b) this implies that

$$\begin{aligned} \Delta_i S_m^{(1)'} &\equiv S_m^{(1)''} - S_m^{(2)''} \\ &= \sum_q \frac{s_q}{a} [S_{m_q}^{(0)'} - S_{m_q}^{(1)'}] \\ &= \Delta_i S_m^{(0)} - r[\Delta_i S_m^{(0)} - \Delta_i S_{m-1}^{(0)}] - l[\Delta_i S_m^{(0)} - \Delta_i S_{m+1}^{(0)}]. \end{aligned} \tag{81}$$

Using Eq. (22) to express r and l in terms of the transport parameters and of the time and length units, we obtain

$$\begin{aligned} \delta\Delta_i S_m = \frac{\tau D}{a^2} \left(1 + \frac{\tau v^2}{2D} \right) [\Delta_i S_{m-1}^{(0)} + \Delta_i S_{m+1}^{(0)} - 2\Delta_i S_m^{(0)}] \\ - \frac{\tau v}{2a} [\Delta_i S_{m+1}^{(0)} - \Delta_i S_{m-1}^{(0)}]. \end{aligned} \tag{82}$$

Since $\Delta_i S_m^{(0)}$ is of order τa [after all, $\Delta_i S_m^{(0)}/(a\tau)$ approaches a finite limit, the irreversible entropy production per unit length (volume)], it is already clear from here that $\delta\Delta_i S_m$ is of order $\tau^2 a$. To see this in detail notice that in Eq. (82) the expressions in square brackets are discrete versions of spatial derivatives. In the limit of large spatial extension therefore we have

$$\delta\Delta_i S = \tau D \left(1 + \frac{\tau v^2}{2D} \right) \partial_x^2 \Delta_i S^{(0)} - \tau v\, \partial_x \Delta_i S^{(0)}. \tag{83}$$

For well-posed physical problems we expect $\Delta_i S_m^{(0)}/(a\tau)$ to approach a function with finite derivatives in x. This implies that $\delta\Delta_i S_m/(a\tau)$ possesses a well-defined limit of $a \to 0$ for any fixed τ, but *vanishes* for $\tau \to 0$. In other words, the corrections to both $\sigma^{(\text{irr})}$ and $P^{(\text{irr})}$ disappear in the large system limit. In this limit different prescriptions using different ways of coarse graining to calculate the rate of irreversible entropy production give indeed the same results. Similarly, one can check that also the expressions of the flux possess a well-defined macroscopic limit. As a consequence, the full entropy balance equation is independent of the way of coarse graining.

For sake of lucidity we only presented the calculations for the two simplest cases. We stress, however, that the argument is valid in general. Indeed, all calculations can be generalized in a straight-forward way to account for averaging only after every t time steps on any finite level ν. All these approaches only differ in terms that may be expressed as a product of τ and spatial derivatives of the macroscopic rate of irreversible entropy production. For larger t and ν more and higher order derivatives appear.

IX. DISCUSSION

In this paper we have illustrated that in dynamical systems modeling transport the following holds true.

(i) A coarse-grained version of the Gibbs entropy is a natural extension of the concept of thermodynamic entropy.

(ii) An entropy balance equation can be derived in properly or improperly thermostated models, provided the intracell dynamics is Hamiltonian.

(iii) The entropy current into the heat bath and into the particle reservoirs can be identified.

(iv) An agreement with nonequilibrium thermodynamics can be found only for the properly thermostated (i.e., dissipative with time reversal symmetry) model ($\epsilon = -1$) in its macroscopic limit.

(v) The details of the phase-space densities can be followed with enhanced resolution, but upon reaching the finest level of observation always the same amount of entropy is produced in the large system limit.

(vi) There is reason to believe that the formula $P^{(\mathrm{irr})} = u^2/D$ for the rate of irreversible specific entropy production in the large system limit is valid beyond linear thermodynamics, since the derivation of entropy production relies upon dynamical concepts.

(vii) The entropy-balance equation cannot be derived from the projected dynamics onto the direction of transport alone if any kind of thermostating (dissipation) is present.

