CHAOS VOLUME 8, NUMBER 2 JUNE 1998

Entropy balance, time reversibility, and mass transport in dynamical systems

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(Received 15 December 1997; accepted for publication 6 April 1998)

We review recent results concerning entropy balance in low-dimensional dynamical systems modeling mass (or charge) transport. The key ingredient for understanding entropy balance is the coarse graining of the local phase-space density. It mimics the fact that ever refining phase-space structures caused by chaotic dynamics can only be detected up to a finite resolution. In addition, we derive a new relation for the rate of irreversible entropy production in steady states of dynamical systems: It is proportional to the average growth rate of the local phase-space density. Previous results for the entropy production in steady states of thermostated systems without density gradients and of Hamiltonian systems with density gradients are recovered. As an extension we derive the entropy balance of dissipative systems with density gradients valid at any instant of time, not only in stationary states. We also find a condition for consistency with thermodynamics. A generalized multi-Baker map is used as an illustrative example. © *1998 American Institute of Physics.* [S1054-1500(98)02602-0]

Trajectories of chaotic dynamical systems closely approach the unstable manifold of an invariant set, namely, a chaotic saddle for open systems, or a chaotic attractor for closed and dissipative systems. Consequently, the Gibbs entropy of smooth initial distributions monotonically decreases in time. We introduce here the concept of coarse-grained phase-space densities and the corresponding entropies, and point out that a local entropy-balance equation with a non-negative irreversible entropy production can always be derived under weak assumptions. The structure of this microscopic balance equation is similar to what is known from thermodynamics, but the contributing terms differ in general from those in the macroscopic case. We show that the macroscopic and the microscopic balance equations are compatible only if it is possible to take the limit of large systems while keeping the transport coefficients fixed. In addition, in the case of a general driving due to an external field, a reversible dissipation mechanism is required, corresponding to a proper thermostating of the system. We also point out that consistency with thermodynamic results can only be achieved when considering the time evolution of the full phase-space density. Even though an entropy-balance equation can also be established for the process projected on the transport direction, this equation can no longer be compatible with thermodynamics, except for the case of unbiased mass transport (pure diffusion).

I. INTRODUCTION

The concept of irreversible entropy production in dynamical systems first appeared in the context of dissipative deterministic thermostats introduced to perform molecular dynamics simulations of transport in spatially periodic systems.[1,2] Since every ensemble of trajectories with smooth initial distributions approaches a chaotic attractor in the phase space,[3] it became clear soon that after an initial transient the Gibbs entropy *decreases* in time. It has a constant negative time derivative which coincides with the sum of all Lyapunov exponents on the attractor.[1,4] It was tempting to identify the modulus of this quantity with the irreversible entropy production. A qualitative explanation corroborating this view was based on the idea that the system together with the thermostat forms a larger closed system and, consequently, the thermostat's entropy should increase with at least the rate of decrease of the Gibbs entropy.[2,5,6]

Support of this picture is based on the observation that the negative sum of the Lyapunov exponents is the average phase-space contraction rate, which is expected to be non-negative in physically relevant cases. It is then natural to say that the average phase-space contraction rate should be considered as the irreversible entropy production.[4,6–13] Rigorous mathematical statements have been proved concerning properties of this entropy production.[10–12] On the other hand, there is a conceptual difficulty in these results because entropy production is referred to without specifying the underlying concept of entropy.

The cornerstone of nonequilibrium thermodynamics is an entropy which is (i) constant in a steady state (in contrast to the Gibbs entropy of thermostated systems), and (ii) has a time derivative which contains two contributions: the entropy flux $\mathrm{d}_e S/\mathrm{d}t$ and the irreversible entropy production $\mathrm{d}_i S/\mathrm{d}t \geqslant 0$[14]

$$\frac{\mathrm{d}S}{\mathrm{d}t}=\frac{\mathrm{d}_eS}{\mathrm{d}t}+\frac{\mathrm{d}_iS}{\mathrm{d}t}. \tag{1}$$

In any finite volume, the entropy density s, i.e., the entropy per unit volume, fulfills the balance equation

$$\frac{\mathrm{d}s}{\mathrm{d}t}=\Phi+\sigma^{(\mathrm{irr})}, \tag{2}$$

where $\mathrm{d}s/\mathrm{d}t$ is the time derivative of entropy density, Φ denotes the entropy flux *into* that volume, and the rate of irreversible entropy production $\sigma^{(\mathrm{irr})}\geqslant 0$ can be viewed as the source strength of entropy. In a steady state the entropy flux balances the irreversible entropy production, i.e., $\Phi=-\sigma^{(\mathrm{irr})}$, so that $\mathrm{d}s/\mathrm{d}t=0$.

The relation between the Gibbs entropy, which is continually decreasing in a steady state, and the thermodynamic entropy needs clarification. It is not *a priori* obvious why the temporal change of the Gibbs entropy should be fully attributed to the irreversible entropy production and not (at least partially) to an entropy flux into an attached heat bath or particle reservoir.

To find a consistent description, the use of a coarse-grained entropy has recently been proposed for dynamical systems.[15–22] This concept emphasizes the importance of finite resolution in any observation, which is mimicked by coarse graining the density over phase-space cells of a fixed size.[23] The coarse-grained entropy computed with respect to the coarse-grained density (or the ϵ-entropy[24]) differs qualitatively from the Gibbs entropy. After a long time, the coarse-grained density approaches a *stationary* distribution localized around the unstable manifold of the chaotic set. This limiting distribution is a finite-precision approximation of the natural measure on this manifold, which typically has a fractal structure. Correspondingly, the coarse-grained entropy eventually becomes independent of time. Then the irreversible entropy production can be defined as the loss of information on the microscopic state of the system due to the coarse-grained description. It is reflected in the growth of the difference between the coarse-grained and the Gibbs entropy.[15]

In open systems the concept of phase-space contraction has to be generalized since there is an effective phase-space contraction even in Hamiltonian cases because trajectories can escape from the relevant part of the phase space. This leads to the observation that the escape rate has to be added to the previous result.[10,15]

To understand boundary driven problems, it turned out to be essential to use the balance equations in addition to the coarse-grained entropies. The first attempt to derive entropy balance for a deterministic dynamical system is due to Gaspard[16] (in a noisy system to Nicolis and Daems[17]). To describe a one-dimensional diffusive current induced by flux boundary conditions, Gaspard considered a purely Hamiltonian model (a multi-Baker map). The rate of entropy production he derived was consistent with the thermodynamic expression in the large-system limit.

In the present paper we consider one-dimensional mass transport that is driven not only by density gradients but also by an external bias (a field). The entropy balance for maps modeling this process is worked out for arbitrary nonstationary states, and a general expression for the irreversible entropy production is derived. It turns out that the entropy production stems from *both* phase-space contraction and mixing. In other words, whenever mixing of phase-space volumes with different mass densities plays a role in the transport process, the irreversible entropy production does not coincide with the average phase-space contraction rate. We also show that the inclusion of dissipation is *unavoidable* in order to be consistent with classical thermodynamics in this general case. The only choice consistent with this requirement is a time-reversible dissipation mechanism that models proper thermostating of the system.

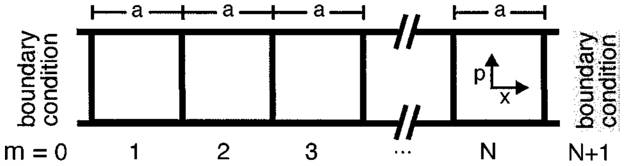

FIG. 1. General scheme of a map modeling mass transport. The mapping is defined on a domain of N identical cells of phase-space volume $\Gamma=ab$ where a is the width in the direction of an applied bias. Different boundary conditions can be imposed by suitably defined action of the map on two additional cells 0 and $N+1$.

In Sec. II we derive the entropy-balance equation for a general dynamical system. Different levels of description will be considered. We will find balance equations at all levels but an agreement with thermodynamics can be achieved only if the phase-space density is used to define the entropy, and if the system size is large. In Sec. III we introduce the biased multi-Baker model. The microscopic balance for this model is derived in Sec. IV, and its macroscopic limit is presented in Sec. V. In the conclusion we discuss the role of coarse graining for the concept of entropy (Sec. VI). The paper is augmented by three appendices. For reference, in Appendix A relevant thermodynamic relations are derived in a form not relying on temperature. The discussion of the entropy balance for the process projected on the transport direction is relegated to Appendix B. A generalization of the irreversible entropy-production formula to maps more general than the multi-Baker is given as Appendix C.

