Multibaker map for thermodynamic cross effects in dynamical systems

László Mátyás,[1] Tamás Tél,[1] and Jürgen Vollmer[2,3]

[1]*Institute for Theoretical Physics, Eötvös University, P. O. Box 32, H-1518 Budapest, Hungary*
[2]*Fachbereich Physik, Universität-GH Essen, 45117 Essen, Germany*
[3]*Max-Planck-Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany*
(Received 14 December 1999)

A consistent description of simultaneous heat and particle transport, including cross effects, and the associated entropy balance is given in the framework of a deterministic dynamical system. This is achieved by a multibaker map where, in addition to the phase-space density of the multibaker, a second field with appropriate source terms is included in order to mimic a spatial temperature distribution and its time evolution. Conditions are given to ensure consistency in an appropriately defined continuum limit with the thermodynamic entropy balance. They leave as the only free parameter of the model the entropy flux let directly into the surroundings. If it vanishes in the bulk, the transport properties of the model are described by the thermodynamic transport equations. Another choice leads to a uniform temperature distribution. It represents transport problems treated by means of a thermostating algorithm, similar to the one considered in nonequilibrium molecular dynamics.

I. INTRODUCTION

Irreversibility in transport models based on dynamical systems with only a *few degrees of freedom* has become the subject of intensive recent studies [1–11]. 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 [4,6,7,9,12–20]. This development opens the possibility of requiring for a consistent dynamical-system modeling of an irreversible process the derivation of both the transport equations and the entropy balance. In our approach we shall observe this constraint.

Many models [4–10] were originally designed to rely on equations of motion, where transport is induced by an external field and the (average) work done by the field on the systems is removed by a so-called Gaussian thermostat. This approach is commonly implemented with periodic boundary conditions. In spite of extensive numerical investigations, however, there are conceptual problems in the interpretation of the results as far as the entropy (heat) flux is concerned. After all, it is not obvious how this flux can come about in a system with periodic boundaries. Moreover, the average phase-space contraction is commonly taken as a measure of entropy production. This limits these considerations to the overall entropy balance of the full system. It is not possible to address the local balance of nonequilibrium thermodynamics. The aim of the present article is to investigate a class of dynamical systems tailored to describe simultaneous particle and heat transport, driven by appropriate boundary conditions and an external field. We work out the *local* entropy balance, and identify conditions under which the model can be consistent with nonequilibrium thermodynamics.

Earlier low-dimensional models were devoted exclusively to either particle (mass, charge) transport [5,6,21–26] or to heat conductivity [27,28]. These transport processes are driven by a single thermodynamic force. It is of basic interest, however, to understand how thermodynamic cross effects generated by the presence of two *independent* driving forces can be described in the framework of dynamical-system theory (as for many-particle systems see, e.g., [29]). The case of thermoelectric phenomena in which the driving forces are (i) the temperature difference and (ii) the electric field and/or a density gradient is illustrated by Fig. 1. The cross effects imply that the temperature gradient contributes to the electric current, and the density gradient to the heat current. Recently, the authors of the present paper suggested an elementary model to study these effects [30]. Here, we generalize it to explore the conditions under which consistency with thermodynamics can be found.

A part of the above mentioned problems with the entropy balance has recently been clarified [16–18] in the framework of multibaker maps modeling quasi-one-dimensional particle transport at constant temperature. These models are given in terms of the time evolution of the (multibaker) phase-space density in a corresponding two-dimensional *single-particle phase space*, which in this case consists of a band of length L. The fixed width represents a phase-space variable p in addition to the spatial coordinate x along the band. The multibaker map defines a discrete dynamics (cf. below), which is one-to-one on the band, but does not necessarily preserve the volume locally. A recent paper by Tasaki and
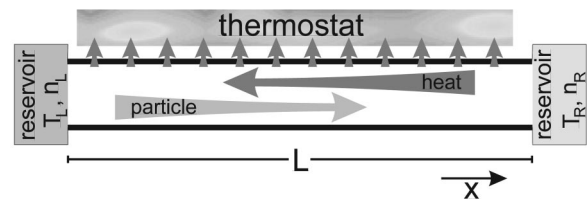

FIG. 1. Graphic illustration of the transport process considered. A system of spatial extension L is attached to reservoirs inducing particle and heat currents due to the differences in the densities (n) and temperatures (T) at the two ends, as indicated by the arrows. Along the system heat can be exchanged with a thermostat.

