Equivalence of Irreversible Entropy Production in Driven Systems: An Elementary Chaotic Map Approach

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A multibaker map is generalized in order to mimic the thermostating algorithm of transport models. Elementary calculations yield the irreversible entropy production caused by coarse graining of the phase-space density. For different systems, either in steady states (periodic or flux boundaries) or subjected to absorbing boundaries, the specific irreversible entropy production is shown to be u^2/D , where *u* denotes the local streaming velocity (current per density) and *D* is the diffusion coefficient. [S0031-9007(97)04219-1]

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The connection between nonequilibrium statistical physics and the underlying chaotic dynamics has become a subject of vivid interest [1-15]. The central questions are how the microscopic reversible dynamics can appear as an irreversible process on the macroscopic level, and how the macroscopic transport coefficients are related to microscopic characteristics of the chaotic dynamics. A careful analysis of the rate of irreversible entropy production is at the heart of this problem [16-20], but the relation between complementary approaches has been poorly understood. Here, we present a consistent derivation of the irreversible entropy production for three main approaches to describe transport in driven systems producing currents. They model either *nonequilibrium steady states* (*A*) or the *relaxation* towards steady states (*B*):

(A1) In the *thermostating algorithm* a special force is introduced to avoid an uncontrolled growth of the kinetic energy of particles moving in external fields [2– 9]. The force mimics the presence of a thermostat and makes the particle dynamics dissipative on average, although it preserves time reversibility. The systems investigated up to now were assumed to be periodic of large spatial extension, and hence to be closed. The long time dynamics exhibits permanent chaos on an underlying chaotic attractor. Transport coefficients and the irreversible entropy production are connected with the average phase-space contraction rate $\bar{\sigma}^{(p)}$ on the attractor.

(A2) By applying *flux boundary conditions* to an open Hamiltonian system it was shown that the steady-state density follows Fick's law [10], and the irreversible entropy production has been calculated [19]. In this case the current running through the system is due to the boundary condition only, and the phase-space contraction rate is zero, $\bar{\sigma}^{(f)} = 0$.

(B) The escape-rate formalism of transport processes is based on the investigation of open systems of large spatial extensions subjected to absorbing boundary conditions [11-13]. In such cases the particle dynamics is chaotic in the sense of transient chaos, and there exists an underlying nonattracting chaotic set (a chaotic saddle) in the phase space. In the regime of linear response, at least, relaxation is closely related to steady-state transport. The transport coefficients of Hamiltonian systems are related [1,11–13] to the chaotic saddle's escape rate κ . In a recent paper [17] dissipation was also taken into account, and the irreversible entropy production was shown to be the sum of the escape rate κ and the average phase-space contraction rate $\bar{\sigma}^{(a)}$ on the chaotic saddle.

As the list indicates, complementary dynamical approaches have traditionally been associated with different boundary conditions. Here we show that a thermostated approach can be defined irrespective of boundary conditions, which, in the following, will be referred to by (A1)–(B). Even multibaker maps [9–11,13] can be generalized to mimic thermostating. They will be used to analytically work out expressions for the irreversible entropy production from the point of view of dynamical systems.

The multibaker map acts on a chain of N elementary cells of size $a \times a$ (cf. Fig. 1). It will be subjected to the different boundary conditions A1, A2, or B. The discrete time dynamics acts at integer multiples of a time unit τ . The square is divided into four vertical columns. The rightmost (leftmost) column of width s_R (s_L) is mapped onto a strip of width a and height s'_R (s'_L) in the square to the right (left). These columns



FIG. 1. Action of the multibaker map on a single cell m. Four vertical columns are squeezed and stretched by the map such that the resulting horizontal strips exactly fit into the cell or its neighbors.