II. ENTROPY BALANCE FOR MAPS MODELING MASS TRANSPORT

We consider a system whose phase space is part of the (x,p) plane and consists of N identical cells which are aligned along the direction of an external field. The cells are coupled such that a trajectory can proceed from one cell to its neighbors. Since there are no temperature gradients in the system, all cells can be taken equivalent as far as their geometry and dynamics is concerned. They are of linear size a with phase-space volume $\Gamma=ab$ (Fig. 1). The time evolution is given by a mapping acting at integer multiples of the time unit τ. Since we are interested in ensembles of trajectories, we consider the dynamics of phase-space densities. In order to model the effect of finite accuracy of observation, we will consider coarse-grained densities where only the average phase-space density in the bins of a preselected fixed grid is specified. For simplicity, in the present paper this grid is taken to coincide with the cells depicted in Fig. 1.[25] Thus the mapping describing the time evolution of the coarse-grained densities will be considered as always acting on densities which are uniform within each cell. Such a density is also the initial condition for the time evolution of the phase-space density.

Let $\varrho_m(x,p)$ denote the phase-space density in cell m at some time t. For later reference we mention that the mass density $\rho_m(x)$ in cell m is obtained by integrating the phase-space density over the momentum coordinate

$$\rho_m(x)=\int_0^b \varrho_m(x,p)\mathrm{d}p. \tag{3}$$

The difference between these quantities is also stressed by labeling them with different letters, ρ and ϱ.

The Gibbs entropy $S_m^{(G)}$ of cell m is defined as

$$S_m^{(G)}=-\int_{\text{cell } m} \varrho_m(x,p)\ln\frac{\varrho_m(x,p)}{\varrho^\star}\,\mathrm{d}x\ \mathrm{d}p, \tag{4}$$

where the Boltzmann constant k_B has been suppressed, and $\varrho^\star$ is a constant reference density which fixes the origin of the entropy scale. It does *not* depend on spatial coordinates, time or the boundary conditions, and must not be confused with an equilibrium or steady-state density of the physical system under consideration.

The coarse-grained or *cell density* ϱ_m is the average density

$$\varrho_m=\frac{1}{\Gamma}\int_{\text{cell } m} \varrho_m(x,p)\mathrm{d}x\ \mathrm{d}p \tag{5}$$

in cell m. The corresponding entropy

$$S_m=-\Gamma\varrho_m\ \ln\frac{\varrho_m}{\varrho^\star} \tag{6}$$

is in general different from the Gibbs entropy. It will be called the *coarse-grained entropy* (coarse grained on the full cell). We argue below that it is a natural candidate for a generalization of the thermodynamic entropy to dynamical systems. When the coarse-grained entropies are defined on a grid with bins smaller than the full cell, the results depend on the form of the partitioning. In the macroscopic limit, however (cf. Sec. V), the chain consists of many cells ($N\gg 1$), and coarse graining over each cell corresponds to a rather fine resolution. In this limit the time derivatives and the contributions to the entropy balance become independent of the details of the partitioning inside the cell, as corroborated in Ref. 22.

To derive an entropy-balance equation, we compare quantities computed at two successive time steps, $t=t_0=n\tau$ and $t'=t_0+\tau=(n+1)\tau$. The temporal variation of the Gibbs entropy in cell m during one time step is

$$\Delta S_m^{(G)}=S_m^{(G)\prime}-S_m^{(G)}, \tag{7}$$

and, similarly, for the coarse-grained entropy we write

$$\Delta S_m \equiv S_m'-S_m. \tag{8}$$

In meaningful models of transport, the entropy change should always be related to particle motion contributing to transport. This means that for localized trajectories (as long as they stay inside a given cell) phase-space volume should be preserved. In view of this requirement we let the dynamics inside a cell be phase-space preserving (Hamiltonian), i.e., localized trajectories cannot contribute to the temporal change of a cell's Gibbs entropy. Consequently, the change of $\Delta S_m^{(G)}$ is entirely due to the entropy *flux* into the cell. The entropy fluxes in the coarse grained and in the microscopic description do not differ,

$$\Delta_e S_m=\Delta S_m^{(G)}. \tag{9}$$

This equation states that the coarse-grained entropy flux is *entirely* due to a change of the Gibbs entropy.

With this result Eq. (8) can also be written as

$$\Delta S_m=S_m^{(G)\prime}-S_m^{(G)}+[(S_m'-S_m^{(G)\prime})-(S_m-S_m^{(G)})]. \tag{10}$$

In view of (7) and (9),

$$\Delta S_m=\Delta_e S_m+\Delta_i S_m, \tag{11}$$

where

$$\Delta_i S_m \equiv (S_m'-S_m^{(G)\prime})-(S_m-S_m^{(G)}). \tag{12}$$

Here, the expressions for ΔS_m, $\Delta_e S_m$, and $\Delta_i S_m$ take the form of discrete time derivatives, so that Eq. (11) has the structure of an entropy-balance equation [cf. (1)]. Consequently, $\Delta_i S_m/\tau$ is a natural extension of the irreversible entropy production to dynamical systems. Being the change in time of the difference between the coarse-grained and the Gibbs entropy, it exactly measures the amount of information lost per time unit τ because of coarse graining.[15]

We remark that for the present choice of initial densities, which are uniform over full cells, the initial Gibbs and coarse-grained entropies coincide: $S_m=S_m^{(G)}$. In (10)–(12) the term $S_m-S_m^{(G)}$ was nevertheless written out explicitly, to make clear that $\Delta_i S_m$ is indeed a discrete time derivative.

Note that the Gibb's entropy $S_m^{(G)\prime}$ contains more information about the phase-space structure than the coarse-grained entropy S_m' and, therefore, must be less than or equal to S_m'. This ensures that the irreversible entropy production is always non-negative

$$\Delta_i S_m \geqslant 0. \tag{13}$$

The irreversible entropy production $\Delta_i S_m$ vanishes only when, under the dynamics, the phase-space densities are no longer developing fine structures. The absence of temporal changes in the structure of the phase-space density can therefore be viewed as a signature of thermal equilibrium.

In a nonequilibrium steady state we have $S_m'=S_m$, and the rate of irreversible entropy production

$$\left.\frac{\Delta_i S_m}{\tau}\right|_{ss}=-\frac{\Delta S_m^{(G)}}{\tau} \tag{14}$$

coincides with the *negative* time derivative of the Gibbs entropy. Thus the rule that, after a long time, the irreversible entropy production is the negative of the Gibbs entropy's time derivative appears as a natural consequence of the fundamental fact that any observation has finite precision. By that, the present approach also provides a foundation, within the framework of entropy balance, for the qualitative arguments mentioned in the Introduction.

Although the structure of the microscopic balance equation (11) is identical with that of the macroscopic equation (1), each term is yet a function of the microscopic parameters of the dynamics, e.g., of the cell size a, the time unit τ, and typically also of additional parameters symbolically denoted by ε. Therefore, the terms on the right hand side of Eq. (11) will not coincide with the corresponding terms of the macroscopic equation (1).

In the *macroscopic limit* the microscopic parameters a, and τ tend to zero in such a way that the transport coefficients stay finite. In that limit we expect that a finite entropy density is obtained as the limit of S_m/a. Furthermore, we also expect that the *rates* of entropy changes obtained from Eqs. (9), (8), and (12) by dividing these equations by $a\tau$ are also well-defined and finite. Thus $\Delta S_m/(a\tau)\to \mathrm{d}s/\mathrm{d}t(\varepsilon)$, $\Delta_e S_m/(a\tau)\to\Phi(\varepsilon)$, and $\Delta_i S_m/(a\tau)\to\sigma^{(\mathrm{irr})}(\varepsilon)$, so that the canonical form of entropy balance (2) is recovered

$$\frac{\mathrm{d}s}{\mathrm{d}t}(\varepsilon)=\Phi(\varepsilon)+\sigma^{(\mathrm{irr})}(\varepsilon). \tag{15}$$

Note, however, that in general all terms still depend on the system parameter(s) ε. Only for special values of ε, these terms can coincide with the expressions known from irreversible thermodynamics.

To facilitate comparison with thermodynamics, the temperature must be eliminated from the classical expressions for $\mathrm{d}s/\mathrm{d}t$, Φ and $\sigma^{(\mathrm{irr})}$. After all, in low-dimensional dynamical systems the concept of temperature is ill-defined. Appendix A shows how this can be achieved. In the next paragraphs we present temperature-independent expressions for the entropy flux Φ and the irreversible entropy production $\sigma^{(\mathrm{irr})}$.