Gaspard [31] shows that analogous results can be obtained with area-preserving maps by making the width of the band position dependent. This varying height was connected to changes in the (potential) energy, and does not appear as a driving force independent of the density gradient or the external field.

Multibaker maps have no natural momentum variable conjugated to the spatial coordinate x. Therefore, we characterize the thermodynamic states by *two independent* fields. Besides the phase-space density ϱ, a new field w is introduced, whose dynamics describes the evolution of the *kinetic energy per particle*, i.e., ϱw corresponds to the kinetic-energy density [32].

To make contact with nonequilibrium thermodynamics, the time evolution of average densities in regions of small spatial extension along the x axis is considered. They will be called *coarse-grained densities*. Transport equations in the form of differential equations are obtained in a continuum limit, where the spatial resolution of coarse graining is much smaller than the linear size L of the system and the time unit τ of the discrete dynamics is much shorter than that of the macroscopic relaxations. In this *macroscopic limit* the phase-space density ϱ and the kinetic energy per particle w are related to the particle density n and to the local temperature T, respectively.

It is not obvious that a deterministic dynamical system as simple as a multibaker can fulfill all constraints required for consistency with thermodynamics [33]—not even when taking the macroscopic limit. The thermodynamic entropy balance relates the time derivative of the entropy density s to the entropy production $\sigma^{(\mathrm{irr})}$ per unit volume and to the entropy flux Φ,

$$\partial_t s = \sigma^{(\mathrm{irr})} + \Phi. \tag{1}$$

We consider thermoelectric phenomena induced by particles of charge e in a transport process along the x axis. In a system that is translation invariant perpendicular to the x axis, the quantities causing entropy changes can be expressed as [34]

$$\sigma^{(\mathrm{irr})} = \frac{e^2 j^2}{\sigma_{el} T} + \lambda \left(\frac{\partial_x T}{T} \right)^2, \tag{2a}$$

$$\Phi = -\partial_x j^{(s)}. \tag{2b}$$

Here σ_{el} and λ denote the electric and the heat conductivity, respectively, and

$$j = n v_{el} - \frac{\sigma_{el}}{e^2} (\partial_x \mu_c + e \alpha \partial_x T), \tag{3a}$$

$$j^{(s)} = \frac{e \Pi}{T} j - \lambda \frac{\partial_x T}{T} \tag{3b}$$

are the particle and the entropy current densities, respectively. In Eq. (3), μ_c denotes the chemical potential of the particles, and v_{el} is the drift velocity due to an external electric field E, which is related to σ_{el} by

$$v_{el} = \frac{\sigma_{el} E}{en}. \tag{4}$$

Π is the Peltier coefficient, and α the thermoelectric power (or Seebeck coefficient). Thermodynamic cross effects are manifest in Eq. (3), and the corresponding Onsager relations imply a relation between the transport coefficients α and Π.

Since the entropy plays a central role in these relations, one has to choose an appropriate entropy concept for the multibaker. One obvious candidate is the Gibbs entropy $S^{(G)}$ defined with respect to the phase-space density ϱ. Because of the ever refining phase-space structures that chaotic dynamics generates from every smooth initial density, this entropy *never* becomes time independent, not even in a macroscopically steady state. In contrast, the corresponding entropy S, whose definition is based on coarse-grained densities, is thermodynamically well behaved, and its value per unit length is the analog of the entropy density s appearing in Eq. (1). This entropy will be called the *coarse-grained entropy*. The irreversible entropy production of arbitrary steady and nonsteady states has been identified as the time derivative of the difference between the Gibbs and the coarse-grained entropy [17,18].

Although the thermodynamic relation (2b) requires the entropy flux to be the divergence of the entropy current, we allow for deviations from thermodynamics in that we do not exclude the presence of an additional term. This term is interpreted as the consequence of a thermostat, which can *locally* remove or release heat, leading to an additional entropy flux $\Phi^{(\mathrm{thermostat})}$. In such cases

$$\Phi = -\partial_x j^{(s)} + \Phi^{(\mathrm{thermostat})}. \tag{5}$$

We say a system is thermostated whenever $\Phi^{(\mathrm{thermostat})}$ differs from zero. Depending on the details of the model, we are able to study both nonthermostated and thermostated systems, and in the latter case we shall be able to generate arbitrary stationary temperature profiles. To our knowledge, these features have not yet been explored in nonequilibrium molecular dynamics simulations [4,29].