induce transport along the x direction. The two middle columns of width s_1 and s_2 are transformed into strips of width *a* and respective heights s'_1 and s'_2 , and model the chaotic motion of trajectories not contributing to transport in a single time step. Subscript k will be used to label the four columns or rows of a cell, and i = 1, 2 will denote the inner strips only. By definition $s_k > 0$ and $\sum_{k} s_{k} = a$, so that the local phase-space contraction rates are $\sigma_k = -(1/\tau) \ln(s'_k/s_k)$. Such maps are known to be prototypes of strongly chaotic systems [21]. They possess probability densities $\rho(x, y)$ which take constant values along the x direction in each cell and might depend on time. The conditional hopping probabilities from a cell to its right or left neighbors are then $r = s_R/a$ and $l = s_L/a$, respectively. For every $0 \le m \le N$ the current density j_m flowing from cell m to m + 1 is related to the hopping probabilities and to the cell densities by $j_m = (r\varrho_m - l\varrho_{m+1})(a/\tau).$

A map modeling driven thermostated systems has to be area contracting (expanding) if the trajectory moves in the direction of (against) the driving force in order to model the work done by the thermostat on particles moving parallel to the external field (cf. [1,2,7]). Furthermore, the local contraction rate σ_R should coincide with $-\sigma_L$, because for a trajectory going *n* cells to the right and then *n* cells to the left, the overall dissipation should be zero. In addition, the mapping of the phase space must be oneto-one in order to preserve time reversibility [22]. In the multibaker model this is fulfilled by the choice

$$s'_{L} = s_{R}, \qquad s'_{R} = s_{L}, \qquad \text{and} \quad s_{i} = s'_{i}.$$
 (1)

The local phase-space contraction rates are then $\sigma_R = -\sigma_L$, and $\sigma_1 = \sigma_2 = 0$, expressing that thermostating is needed only for trajectories contributing to transport.

We emphasize that results comparable with thermodynamics can be obtained only if, in the macroscopic limit $a \rightarrow 0$ and $\tau \rightarrow 0$, the hopping probabilities $r = s_R/a$ and $l = s_L/a$, which define a random walk along the chain, are compatible with a diffusion process [13]. Irrespective of the thermostating condition (1), this leads to the following restrictions [23] on the parameters

$$l + r = \frac{2\tau}{a^2}D, \qquad r - l = \frac{\tau}{a}v.$$
 (2)

Here, D and v, respectively, denote the diffusion and drift coefficients of the associated advection diffusion (Fokker-Planck) equation [13]. They are assumed to be constant.

Let us consider the Gibb's entropy S defined with respect to the phase-space density $\varrho(x, y)$ as

$$S = -\int \varrho(x, y) \ln \varrho(x, y) \, dx \, dy \,, \tag{3}$$

where the Boltzmann constant k_B has been suppressed. We shall assume that a stationary state has set in characterized by constant cell densities Q_m . Nevertheless, after a single time step there will be a change $\Delta S^{(1)}$ of S because inhomogeneities develop in Q(x, y). $\Delta S^{(1)}$ is unobservable, however, in a coarse-grained description where only cell densities are considered. This change will be related to the irreversible entropy production. Owing to the strict self-similarity of the dynamics, the entropy change $\Delta S^{(n)}$ after *n* time steps is $n\Delta S^{(1)}$. Therefore, it is sufficient to compute $\Delta S^{(1)}$ only. The different boundary conditions give rise to different densities ϱ , thereby inducing significant differences in the evaluation of $\Delta S^{(1)}$. In the following we demonstrate that, nevertheless, the respective irreversible entropy productions are the same.