According to irreversible thermodynamics, mass transport is characterized by the drift coefficient v and the diffusion coefficient D, and by two density distributions, namely, the mass density $\rho(x)$ and the current density $j(x)$. The current density j is the sum of the *diffusion current*, $-D\,\partial_x\rho$, and the *drift current*, $v\rho$

$$j=v\rho-D\partial_x\rho. \tag{16}$$

The conservation of particles leads to a continuity equation which is a kind of transport (Fokker–Planck) equation

$$\partial_t\rho=-\partial_x j=-v\,\partial_x\rho+D\partial_x^2\rho. \tag{17}$$

The entropy flux, which is the sum of a convective term and of the heat flow, can be written as

$$\Phi=\partial_x[j(c+\ln\varrho)]-\frac{v}{D}\,j \tag{18}$$

with c as a constant. The second term corresponds to the entropy flow related to the heat current into the thermostat (Joule's heat, cf. Appendix A).

The expression of the irreversible entropy production formula is obtained as

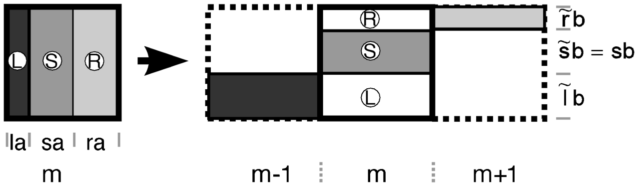

FIG. 2. Graphical illustration of the action of the multi-Baker map. Three vertical columns are squeezed and stretched to obtain horizontal strips of width a. Note the corresponding free spaces (white strips labeled R and S) where strips from the neighboring boxes are mapped to $(r+l=\tilde{r}+\tilde{l})$.

$$\sigma^{(\mathrm{irr})}=\frac{j^2}{\rho D}, \tag{19}$$

an expression quadratic in the total current density (16).

At this point general statements about the ε dependence of the flux and entropy production appearing in (15) cannot be made. For the particular example of the next section there is one and only one set of parameters which corresponds to the thermodynamic forms, namely, the one describing a *time-reversible dissipation mechanism* which models a proper thermostating of the system.

We show in Appendix B that an entropy balance similar to (15) also holds for the transport process projected on the transport direction. However, this ''projected'' entropy balance is in general inconsistent with thermodynamics.

III. THE MULTI-BAKER MODEL

Baker maps[26–28] are archetype models for strongly chaotic systems,[26] and multi-Baker maps[29–31,21,22] play an essential role in understanding the connection between chaotic microscopic dynamics and macroscopic irreversibility, which has also been a subject investigated by means of several other approaches.[32–39]

The phase-space of the multi-Baker model to be treated here consists of a chain of identical cells of linear size a and area $\Gamma=ab$ (cf. Fig. 1). To define the dynamics every cell is divided into three vertical columns (see Fig. 2): the rightmost (leftmost) column of width $ra(la)$ of each cell is mapped onto a strip of width a and height $\tilde{r}b(\tilde{l}b)$ in the square to the right (left). These columns are responsible for transport in one time step τ. The middle column of width sa stays inside the cell, thus modeling the motion that does not contribute to transport during a single iteration. This column is mapped onto a strip of width a and height $\tilde{s}b$. According to the argument of the previous section, the internal dynamics should be area preserving, i.e., $s=\tilde{s}$. Motivated by other models of transport, *global* phase-space conservation is assumed, which implies the sum rules $s+l+r=1=s+\tilde{l}+\tilde{r}$. In order to characterize the local dissipation mechanism, we introduce the parameter

$$\varepsilon\equiv\frac{\tilde{r}-\tilde{l}}{r-l}, \tag{20}$$

which measures the deviation from uniform phase-space contraction on the strips R and L. For $\varepsilon=1$ the Jacobians of the strips R and L are identical, while for $\varepsilon=-1$ they are reciprocal to each other. Besides the microscopic units (τ, a, and b), the thermodynamic and transport properties of the model are characterized by three independent parameters: the transition probabilities to neighboring cells r and l, and the dissipation parameter ε.

The phase-space contraction rates $\sigma_L=(1/\tau)\ln(l/\tilde{l})$ and $\sigma_R=(1/\tau)\ln(r/\tilde{r})$ on the respective strips L and R depend on the parameter ε. According to their value, different transport dynamics can be modeled:

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

$$\sigma_L=\sigma_R=0 \tag{21a}$$

($\varepsilon=1\Rightarrow r=\tilde{r},\ l=\tilde{l}$).

(ii) Dissipative dynamics with time-reversal symmetry:

$$\sigma_R=-\sigma_L=\frac{1}{\tau}\ln\frac{r}{l} \tag{21b}$$

($\varepsilon=-1\Rightarrow r=\tilde{l},\ l=\tilde{r}$). This choice mimics the effect of a thermostat.[21] Indeed, in order to model the decelerating effect of the heat bath on particles accelerated by the external field, a map modeling driven thermostated systems has to be area contracting if the trajectory moves in the direction of the bias. Similarly, the map should be expanding for trajectories moving against the bias, on which the heat bath has an accelerating effect to compensate for the slowing down by the external field (cf. Refs. 2, 5, 9). In addition, the overall dissipation should vanish for closed trajectories which do not contribute to transport. Since this is also true for period-2 orbits, the overall contraction rates $\sigma_R+\sigma_L$ for making a step to the right and a step to the left should add up to zero. It is worth noting that the map is then time-reversible.[40]

(iii) General dissipative dynamics:

$$\sigma_L\neq-\sigma_R\neq 0 \tag{21c}$$

($\varepsilon\neq\pm 1$). This case has similarities with the thermostating algorithm but does not fulfill the time-reversal symmetry.[40] We consider it as a model for improper thermostatting.

Finally, we stress that also the coarse-grained densities depend, in general, on time. Due to the conservation of probability, we have the following expression for the cell density ϱ_m' after one time step:

$$\varrho_m'=(1-r-l)\varrho_m+r\varrho_{m-1}+l\varrho_{m+1}. \tag{22}$$

This is a discrete-time master equation[42] governing the dynamics of the cell densities. In contrast to the full dynamics, it does not depend on the dissipation parameter ε. Because the average mass density ρ_m of cell m is $\rho_m=b\varrho_m$, Eq. (22) also holds for the average mass density. It provides a closed set of equations for the time evolution of the coarse-grained densities, which can rigorously be derived from the microscopic dynamics (cf. Refs. 31, 29). By this, modeling transport by means of multi-Baker maps allows us to work out the relation between self-contained descriptions of transport behavior on the microscopic level (phase-space densities and Gibbs entropy) and a macroscopic level (coarse-grained densities and coarse-grained entropy).

IV. ENTROPY BALANCE FOR THE MULTI-BAKER MODEL

In this section we calculate the different contributions (8), (9), (12) to the entropy balance (11) for the general multi-Baker map depicted in Fig. 2. As discussed above, we choose the initial density $\varrho_m(x,p)$ to be uniform in every cell. Then the coarse-grained entropy of cell m at time t and $t'=t+\tau$ takes the form

$$S_m=-\Gamma\varrho_m\ln\frac{\varrho_m}{\varrho^\star}=S_m^{(G)} \tag{23a}$$

and

$$S_m'=-\Gamma\varrho_m'\ln\frac{\varrho_m'}{\varrho^\star}, \tag{23b}$$

respectively. In order to compute the Gibbs entropy at time t', we note that the densities on the three horizontal strips depicted in Fig. 2 differ after having applied the map. On the strips R, S and L the density assumes the new values $\varrho_R'=\varrho_{m-1}r/\tilde{r}$, $\varrho_S'=\varrho_m$, and $\varrho_L'=\varrho_{m+1}l/\tilde{l}$, respectively. (The initial densities on these strips were $\varrho_R=\varrho_S=\varrho_L=\varrho_m$.) Consequently, the Gibbs entropy $S_m^{(G)\prime}$ is

$$S_m^{(G)\prime}\equiv-\Gamma\left[s\varrho_S'\ln\frac{\varrho_S'}{\varrho^\star}+\tilde{r}\varrho_R'\ln\frac{\varrho_R'}{\varrho^\star}+\tilde{l}\varrho_L'\ln\frac{\varrho_L'}{\varrho^\star}\right] \tag{24a}$$

$$=-\Gamma\left[(1-r-l)\varrho_m\ln\frac{\varrho_m}{\varrho^\star}+r\varrho_{m-1}\ln\left(\frac{\varrho_{m-1}}{\varrho^\star}\frac{r}{\tilde{r}}\right)\right.$$
$$\left.+l\varrho_{m+1}\ln\left(\frac{\varrho_{m+1}}{\varrho^\star}\frac{l}{\tilde{l}}\right)\right] \tag{24b}$$

$$=-\Gamma\left[\varrho_m'\ln\frac{\varrho_m}{\varrho^\star}+r\varrho_{m-1}\ln\left(\frac{\varrho_{m-1}r}{\varrho_m\tilde{r}}\right)\right.$$
$$\left.+l\varrho_{m+1}\ln\left(\frac{\varrho_{m+1}l}{\varrho_m\tilde{l}}\right)\right], \tag{24c}$$

where Eq. (22) has been used to arrive at the latter equality. It is clear from these relations that the Gibbs entropy $S_m^{(G)\prime}$ coincides with the coarse-grained one, S_m', only if the map does not generate any local inhomogeneities of the phase-space density.