The paper is organized as follows. In Sec. II we revisit the thermodynamics of irreversible processes by rewriting the expressions of entropy production as well as of particle and entropy currents in forms amenable to a comparison with the results of multibaker maps. Subsequently (Sec. III), we introduce the multibaker map, and discuss the time evolution of the phase-space density and the kinetic-energy density. The Gibbs and coarse-grained entropies and their dynamics are studied in Sec. IV. In Sec. V the macroscopic limit of the obtained expressions is taken. Conditions on the baker dynamics to make it consistent with thermodynamics are explored in Sec. VI. A short discussion is devoted to thermostated cases (Sec. VII), and our main results are summarized in Sec. VIII. The paper is augmented by two Appendixes. Appendix A is devoted to a formal definition of the map and the resulting time evolution of the densities. In Appendix B it is shown that the macroscopic results do not depend on the prescription for coarse graining.

II. NONEQUILIBRIUM THERMODYNAMICS

In this section we recall the thermodynamic description of thermoelectric transport induced by two independent driving fields [33]. The most general situation is treated, which comprises the presence of an external field, as well as gradients in the particle density and the temperature.

A. Thermodynamic forces and currents

We consider a system of particles of charge e, which interact with a lattice forming a background which ensures the electric neutrality of the system. The frame of reference is fixed to this background. The degrees of freedom of the lattice are not considered. As demonstrated explicitly for the periodic Lorentz gas, this setting leads to a chaotic, diffusionlike motion of the particles. Due to an (electro)chemical potential gradient and a temperature gradient, both a particle and an energy current are flowing through the system. Let j and $j^{(u)}$, respectively, denote the density of these currents in a frame of reference fixed to the lattice. In this setting the number density of particles n and the density u of the total energy are locally preserved. (The density u also contains the potential energy due to an external field and the kinetic energy of the ordered motion.)

In order to derive the entropy balance in a region of fixed volume, we start from the conservation laws

$$\partial_t n = -\nabla j, \tag{6a}$$

$$\partial_t u = -\nabla j^{(u)}, \tag{6b}$$

and express the time derivative of the entropy density per unit volume s,

$$\partial_t s = -\nabla j^{(s)} + \sigma^{(\mathrm{irr})}, \tag{6c}$$

in terms of the entropy current density $j^{(s)}$ and the irreversible entropy production $\sigma^{(\mathrm{irr})}$.

Considering a system in local equilibrium, the Gibbs relation

$$T\,ds = du - \mu\,dn, \tag{7}$$

holds, with T and μ denoting the local temperature and electrochemical potential, respectively. To find the time derivative of s, we write the local temporal change of Eq. (7),

$$\partial_t s = \frac{1}{T}\partial_t u - \frac{\mu}{T}\partial_t n, \tag{8}$$

in the form of Eq. (6c) by identifying

$$j^{(s)} = \frac{j^{(u)} - \mu j}{T} \tag{9a}$$

as the total entropy current, and

$$\sigma^{(\mathrm{irr})} = j^{(u)}\nabla\frac{1}{T} - j\nabla\frac{\mu}{T} = -(j^{(s)}\nabla T + j\nabla\mu)\frac{1}{T} \tag{9b}$$

as the irreversible entropy production.

Equation (9b) shows that the currents j and $j^{(s)}$ are conjugate to the thermodynamic forces $-\nabla\mu/T$ and $-\nabla T/T$,

respectively. Therefore, in the spirit of nonequilibrium thermodynamics, these currents can be expressed in terms of the forces as

$$j = -L_{11}\frac{\nabla\mu}{T} - L_{12}\frac{\nabla T}{T}, \tag{10a}$$

$$j^{(s)} = -L_{21}\frac{\nabla\mu}{T} - L_{22}\frac{\nabla T}{T} \tag{10b}$$

$$= -\frac{L_{11}L_{22} - L_{12}L_{21}}{L_{11}}\frac{\nabla T}{T} + \frac{L_{21}}{L_{11}}j, \tag{10c}$$

where the latter expression for $j^{(s)}$ was obtained by inserting Eq. (10a) into Eq. (10b). Moreover, by inserting Eq. (10b) into Eq. (9b), one expresses the irreversible entropy production as

$$\sigma^{(\mathrm{irr})} = \frac{L_{11}L_{22} - L_{12}L_{21}}{L_{11}}\left(\frac{\nabla T}{T}\right)^2 + \frac{j^2}{L_{11}} + \frac{L_{12} - L_{21}}{L_{11}}\frac{\nabla T}{T}j. \tag{11}$$

After using the Onsager relation $L_{12} = L_{21}$, this expression for the irreversible entropy production is a quadratic form, which takes only non-negative values provided that the matrix of kinetic coefficients is positive definite, i.e., the well-known condition $L_{11}L_{22} - L_{12}L_{21} > 0$ is fulfilled [33,35].