(A1) Periodic boundary conditions.—All cells are equivalent in this case so that there is a constant stationary coarse-grained density $\rho^* = \rho_m$ for all m. It is sufficient to consider a single cell with periodic boundaries, implying that the strip mapped out of the cell at one side is injected back from the other. The density is normalized so that $\int \varrho^* dx \, dy$ gives the number of particles in the cell. The corresponding entropy for the constant density is $S^* = -\varrho^* a^2 \ln \varrho^*$. An application of the map introduces microscopic inhomogeneities into the system: the densities after time τ on the different strips will be the constant values $\varrho_k = \varrho^* s_k / s'_k$. Thus, there is an entropy change $\Delta S^{(1)} = \varrho^* a [-\sum_k s_k \ln(\varrho^* s_k / s'_k)] S^*$. Averaging the density over the cell leads to ρ^* again. Thus, the loss of information due to coarse graining is $-\Delta S^{(1)}$. Since the entropy computed from the coarsegrained density remains constant, the irreversible entropy production $P_{irr}^{(p)}$ per particle is $P_{irr}^{(p)} = -\Delta S^{(1)}/\varrho^* a^2 \tau = [\sum_k s_k \ln(s_k/s'_k)]/a\tau$. In accordance with previous statements [2,4,7], the right-hand side is nothing but the average phase-space contraction rate $\bar{\sigma}^{(p)}$ on the attractor.

Using Eq. (1) one obtains for the irreversible entropy production in the thermostated case

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Here, we have introduced a characteristic length scale $l_v \equiv D/v$ and used (2). Since *D* and *v* are macroscopically relevant quantities, l_v is a macroscopic length. Hence, the second term in the square brackets is a finite-size correction, and the macroscopic entropy production is v^2/D .

(A2) Flux boundary conditions.—We assume Fick's law to hold in the steady state with a density gradient $Q_m\delta$, and consider a cell *m* in the interior of a long chain. In general the entropy change $\Delta S^{(1)}$ is due to the mixing of the density Q_m with $Q_L \equiv Q_m(1 + \delta a)$ and $Q_R \equiv Q_m(1 - \delta a)$ in the neighboring cells, and to the phase-space contraction. For an unbiased dynamics $l = l' = r = r' = \tau D/a^2$ the latter effect is not present, implying $\Delta S^{(1)} = \tau Q_m D[-(1 - \delta a) \ln(1 - \delta a) - (1 + \delta a) \ln(1 + \delta a)]$ (for the biased case cf. Ref. [24]). By construction, the average density Q_m in the cell is unchanged, so that it is coarse graining that causes the information loss $-\Delta S^{(1)}$ about the microscopic state of the system. Consequently, the irreversible entropy production per particle is

$$P_{\rm irr}^{(f)} = \frac{-\Delta S^{(1)}}{\varrho_m a^2 \tau} = \frac{D}{a^2} \bigg[\ln(1 - \delta^2 a^2) + \delta a \ln \frac{1 + \delta a}{1 - \delta a} \bigg] = D \delta^2 \bigg[1 + \frac{1}{6} (\delta a)^2 + \dots \bigg].$$
(5)

This expression is equivalent to the local irreversible entropy production initially found in [19]. Moreover, for an unbiased dynamics and a density fulfilling Fick's law, the streaming velocity [2] is $u_m \equiv j_m/\varrho_m = -D(\nabla \varrho)/\varrho_m = -D\delta$. Thus, we find that the macroscopic term of Eq. (5) agrees with those obtained for the periodic case [Eq. (4)], where u = v.

(B) Absorbing boundary conditions.—Owing to escape, the phase-space density ρ is decreasing in time. Therefore, the change of the entropy (3) contains a contribution of entropy flow into the surroundings in addition to irreversible entropy production. It is worth concentrating only on the effect of the fractal foliation induced by the dynamics (cf. [17]) by considering a specific entropy s (entropy per particle) defined in the same form as (3), except that ρ is replaced by the conditional phase-space density $\tilde{\rho}(x, y)$. This density represents the probability to find a particle around a phase-space point under the condition that it has not yet escaped. It is defined on the whole phase space and normalized to unity at any time: $\int \tilde{\rho} \, dx \, dy = 1$. After a long time, the conditional density of cell *m* tends to the invariant conditional density $\tilde{\varrho}_m$, for which the flux through the boundaries is counterbalanced by the normalization $\exp(\kappa \tau)$ [13]. For $1 \le m \le N$ this implies the eigenvalue equation

$$e^{-\kappa\tau}\tilde{\varrho}_m = \left(\frac{1}{a}\sum_i s_i\right)\tilde{\varrho}_m + r\tilde{\varrho}_{m-1} + l\tilde{\varrho}_{m+1}.$$
 (6)