Inserting Eqs. (23b) and (24) into the expressions for the change ΔS_m of the coarse-grained entropy [Eq. (8)], the change $\Delta_e S_m$ due to the flux [Eq. (9)], and the irreversible entropy change $\Delta_i S_m$ [Eq. (12)], one obtains

$$\Delta S_m=-\Gamma\left[\varrho_m'\ln\frac{\varrho_m'}{\varrho^\star}-\varrho_m\ln\frac{\varrho_m}{\varrho^\star}\right], \tag{25a}$$

$$\Delta_e S_m=-\Gamma\left[(\varrho_m'-\varrho_m)\ln\frac{\varrho_m}{\varrho^\star}+r\varrho_{m-1}\ln\left(\frac{\varrho_{m-1}}{\varrho_m}\frac{r}{\tilde{r}}\right)\right.$$
$$\left.+l\varrho_{m+1}\ln\left(\frac{\varrho_{m+1}}{\varrho_m}\frac{l}{\tilde{l}}\right)\right], \tag{25b}$$

$$\Delta_i S_m = \Gamma\left[r\varrho_{m-1} \ln\left(\frac{\varrho_{m-1}}{\varrho_m} \frac{r}{\tilde{r}} \right) + l\varrho_{m+1} \ln\left(\frac{\varrho_{m+1}}{\varrho_m} \frac{l}{\tilde{l}} \right) \right.$$
$$\left. - \varrho'_m \ln\frac{\varrho'_m}{\varrho_m} \right]. \tag{25c}$$

The sum of $\Delta_e S_m$ and $\Delta_i S_m$ is indeed the total change ΔS_m of entropy. Consequently, the balance equation (11) is fulfilled. In Appendix C we consider a map much more general than the multi-Baker model and show that, under very weak assumptions, an expression structurally very similar to (25c) follows for the irreversible change of entropy.

Let us discuss expression (25c) for $\Delta_i S_m$ in some more detail. First, we consider a steady state. Then the discrete version of the rate of irreversible entropy production is

$$\left.\frac{\Delta_i S_m}{\tau}\right|_{ss} = \Gamma \varrho_m \left[r\, \frac{\varrho_{m-1}}{\varrho_m} \ln \frac{\varrho'_R}{\varrho_R} + l\, \frac{\varrho_{m+1}}{\varrho_m} \ln \frac{\varrho'_L}{\varrho_L} \right]. \tag{26}$$

Notice that ϱ'_R/ϱ_R is the ratio of the local densities at time t' and t on strip R, and ϱ'_L/ϱ_L the corresponding quantity on strip L.

The probability to be mapped onto these strips by time t' is $r\varrho_{m-1}/\varrho_m$ (or $l\varrho_{m+1}/\varrho_m$). Therefore, we can say that the irreversible entropy production is related to the average of the *growth* rates

$$\sigma_\varrho(x,p) \equiv \frac{1}{\tau} \ln \frac{\varrho'(x,p)}{\varrho(x,p)} \tag{27}$$

of the *local* (non coarse-grained) phase-space densities. In other words,

$$\left.\frac{\Delta_i S_m}{\tau\Gamma \varrho_m}\right|_{ss} = \left.\frac{\Delta_i S_m}{\tau a \rho_m}\right|_{ss} = \langle \sigma_\varrho \rangle_{ss}\,. \tag{28}$$

Thus the irreversible entropy production per particle (degree of freedom) is the average growth rate of the local phase-space density, where the average has to be taken with respect to the steady-state distribution. In the special case when the coarse-grained density is constant along the chain ($\varrho_{m-1} = \varrho_m$ for every m), the local density growth rates reduce to the phase-space contraction rates $\sigma(x,p)$ and we recover the relation $(\Delta_i S_m/(\tau a \rho_m))_{ss} = \langle \sigma \rangle_{ss}$ valid for thermostated systems with periodic boundary conditions.[1,4,6–13] We believe (28) to be a proper generalization that holds in every steady state of a dynamical systems where mixing (i.e., intertwining of different neighboring average cell densities) plays a role.

To underline this observation, it is useful to separate the contributions stemming from mixing and phase-space contraction. To this end we split the full entropy change (25c) into a term with only ϱ dependence under the logarithms, a term which accounts for the change of phase-space volumes, and a time-dependent rest:

$$\Delta_i S_m = \Delta S_m^{(\mathrm{mix})} + \Delta S_m^{(\mathrm{con})} + \Delta S_m^{(\mathrm{evo})}\,. \tag{29}$$

Here,

$$\Delta S_m^{(\mathrm{mix})} \equiv \Gamma \left[r\varrho_{m-1} \ln \frac{\varrho_{m-1}}{\varrho_m} + l\varrho_{m+1} \ln \frac{\varrho_{m+1}}{\varrho_m} \right] \tag{30}$$

is the *mixing entropy* based on neighboring cell densities, and the contribution

$$\Delta S_m^{(\mathrm{con})} \equiv \Gamma [\varrho_{m-1} \tau \sigma_+ + \varrho_{m+1} \tau \sigma_-], \tag{31}$$

accounts for an average *contraction* of phase space. The quantities

$$\sigma_+ = \frac{1}{\tau} r \ln \frac{r}{\tilde{r}} \quad \text{and} \quad \sigma_- = \frac{1}{\tau} l \ln \frac{l}{\tilde{l}} \tag{32}$$

are the *conditional phase-space contraction rates* for the motion in the positive and negative direction, respectively. (By conditional we mean that for a constant distribution of the coarse-grained density these rates would be the average phase-space contraction rates for the two directions.) The third term of (29),

$$\Delta S_m^{(\mathrm{evo})} = -\Gamma \varrho'_m \ln \frac{\varrho'_m}{\varrho_m}, \tag{33}$$

vanishes in a steady state. It accounts for irreversible entropy production due to the temporal change of the cell densities, in addition to the contributions due to mixing and phase-space contraction which are found in both stationary and nonstationary situations. In particular, the splitting of Eq. (29) shows that in a steady state with constant cell densities, only the phase-space contraction contributes to the irreversible entropy production. In the other limiting case, namely, for a steady state where the dynamics is everywhere Hamiltonian, the mixing entropy provides the entire entropy production (see Ref. 16).

It is worth briefly mentioning the case of a homogenous temporal decay of the density towards an empty state, which corresponds to the decay with the most stable eigenstate of a system displaying transient chaos (escape rate formalism, cf. Refs. 5, 32, 31, 21). One can then write $\varrho'_m = \exp[-\kappa(t_0 + \tau)]\tilde{\varrho}_m$, where κ is the decay rate (escape rate from a saddle), and $\tilde{\varrho}_m$ is the conditional cell density which does not depend on time. An analogous form holds for the phase-space density $\varrho'_m(x,p) = \exp[-\kappa(t_0+\tau)]\tilde{\varrho}_m(x,p)$, where $\tilde{\varrho}_m(x,p)$ is the so-called conditional phase-space density. In contrast to its cell average, $\tilde{\varrho}_m(x,p)$ is time-dependent, expressing the approach towards the chaotic saddle's unstable manifold. From (25c) we obtain for such a **d**ecaying **s**tate (ds)

$$\left.\frac{\Delta_i S_m}{\tau a \rho_m \exp(-\kappa\tau)}\right|_{ds} = \kappa + \langle \sigma_{\tilde{\varrho}} \rangle_{ds}\,, \tag{34}$$

where κ stems from $\Delta S_m^{(\mathrm{evo})}$, and

$$\langle \sigma_{\tilde{\varrho}} \rangle_{ds} = \frac{e^{\kappa\tau}}{\tau} \left[r\, \frac{\tilde{\varrho}_{m-1}}{\tilde{\varrho}_m} \ln \frac{\tilde{\varrho}'_R}{\tilde{\varrho}_R} + l\, \frac{\tilde{\varrho}_{m+1}}{\tilde{\varrho}_m} \ln \frac{\tilde{\varrho}'_L}{\tilde{\varrho}_L} \right] \tag{35}$$

is the average growth rate of the conditional phase-space density evaluated under the condition that particles have not yet escaped. Note that $\sigma_{\tilde{\varrho}} = (1/\tau)\ln(\tilde{\varrho}'/\tilde{\varrho})$ appearing here is the direct generalization of σ_ϱ [cf. Eq. (27)] for the conditional density $\tilde{\varrho}_m(x,p)$.