In order to have a better understanding of the last statement, it is worth mentioning that a ''projected'' entropy S_p different from $S^{(G)}$ can be defined with respect to the mass density $\rho(x,t)$ [i.e., the phase-space density projected onto the direction of transport]:

$$S_p(t) = -\int \rho(x,t) \ln \rho(x,t)\, dx. \tag{84}$$

This entropy contains information about the inhomogeneities of the distribution along the x axis. The dynamics of the density $s_p(x,t) = -\rho(x,t)\ln\rho(x,t)$ of this entropy immediately follows from the advection-diffusion equation (5). A direct substitution shows that an entropy balance equation exists in the form

$$\partial_t s_p = -\partial_x j_{s_p} + \sigma_p \tag{85}$$

with

$$j_{s_p}(x,t) = -j(x,t)[1 + \ln\rho(x,t)] + v\rho(x,t) \tag{86}$$

as the entropy current, and

$$\sigma_p = D\frac{[\partial_x \rho(x,t)]^2}{\rho(x,t)} \tag{87}$$

as the entropy production of s_p. This rate of irreversible entropy production is always positive. However, in the case of a nonvanishing drift it is markedly different from the thermodynamic form $\varrho u^2/D$. This is in agreement with our previous observation that the projected density cannot contain information about the phase-space contraction along the y axis giving rise to the heat current into a thermostat. The projected density merely reflects the entropy changes related to the coupling to particle reservoirs.

To find a proper interpretation for the term $v\varrho$ in j_{s_p}, let us consider the balance of s_p from the point of view of an observer moving with velocity u_0 to the right. This corresponds to the transformation $\varrho(x,t) \to \varrho(x - u_0 t, t)$, which implies $v \to v - u_0$ and $j \to j - u_0 \varrho$ in the advection-diffusion equation. In the entropy balance equation the change in the time derivative is exactly compensated by the change of the flux so that the rate of irreversible entropy production remains *invariant*. For the special choice of $u_0 = v$ the case of a pure diffusion is recovered. Then, and only then, the projected density gives rise to an entropy production corresponding to Gaspard's result [25], i.e., $\sigma^{(\mathrm{irr})} = \sigma_p$.

In view of these observations we can say that the Hamiltonian version ($\epsilon = 1$) of our multibaker model corresponds to a purely diffusive problem observed from the reference frame moving to the left with velocity v. The presence of a term $v\rho$ in the total current j in this system is then due to a Galilei transformation and must not be identified with a current generated by an external field.

We expect our results to be generic for generalized Anosov systems. Although our model is piecewise linear, the general features are valid in a much broader class of systems since smooth dynamical systems appear on sufficiently (but not infinitesimally) small scales to be piecewise linear [39]. Thus we expect more general transport models to be well-approximated on small scales via multibaker maps that might have many more strips and columns (but of finite number) than ours, in different geometrical arrangements. At this point our work complements the chaoticity hypothesis of Gallavotti and Cohen [6,24,27]. In order to derive thermodynamic behavior, they assume hyperbolicity, and that the average phase-space contraction of the system is just the rate of irreversible entropy production. The requirement of hyperbolicity was stated as an extension of the ergodicity hypothesis in order to cover also nonequilibrium phenomena. Together with time reversibility, it might very well be a sufficiently good approximation to construct models for transport. However, the requirement about the equivalence of average phase-space contraction and the rate of irreversible entropy production was up to now based on plausible physical arguments [2,7,20] without introducing the concept of entropy and its balance equation. Here, we were able to demonstrate that this property can be derived for periodic driven thermostated systems with the use of coarse-grained entropies. As we also pointed out, this relation is a special case of a more general relation: in the presence of particle reservoirs giving rise to diffusion currents, there are additional contributions to the entropy production from the mixing of phase-space regions with different (coarse-grained) densities. In the case of pure diffusion when no dissipation is needed, this effect is responsible for the entire entropy production [25], but in the simultaneous presence of both diffusion and driving (thermostating) an interplay of both effects can be observed.

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