With the boundary conditions $\tilde{\varrho}_0 = \tilde{\varrho}_{N+1} = 0$ this leads to $\tilde{\varrho}_m = Z e^{\alpha m} \sin[\pi m/(N+1)]$, where Z is a normalization constant and $\alpha = (1/2) \ln(r/l)$. The associated eigenvalue is

$$e^{-\kappa\tau} = 1 - l - r + 2\sqrt{lr} \cos\left(\frac{\pi}{N+1}\right).$$
 (7)

Here κ is the escape rate from the chaotic saddle underlying transport. In the present paper, we only discuss the large-system result $N \gg 1$, where the cosine function can be replaced by unity.

The total irreversible entropy production is the sum of contributions from every single cell. In cell *m* the change of specific entropy $\Delta s_m^{(1)}$ in one time step is due to the distribution of conditional densities $\tilde{\varrho}_{m,i} = \tilde{\varrho}_m s_i/s_i' \exp(\kappa \tau)$, $\tilde{\varrho}_{m,R} = \tilde{\varrho}_{m-1} s_R/s_R' \exp(\kappa \tau)$, and $\tilde{\varrho}_{m,L} = \tilde{\varrho}_{m+1} s_L/s_L' \exp(\kappa \tau)$ on the strips 1, 2, *R*, *L*, respectively, where the factors $\exp(\kappa \tau)$ ensure normalization [cf. Eq. (6)]. Consequently, the change is $\Delta s_m^{(1)} = -a \sum_k s_k' \tilde{\varrho}_{m,k} \ln \tilde{\varrho}_{m,k} + a^2 \tilde{\varrho}_m \ln \tilde{\varrho}_m$. The information loss due to coarse graining is $-\Delta s_m^{(1)}$ in cell *m*, and the rate of irreversible entropy production is obtained as $P_{\rm irr}^{(a)} = -\Delta s_m^{(1)}/(\varrho_m a^2 \tau)$. Inserting the expressions for $\tilde{\varrho}_{m,k}$ and taking into account Eq. (6), one obtains

$$P_{\rm irr}^{(a)} = -\frac{\Delta s_m^{(1)}}{\tilde{\varrho}_m a^2 \tau} \kappa + \frac{1}{\tau} e^{\kappa \tau} \left[\sum_{i=1}^2 \frac{s_i}{a} \ln \frac{s_i}{s_i'} + \frac{\tilde{\varrho}_{m-1}}{\tilde{\varrho}_m} r \ln \frac{r \tilde{\varrho}_{m-1}}{r' \tilde{\varrho}_m} + \frac{\tilde{\varrho}_{m+1}}{\tilde{\varrho}_m} l \ln \frac{l \tilde{\varrho}_{m+1}}{l' \tilde{\varrho}_m} \right].$$

Except for a narrow boundary layer around the two ends, the evaluation of $P_{irr}^{(a)}$ is elementary since for $N \gg 1$ we can use $\tilde{\varrho}_{m+1}/\tilde{\varrho}_m = \exp(\alpha) [1 + \mathcal{O}(N^{-1})]$, obtaining

$$P_{\rm irr}^{(a)} = \kappa + \frac{e^{\kappa\tau}}{\tau} \left[\sum_{i} \frac{s_i}{a} \ln \frac{s_i}{s_i'} + (lr)^{1/2} \ln \frac{lr}{l'r'} \right] = \kappa + \bar{\sigma}^{(a)}.$$
(8)

Here, $\bar{\sigma}^{(a)}$ represents the average phase-space contraction rate [25] on the saddle. The rightmost equality of (8) was argued to be the irreversible entropy production for general open systems [17]. Here, we have illustrated this by an explicit calculation for the long baker chain.