Equation (34) is an extension of the results of Ref. 15, which are recovered for two special cases: a homogeneous cell density distribution, $\varrho_m = \varrho_{m+1}$, or averaging over the whole system. If the deviation from a homogeneous cell density distribution is important (or averaging takes place over, e.g., individual cells), there is, according to (34), (35), also a contribution due to the mixing entropy, just as in a steady state.

V. THE MACROSCOPIC LIMIT

As a first step towards a meaningful macroscopic limit, we assume that the system consists of a large number $N \gg 1$ of cells. This implies that the total length $L \equiv Na$ is much larger than the cell size a. We are interested in the *large-system limit* corresponding to $a \ll L$, i.e., to $a \to 0$ at fixed length L.

The spatial variation of the average phase-space density ϱ_m, i.e., of the cell density, follows the one of the mass density ρ_m in the large system limit ($b\varrho_m = \rho_m$). Thus the cell densities for the neighbors of cell m [i.e., at positions $x+\delta x = (m \pm 1)a$] can be expressed through spatial derivatives of the mass density distribution $\rho(x)$ at $x = ma$. Up to second order in a,

$$b\varrho_{m\pm 1} = \rho(x) \pm a\,\partial_x \rho(x) + \frac{a^2}{2}\,\partial_x^2 \rho(x). \tag{36}$$

In the same spirit, the temporal variation of the cell density reads

$$b(\varrho_m' - \varrho_m) = -a(r-l)\,\partial_x \rho + \frac{a^2}{2}(r+l)\,\partial_x^2 \rho. \tag{37}$$

Substituting these relations for the phase-space densities in (25c) yields for the irreversible entropy production in the large system limit

$$\frac{\Delta_i S_m}{a\tau} = (\sigma_+ + \sigma_-)\left(\rho + \frac{a^2}{2}\,\partial_x^2 \rho\right) - a(\sigma_+ - \sigma_-)\,\partial_x \rho + \frac{a^2}{2\tau}\left[(r+l) - (r-l)^2\right]\frac{(\partial_x \rho)^2}{\rho}. \tag{38a}$$

The first two terms are consequences of the phase-space contraction, while the third one arises from $\Delta S^{(\mathrm{mix})}$ and $\Delta S^{(\mathrm{evo})}$. A similar rearrangement of (25b) yields for the entropy flux

$$\begin{aligned}\frac{\Delta_e S_m}{a\tau} = {} & -(\sigma_+ + \sigma_-)\left(\rho + \frac{a^2}{2}\,\partial_x^2 \rho\right) \\ & + a\left[\sigma_+ - \sigma_- - \frac{r-l}{\tau}\right]\partial_x \rho \\ & + \partial_x\left[\left(a\,\frac{r-l}{\tau}\,\rho - \frac{a^2}{2}\,\frac{r+l}{\tau}\,\partial_x \rho\right)\left(1 + \ln\frac{\rho}{\rho^\star}\right)\right],\end{aligned} \tag{38b}$$

where $\rho^\star \equiv b\varrho^\star$ denotes the reference mass density.

The fact that these equations are expressed solely by spatial derivatives of the mass density distribution does not yet ensure the existence of a well defined macroscopic limit for $\sigma^{(\mathrm{irr})}$ and Φ. We see that the limit $\tau \to 0$ strongly depends on how the transition probabilities r and l behave. In order to find a sufficient condition for the existence of this limit, we go back to the microscopic model. The cell-to-cell dynamics of the multi-Baker model is equivalent to a random walk with fixed step length a.[31,42,43] Such random walks are characterized by well defined drift (v) and diffusion (D) coefficients, which can be expressed in terms of r and l as $(r-l)a = v\tau$ and $(r+l)a^2 = 2D\tau$, respectively.[44] Thus,

$$r = \frac{\tau D}{a^2}\left(1 + \frac{av}{2D}\right), \quad l = \frac{\tau D}{a^2}\left(1 - \frac{av}{2D}\right). \tag{39}$$

If v and D are fixed, these relations determine the scaling behavior of the transition probabilities r and l as a function of the length unit a and the time unit τ.

Via the conditional contraction rates $\sigma_\pm$, Eqs. (38a) and (38b) contain the parameters $\tilde{r}$ and $\tilde{l}$. It is convenient to express $\tilde{r}$ and $\tilde{l}$ in a similar way as r and l, which, however, now also contain the dissipation parameter ε

$$\tilde{r} = \frac{\tau D}{a^2}\left(1 + \varepsilon\,\frac{av}{2D}\right), \quad \tilde{l} = \frac{\tau D}{a^2}\left(1 - \varepsilon\,\frac{av}{2D}\right). \tag{40}$$

Since ε is also a parameter which is relevant for the macroscopic behavior we *define* the macroscopic limit as

$$a \to 0, \quad \tau \to 0, \quad \text{with} \quad v, D, \varepsilon \quad \text{fixed} \tag{41}$$

(or $a \ll L, D/v$; $\tau \ll L^2/D, D/v^2$). It is in this limit that the dynamics (37) of the cell (or mass) densities reduces to the macroscopic mass transport equation (17). However, this requirement only ensures that the transport process can be described by a one-dimensional Fokker–Planck equation. It does not yet imply that the model also has a meaningful thermodynamics.

In the macroscopic limit one immediately finds

$$\sigma_+ + \sigma_- = \frac{v^2(1-\varepsilon)^2}{4D}, \quad \sigma_+ - \sigma_- = \frac{v(1-\varepsilon)}{a}. \tag{42}$$

Inserting these relations, as well as (39) and (40), into Eq. (38a), we obtain the asymptotic expression

$$\sigma^{(\mathrm{irr})}(\varepsilon) = \frac{\rho}{D}\left(\frac{v(1-\varepsilon)}{2} - D\,\frac{\partial_x \rho}{\rho}\right)^2. \tag{43}$$

In the same way we find for the entropy flux Eq. (38b)

$$\Phi(\varepsilon) = \partial_x\left[j\left(1 + \ln\frac{\rho}{\rho^\star}\right)\right] - \varepsilon v\,\partial_x \rho - \frac{v^2(1-\varepsilon)^2}{4D}\,\rho, \tag{44}$$

where the particle current density j is given by (16). A comparison with the thermodynamic entropy balance also shows that the limit of $-b\varrho_m \ln(\varrho_m/\varrho^\star) = -\rho_m \ln(\rho_m/\rho^\star)$ goes over into the macroscopic expression

$$s(x) = -\rho(x)\ln\frac{\rho(x)}{\rho^\star} \tag{45}$$

of the entropy density given in terms of the mass density. Thus for every ε we find $\mathrm{d}s/\mathrm{d}t = (1 + \ln(\varrho/\varrho^\star))\partial_x j$. We emphasize again that the balance equation and (43), (44) are valid at every instant of time, not only in steady states.

It is remarkable that the asymptotic macroscopic expressions for $\sigma^{(\mathrm{irr})}(\varepsilon)$ and $\Phi(\varepsilon)$ are finite for arbitrary values of the dissipation parameter ε. However, there exists only one value for which the thermodynamic results (18), (19) are recovered, namely $\varepsilon = -1$. [The constant c of Eq. (18) corresponds to $1 - \ln \rho^\star$ and can be set zero by the choice of $\rho^\star = e$.] We thus conclude that (a) although transport caused by an external field (bias) is considered to be a typical many-body phenomenon, it can faithfully be modeled by discrete-time dynamical systems with few degrees of freedom. The heat flow accompanying transport (Joule's heat) is accounted for by a reversible dissipation mechanism. (b) The thermostating condition is fulfilled in one point of the parameter space only.