Notice that owing to (1) the term $\bar{\sigma}^{(a)}$ vanishes for the thermostated model. As a consequence, the thermostat is ineffective for the motion on the chaotic saddle. This surprising result is directly related to the requirement that the thermostated equations of motion preserve phase-space volume globally.

Expressing (7) with the drift and diffusion coefficients (2) and taking the small τ limit, one obtains for the

thermostated model

$$P_{\rm irr}^{(a)} = \kappa = \frac{2D}{a^2} \left\{ 1 - \left[1 - \left(\frac{va}{2D} \right)^2 \right]^{1/2} \right\} \\ = \frac{v^2}{4D} \left[1 + \frac{1}{16} \left(\frac{a}{l_v} \right)^2 + \dots \right], \tag{9}$$

where l_v is defined as in (4). The term in square brackets corresponds to a finite-size correction. Consequently, the irreversible entropy productions expressed in terms of the drift parameter v is by a factor of 4 smaller than in the steady states. Observe, however, that the local current density $j_m = \varrho_m (r - l\varrho_{m+1}/\varrho_m) (a/\tau) \approx \varrho_m (r - l \exp \alpha) (a/\tau) = \varrho_m r [1 - (l/r)^{1/2}]$ tends to $\varrho_m v/2$ for $a \rightarrow 0$; i.e., the local streaming velocity $u_m \equiv j_m/\varrho_m$ is v/2. Consequently, by fixing the streaming velocity one obtains the *same* amount of irreversible entropy production in all approaches.

In spite of the simple model several findings exposed above are apparently of general validity.

(i) Open systems subjected to absorbing boundary conditions and to the same thermostating algorithm as

periodic ones should exhibit *area-preserving* dynamics on the chaotic saddle. Hence, their average phase-space contraction rate (and the sum of the Lyapunov exponents) is *zero*. This is so because for a thermostated system the dissipation is proportional to the average displacement per unit time $\Delta x(t)/t$, where $\Delta x(t)$ is the displacement parallel to the external field after time t. The ratio $\Delta x(t)/t$, however, vanishes in the long-time limit since $\Delta x(t)$ is bounded by the length of the system. Thus, the full irreversible entropy production is given by the escape rate κ , for both thermostated and Hamiltonian systems.

(ii) The irreversible entropy production per particle is independent of the boundary conditions provided the local streaming velocity $u = j/\varrho$ is fixed. The expression $P_{\rm irr} = u^2/D$ holds for arbitrary streaming velocities in the large-system limit, and coincides with the results of thermodynamics in the linear-response regime. To see this, we recall that according to nonequilibrium thermodynamics [26], the irreversible entropy production per unit volume is $\sigma_{irr} = jE/T$ in a system of electric conductance (j denotes the current density, E the electric field, and T the temperature). Using Ohm's law $j = \sigma E \equiv \varrho u$ (σ being the conductivity, ρ the particle density, u the streaming velocity) and Einstein's relation $D = T\sigma/\rho$, we recover for the entropy production per particle the relation $P_{\rm irr} = \sigma_{\rm irr}/\varrho = u^2/D$, in units where the elementary electric charge is unity (for more general cases cf. [24]).

(iii) In a steady state, the thermodynamic expression for the rate of irreversible entropy production per particle can be derived as the information loss due to coarse graining, even when the system is *low dimensional*. We specified minimal requirements for the thermostat [Eq. (1)] and for the scaling of microscopic hopping probabilities with the transport coefficients [Eq. (2)] to obtain physically meaningful macroscopic results. The ultimate reason for the irreversible entropy production is the mixing of the phase-space volume elements due to the *chaoticity* of the dynamics even if, macroscopically, the system is in a steady state. In view of the general validity of the u^2/D expression, this seems to be the origin of the classical irreversible entropy production also in systems with *many degrees of freedom*.

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