Several comments are in order.

(i) For the derivation of Eqs. (43) and (44) we did not specify boundary conditions, i.e., the macroscopic results hold irrespective of their choice. In particular, (43) with ($\varepsilon = -1$) implies that even for periodic boundary conditions there is a non-negligible mixing entropy contribution (the term proportional to $\partial_x \rho$) before the steady state is reached. It is only in the long time limit of such periodic cases that $\sigma^{(\mathrm{irr})}/\rho$ equals v^2/D and coincides with the negative sum of the average Lyapunov exponents.

(ii) The multi-Baker model is an example for which the laws of thermodynamics can be derived without using the concept of temperature and heat. Instead, irreversible entropy production was seen to arise from the mixing of phase-space regions due to a strongly chaotic dynamics. This mechanisms is by no means restricted to low-dimensional systems. We expect it to be the dynamical reason for irreversible entropy production and for the possibility to find an entropy balance in systems with many degrees of freedom, too. In this approach the concepts of heat and temperature appear as convenient tools to characterize certain macroscopically relevant effects of the mixing process.

(iii) Entropy-balance equations have been established for arbitrary values of the external control parameter ε. We would like to point out that although a macroscopic limit exists in all these cases, the expressions obtained for the fluxes and for the irreversible entropy production do, in general, not fulfill the thermodynamic relations between (thermodynamic) forces, induced currents and entropy production. Only for parameter values corresponding to a properly thermostated system (including time reversibility), the thermodynamic relations are recovered. This emphasizes the necessity of both the existence of a meaningful macroscopic limit and proper thermostating.

(iv) It is worth pointing out where the chaoticity of the underlying dynamics plays an essential role. It is the *mixing* property (in the sense of ergodic theory[5,26]) of the multi-Baker map without which an analogy with a random walk, and hence a transport equation, cannot be established. The mixing property leads to the appearance of a diffusion coefficient D which, in our approach, is of *fully dynamical* origin. In view of point (ii), we also see how accurate Gibbs' analogy of irreversible processes with the mixing of a nondiffusive dye in a colorless solvent[45] was, since the latter is of course a chaotic process with mixing properties.[46]

(v) The macroscopic expression $\sigma^{(\mathrm{irr})} = j^2/(\rho D)$ was derived here (for $\varepsilon = -1$) without any assumption about whether or not the system is close to thermal equilibrium. Therefore, we expect this form to hold beyond linear-response theory.

(vi) It was shown that besides for steady states of periodic systems where $\partial_x \rho = 0$, the rate of irreversible entropy production $\sigma^{(\mathrm{irr})}$ contains contributions not only from phase-space contraction but also due to spatial variations of the density. To our knowledge, these contributions can only be derived from dynamical system theory via coarse graining.

VI. DISCUSSION

We conclude this paper with comments on the role of coarse graining when defining entropies. Dividing the phase space into elementary cells of area $\Delta p \Delta q \equiv \Delta \Gamma$ is essential for the foundation of equilibrium statistical mechanics.[43] It is well-known that the equilibrium entropy is defined only up to an additive constant whose value depends on the partition size $\Delta\Gamma$. By the uncertainty principle of quantum mechanics, $\Delta\Gamma$ is bounded from below by Planck's constant h. However, the value of $\Delta\Gamma$ does not affect thermodynamic observables. Indeed, the entropy itself is not an observable, and its derivatives, the observables, are not affected by the additive constant depending on $\Delta\Gamma$.

The same reasoning applies to coarse-grained entropies of dynamical systems. The entropies themselves depend on the way of coarse graining, but their temporal derivatives, which appear in the balance equation, are much less sensitive. In the macroscopic limit the dependence on the coarse graining disappears completely.[16,22]

In the bulk of the paper, we have not discussed the approach to thermal equilibrium in a closed system, i.e., in a Hamiltonian system with a closed phase space. Owing to Liouville's theorem, the Gibbs entropy does not depend on time in that case, its value is preserved. Also in the context of closed systems, one way to find an increase of entropy when starting from nonequilibrium initial conditions is to introduce a coarse-grained entropy. It was already Gibbs who showed that the coarse-grained density approaches some finite limit in the long time limit.[45] He also claimed that the coarse-grained entropy based on this density can increase in time (for polemic discussions, see also Refs. 47–49).

It is interesting to compare the time evolution of the difference $\Delta_i S(t)$ between the coarse-grained and the Gibbs entropy in this Hamiltonian case with the time evolution of the same difference for a transport process approaching a steady state (cf. Fig. 3). For both situations, the Gibbs entropy $S^{(G)}$ is compared at any time with the entropy S computed, for the same initial conditions, with densities coarse grained on a fixed grid. In the case of a closed system, the Gibbs entropy remains unchanged, but $S(t)$ initially grows with time [Fig. 3(a)]. Since closed systems eventually approach equilibrium, the coarse-grained entropy saturates. Consequently, the time derivative of $\Delta_i S(t)$, which can again be considered as irreversible entropy production, first grows but vanishes in the long-time limit. The basic difference between a thermodynamically closed and an open system relaxing towards a nonequilibrium state is that in the

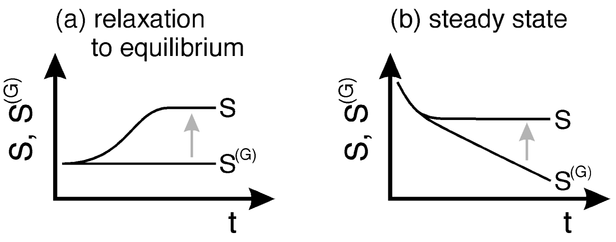

FIG. 3. Schematic time evolution of the coarse-grained density S and the Gibbs entropy $S^{(G)}$ for (a) a closed system where the densities relax to their equilibrium values, and (b) an open system approaching a steady state that carries a nonvanishing mass current. In both cases, the initial condition is smooth and distributed over a region of the phase space much bigger than the cell size used for coarse graining. The arrow indicate the effect of coarse graining on the Gibbs entropy.

latter case the Gibbs entropy decreases forever [Fig. 3(b)].

A jump from the phase-space density to its coarse-grained analog causes the Gibbs entropy to jump up to the curve of S. Because the third column (S) is missing in their model, they can neither find consistency with a Fokker–Planck equation nor with the thermodynamical form of the irreversible entropy production. When such a coarse graining is performed after the closed system has relaxed to equilibrium, S and $S^{(G)}$ remain identical [Fig. 3(a)]. This is a partial extension of the approach of Ref. 22, where only two different refined partitions were investigated but results for arbitrary non-stationary states could be obtained. Even though a jump from the phase-space density to its coarse-grained analog causes the Gibbs entropy to jump up to the curve of S, the coarse-grained and Gibbs entropy always start to differ again after the coarse graining. The central point of the present article was to call attention to this qualitatively different behavior of closed and open systems, which leads to a strictly positive irreversible entropy production in nonequilibrium systems. The ever-lasting decrease of the Gibbs entropy is a striking consequence of the fact that nonequilibrium steady states are associated with chaotic systems whose steady-state distributions are supported by fractal subsets of the phase space.

Note added: After submitting this paper we became aware of a recent preprint by Gilbert and Dorfman[50] dealing with closely related problems. In a multi-Baker model, defined with two columns only, they discuss properties of the entropy in stationary states of the Hamiltonian and of the properly thermostated version (the cases $\varepsilon = \pm 1$ in our notation). By carrying out coarse graining on *arbitrarily* fine Markov-partitions, they derive an expression for the irreversible entropy production in steady states. This is an extension of the results of Ref. 22, where only two different refined partitions were investigated, but for arbitrary nonstationary states. The authors of Ref. 50 show by explicit numerical calculation that in the limit of large system size the irreversible entropy production becomes independent of the partitioning everywhere, except for a narrow boundary layer around the two ends of the chain. Based on the results of Refs. 22 and 50 we firmly believe that in the bulk of every macroscopically large system none of the terms in the entropy-balance equation depends on the details of coarse graining. This is why one recovers the thermodynamic results, as we did in the present paper, even with the most straight-forward choice of coarse-graining size (namely, the full cell size) and the choice of a constant initial density in every cell.

ACKNOWLEDGMENTS

This work was started during a workshop at the ESI in Vienna. We are grateful for enlightening discussions with H. van Beijeren, E. G. D. Cohen, J. R. Dorfman, P. Gaspard, T. Geszti, W. G. Hoover, R. Klages, L. Mátyás, G. Nicolis, L. Rondoni, L. Sasvári, P. Szépfalusy, and S. Tasaki. JV gratefully acknowledges financial support by the Deutsche Forschungsgemeinschaft, and hospitality of the Max-Planck Institute for polymer research (Mainz) where he was a guest scientist upon completion of this work. TT was supported by the Hungarian Science Foundation (OTKA T17493, T19483).

APPENDIX A: NONEQUILIBRIUM THERMODYNAMICS OF MASS TRANSPORT

In this section we summarize the thermodynamic relations describing transport due to the simultaneous presence of drift and diffusion currents.[14] We restrict ourselves to cases where the external field and the density gradient are both parallel to the x-axis so that the diffusion and the conductivity are scalar quantities. The temperature T of the system will be kept constant throughout the system, i.e., we will not consider heat conduction. For the derivation we use the laws of nonequilibrium thermodynamics and linear response. We stress, however, that in spite of this assumption the expressions can very well be of more general validity.

The conductivity σ is the transport coefficient which 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[14]

$$j = \sigma T X = \sigma(E - \partial_x \mu). \tag{A1}$$

Next, we rewrite the current in a convenient form. Substituting, in Eq. (A1), the thermodynamic expression for the diffusion coefficient

$$D = \sigma \left. \frac{\partial \mu}{\partial \rho} \right|_T \tag{A2}$$

we find that $j = \sigma E - D \partial_x \rho$. By introducing the drift velocity

$$v \equiv \mu_0 E \equiv \frac{\sigma E}{\rho}, \tag{A3}$$

(Ohm's law) where μ_0 is the mobility of the particles, we find the full current in the form of (16).

The entropy flux contains[14] a convective contribution

$$\Phi^{(\text{conv})} = \partial_x [j(c + \ln \rho)] \tag{A4}$$

characterizing the entropy carried by the flow of particles (here c is a constant which is typically scaled out to zero). In the presence of a thermostat there must be another contribution, which accounts for the entropy flux due to heat which

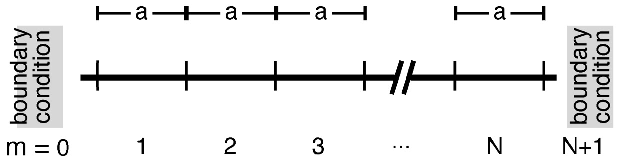

FIG. 4. Chain of intervals along the x axis on which the projected dynamics is defined. (cf. the text).

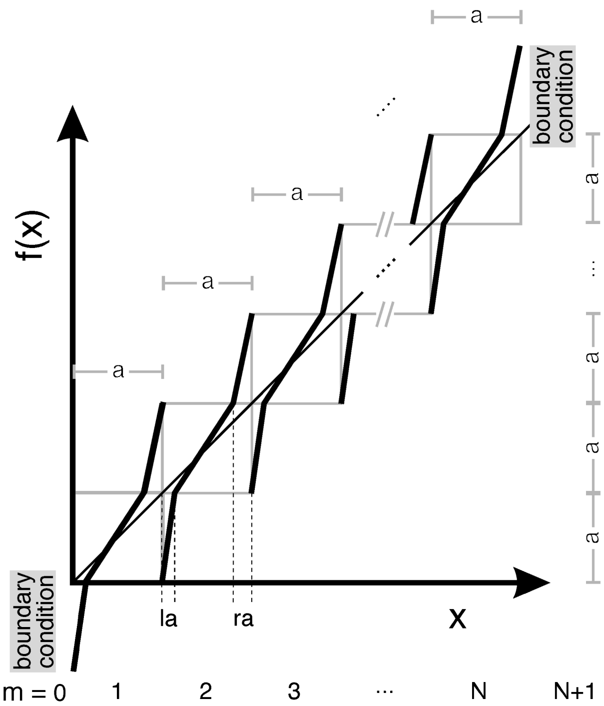

FIG. 5. Piecewise linear map governing the projected dynamics of the multi-Baker model.

dissipates the work done by the external field into a thermostat (Joule's heat). This contribution will be called $\Phi^{(\mathrm{heat})}$, and it takes the form

$$\Phi^{(\mathrm{heat})}=-\frac{Ej}{T}=-\frac{v}{D}\,j. \tag{A5}$$

Here, we used the definition of the drift (A3) and Einstein's relation $\rho D=\sigma T$ to arrive at the last equality. The total flux is the sum: $\Phi=\Phi^{(\mathrm{conv})}+\Phi^{(\mathrm{heat})}$.

Finally, the rate of irreversible entropy production $\sigma^{(\mathrm{irr})}$ is the product of the current density j and the thermodynamic driving force X[14]

$$\sigma^{(\mathrm{irr})}=jX. \tag{A6}$$

In view of Eq. (A1), this leads to

$$\sigma^{(\mathrm{irr})}=\frac{j^2}{\sigma T}=\frac{j^2}{\rho D}, \tag{A7}$$

where again Einstein's relation has been used.

APPENDIX B: ENTROPY BALANCE FOR THE PROCESS PROJECTED ON THE DIRECTION OF TRANSPORT

1. Entropy balance

Since the thermodynamic expressions only contain the mass density distribution $\rho(x)$ along the transport axis, the question arises in which sense the orthogonal direction is relevant. To clarify this, we discuss an entropy balance based on the projected density, i.e., on the mass density distribution inside the cells.

For a general model of the type of Fig. 1, the dynamics of the projected density is generated by an extended one-dimensional map containing identical intervals of size a (see Fig. 4). We define the ''projected'' (Gibbs) entropy as

$$S_m^{(p)}=-\int_{\text{interval } m}\rho_m(x)\ln\frac{\rho_m(x)}{\rho^\star}\,\mathrm{d}x, \tag{B1}$$

which contains information about the inhomogeneities of the projected distribution along the x axis. Here, again, we used $\rho^\star=b\varrho^\star$ as the reference density for the definition of the entropy. We also define a coarse-grained projected entropy computed with the average mass density ρ_m in each interval. In view of Eq. (5), $\rho_m=b\varrho_m$. Therefore, with this choice of $\rho^\star$ the coarse-grained projected entropy $S_m^{(p)}$ *coincides* with the coarse-grained entropy S_m. Thus we can drop the superscript of the coarse-grained entropy: $S_m^{(p)}=S_m$. In spite of this coincidence, however, the balance equation for the projected entropy differs profoundly from its phase-space analog.

For the projected entropy, the derivation of a balance equation is more formal than in the full phase-space approach, because the projected dynamics is no longer invertible. For states with constant mass densities in every interval, the projected Gibbs entropy coincides thus with the coarse-grained entropy although the entropy production might still be strictly positive. What can be done in any case is to identity a flux $\Delta_e S_m^{(p)}$ of the projected entropy into interval m due to the motion of one-dimensional volumes across the boundaries of this interval during one time unit. This quantity is typically different from the full change ΔS_m of the entropy. Therefore, we can *define* the irreversible projected entropy change via a balance equation

$$\Delta S_m^{(p)}=\Delta S_m=\Delta_e S_m^{(p)}+\Delta_i S_m^{(p)}, \tag{B2}$$

i.e., as the difference

$$\Delta_i S_m^{(p)}\equiv\Delta S_m-\Delta_e S_m^{(p)}. \tag{B3}$$

Thus, in this approach the existence of an entropy-balance equation is necessary for the *definition* of entropy production.

2. Entropy balance in the projected multi-Baker map

The dynamics projected onto the x axis is governed by the one-dimensional map depicted in Fig. 5. Since the 1D map is piecewise-linear, the density ρ_m is a step function which is constant within every cell at any instant of time, if the initial density is of this type. Again, we find $\rho_m=b\varrho_m$.

The entropy flux $\Delta_e S_m^{(p)}$ into interval m during one time step corresponds to the flow of S_m through the boundaries of the interval, i.e., it is given by the difference between the respective in- and outgoing fluxes

$$S_m^{(p,\mathrm{in})} = -a\left(r\rho_{m-1} \ln \frac{\rho_{m-1}}{\rho^\star} + l\rho_{m+1} \ln \frac{\rho_{m+1}}{\rho^\star} \right), \tag{B4a}$$

$$S_m^{(p,\mathrm{out})} = -a(r+l)\rho_m \ln \frac{\rho_m}{\rho^\star}. \tag{B4b}$$

The total flux is obtained, after using (22) for the mass density, as

$$\begin{aligned}\Delta_e S_m^{(p)} &\equiv S_m^{(p,\mathrm{in})} - S_m^{(p,\mathrm{out})}\\ &= -a\left[(\rho_m' - \rho_m)\ln \frac{\rho_m}{\rho^\star} + r\rho_{m-1} \ln \frac{\rho_{m-1}}{\rho_m} \right.\\ &\quad \left. + l\rho_{m+1} \ln \frac{\rho_{m+1}}{\rho_m} \right].\end{aligned} \tag{B5}$$

Note that this is exactly the same as Eq. (25b) except that here, the effect of phase-space contraction is missing.

In view of (B3) the irreversible change of the projected entropy reads

$$\Delta_i S_m^{(p)} \equiv a\left[r\rho_{m-1} \ln \frac{\rho_{m-1}}{\rho_m} + l\rho_{m+1} \ln \frac{\rho_{m+1}}{\rho_m} - \rho_m' \ln \frac{\rho_m'}{\rho_m} \right]. \tag{B6}$$

As expected, it is independent of the parameters $\tilde{r}$ and $\tilde{l}$ characterizing the phase-space contraction in the full baker dynamics.

3. Macroscopic limit

The present approach corresponds to the Hamiltonian choice $\varepsilon = 1$ of the previous results [cf. Eq. (25)]. Therefore, in the macroscopic limit when ρ_m tends to $\rho(x)$ we find

$$\Phi^{(p)} = \partial_x \left[j\left(1 + \ln \frac{\rho}{\rho^\star} \right) \right] - v\,\partial_x \rho \tag{B7}$$

and

$$\sigma^{(p,\mathrm{irr})} = D\,\frac{(\partial_x \rho)^2}{\rho}. \tag{B8}$$

Note that the same result is also obtained by directly considering the large-system limit of the projected entropy in (B1). In this limit, $\rho_m(x)$ approaches the thermodynamic mass density $\rho(x)$, and the Fokker–Planck equation (17) can be used to directly evaluate the time derivative of the projected entropy. In this limit, S_m/a approaches s, and one obtains an entropy-balance equation of the form

$$\partial_t s = \Phi^{(p)} + \sigma^{(p,\mathrm{irr})}, \tag{B9}$$

where $\Phi^{(p)}$ and $\sigma^{(p,\mathrm{irr})}$ are again given by Eqs. (B7) and (B8). Although this is a well-defined macroscopic entropy-balance equation with a non-negative entropy production, it is markedly different from the thermodynamic form in the case of a nonvanishing drift. This is consistent with the observation that the projected density cannot contain information about the phase-space contraction along the p axis, which is related to the heat current into a thermostat. The projected density faithfully reflects the entropy changes related to the interaction with particle reservoirs, but it cannot account for the effects related to a heat bath.

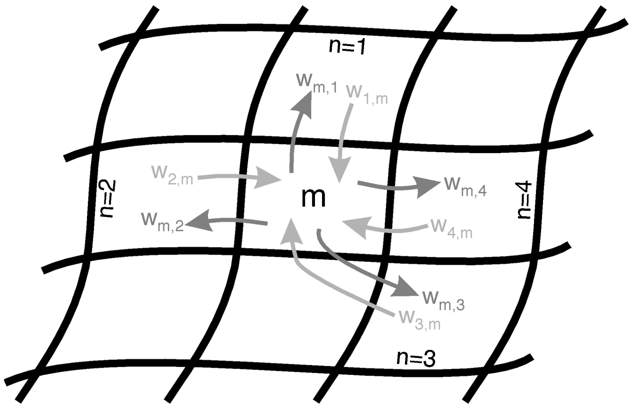

FIG. 6. Notations used for the discussion of entropy production for general maps (cf. the text).

APPENDIX C: IRREVERSIBLE ENTROPY PRODUCTION FOR GENERAL MAPS

We work out the irreversible entropy production Eq. (12) per time step τ in cell m for a general map modeling mass transport on a grid of cells as schematically depicted in Fig. 6.

In order to describe the time evolution of the system on the level of coarse-grained densities, we introduce the following notations:

n: label of the neighbors of cell m.

ϱ_j: the coarse-grained density in cell j.

Γ: the (possibly high dimensional) volume of each cell.

$w_{j,k}$: the transition probability from cell j to k.

$s_{j,k}$: volume fraction of cell j mapped into cell k. $s_{m,m}$ denotes the volume fraction which does not leave cell m in one time step. The $s_{j,k}$'s are subjected to the sum rule

$$\sum_{j\in\{n,m\}} s_{m,j} = 1. \tag{C1}$$

$\tilde{s}_{j,k}$: volume fraction of cell k which contains all points with preimages in cell j. We are only interested in globally phase-space preserving flows implying

$$\sum_{j\in\{n,m\}} \tilde{s}_{j,m} = 1. \tag{C2}$$

Note that $\tilde{s}_{j,j} = s_{j,j}$ for every j because of the assumption that the internal dynamics in every cell is phase-space preserving.

Taking the cell density to be constant because of coarse graining, the transition probability from cell j to k is the volume fraction mapped into cell k

$$w_{j,k} = s_{j,k}. \tag{C3}$$

The volume fraction $\tilde{s}_{m,m}$ of points not leaving cell m in one time step is obtained as

$$s_{m,m}=\tilde{s}_{m,m}=1-\sum_n w_{m,n}. \tag{C4}$$

Conservation of probability leads to a master equation expressing the cell density ϱ'_m after one time step[42]

$$\begin{aligned}\varrho'_m&=\varrho_m-\sum_n (w_{m,n}\varrho_m-w_{n,m}\varrho_n)\\ &=s_{m,m}\varrho_m+\sum_n s_{n,m}\varrho_n .\end{aligned} \tag{C5}$$

At time t' the coarse-grained entropy is

$$S'_m=-\Gamma\varrho'_m \ln\frac{\varrho'_m}{\varrho^\star}. \tag{C6}$$

In order to compute the Gibbs entropy at the same time, we observe that the number of particles entering cell m from the volume $s_{n,m}\Gamma$ of cell n is $\varrho_n s_{n,m}\Gamma$. Therefore, the new density $\varrho'_{n,m}$ on volume $\tilde{s}_{n,m}\Gamma$ of cell m is $\varrho'_{n,m}=\varrho_n s_{n,m}/\tilde{s}_{n,m}$. The density in that part of cell m which is mapped into the same cell does not change. The Gibbs entropy is thus

$$\begin{aligned}S_m^{(G)'}&\equiv-\sum_{j\in\{n,m\}}\Gamma\tilde{s}_{j,m}\varrho'_{j,m}\ln\left(\frac{\varrho'_{j,m}}{\varrho^\star}\right)\\ &=-\sum_{j\in\{n,m\}}\Gamma s_{j,m}\varrho_j\ln\left(\frac{\varrho_j}{\varrho^\star}\frac{s_{j,m}}{\tilde{s}_{j,m}}\right)\\ &=\Gamma\left[-\varrho'_m\ln\varrho_m-\sum_n s_{n,m}\varrho_n\ln\left(\frac{\varrho_n}{\varrho_m}\frac{s_{n,m}}{\tilde{s}_{n,m}}\right)\right],\end{aligned} \tag{C7}$$

where (C5) has been used to arrive at the last equation. Similarly as for the multi-Baker map, the irreversible entropy change becomes

$$\begin{aligned}\Delta_i S_m&=S'_m-S_m^{(G)'}\\ &=\Gamma\left[\sum_n s_{n,m}\varrho_n\ln\left(\frac{\varrho_n}{\varrho_m}\frac{s_{n,m}}{\tilde{s}_{n,m}}\right)-\varrho'_m\ln\left(\frac{\varrho'_m}{\varrho_m}\right)\right].\end{aligned} \tag{C8}$$

Note that this expression is exactly of the same type as (25c), except for a straightforward generalization to general cell shapes, arbitrarily many neighbors, and higher dimension. Hence, it significantly extends the validity of relation (28) and (34), and underlines the general points advanced in Sec. VI when interpreting these results.

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the Lyapunov exponents of the inverted dynamics coincide with those of the forward dynamics. This differs slightly from the irreversibility concept of other authors[41] who demand that the time-reversed dynamics is identical to the original one up to a geometrical transformation. For multi-Baker maps with a dissipative dynamics with time reversal symmetry (21b) the composition with a reflection on the diagonal of every cell complies with the latter requirement.

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