B. Identifying transport coefficients

It is worth expressing the kinetic coefficients L_{ij} by means of directly measurable quantities. The total electrochemical potential can be split as $\mu = \mu_c + e\phi$, where μ_c is the chemical part, and ϕ is the electric potential. Since $E = -\nabla\phi$ and $j_{el} = ej$ is the electric current, we find that L_{11} is proportional to the electric conductivity $\sigma_{el} > 0$:

$$L_{11} = \frac{\sigma_{el}T}{e^2}. \tag{12a}$$

In the absence of a particle current (i.e., for $j = 0$), $Tj^{(s)}$ provides the heat current, such that in view of Eq. (10c)

$$\frac{L_{11}L_{22} - L_{12}L_{21}}{L_{11}} = \lambda, \tag{12b}$$

where $\lambda > 0$ is the heat conductivity. At zero particle current and constant chemical potential, a temperature gradient induces an electric field, which is conventionally written as $\alpha\nabla T$, where α is called the thermoelectric power (or the Seebeck coefficient). Consequently, from Eq. (10a) one finds

$$L_{12} = \frac{\alpha\sigma_{el}}{Te}. \tag{12c}$$

Finally, in a system without temperature gradients, the entropy current due to the presence of an electric current ej amounts to $\Pi ej/T$, where Π is the Peltier coefficient. Hence, Eq. (10c) implies

$$L_{21} = \frac{\Pi\sigma_{el}}{e}. \tag{12d}$$

Using the phenomenological coefficients (12) we write

$$j = -\frac{\sigma_{el}}{e^2}(\nabla\mu + e\alpha\nabla T), \qquad (13a)$$

$$j^{(s)} = -\lambda\frac{\nabla T}{T} + \frac{e\Pi}{T}j. \qquad (13b)$$

Note that the Onsager relation $L_{12} = L_{21}$ makes the Peltier and Seebeck coefficients connected as

$$\Pi = T\alpha. \qquad (14)$$

Substituting Eqs. (12) into (11) one thus derives Eq. (2a).

C. Relating transport and diffusion coefficients

It is worth replacing the chemical potential in the expressions for the currents and entropy production by the density n and temperature T. We write

$$\nabla\mu_c = \frac{De^2}{\sigma_{el}}\nabla n - s\nabla T, \qquad (15)$$

where the diffusion coefficient is defined as

$$D = \frac{\sigma_{el}}{e^2}\left(\frac{\partial\mu_c}{\partial n}\right)\bigg|_T, \qquad (16a)$$

and

$$s \equiv -\left(\frac{\partial\mu_c}{\partial T}\right)\bigg|_n \qquad (16b)$$

is a quantity of dimension entropy per particle. By means of the drift velocity v_{el} [Eq. (4)] one can rewrite the particle current density (13a) as

$$j = v_{el}n - D\nabla n - k\frac{nD}{T}\nabla T \qquad (17)$$

where

$$k\frac{nD}{T} \equiv \frac{\sigma_{el}}{e^2}(e\alpha - s). \qquad (18)$$

The entropy current then takes the form

$$j^{(s)} = -\left(\lambda + knD\frac{e\Pi}{T}\right)\frac{\nabla T}{T} + \frac{e\Pi}{T}(v_{el}n - D\nabla n), \qquad (19)$$

and in view of Eqs. (14), (16a), and (18) one obtains

$$e\Pi = kn\left(\frac{\partial\mu_c}{\partial n}\right)\bigg|_T - T\left(\frac{\partial\mu_c}{\partial T}\right)\bigg|_n. \qquad (20)$$

Note that in the entropy current (19) the coefficients in front of the $v_{el}n$ and $-D\nabla n$ terms coincide.

We finally mention that by taking the limit $E, e \to 0$ at constant $e\Pi, e\alpha$, and σ_{el}/e^2, the thermoelectric problem is formally mapped onto the problem of thermal diffusion in a binary mixture. In that case n stands for the concentration of
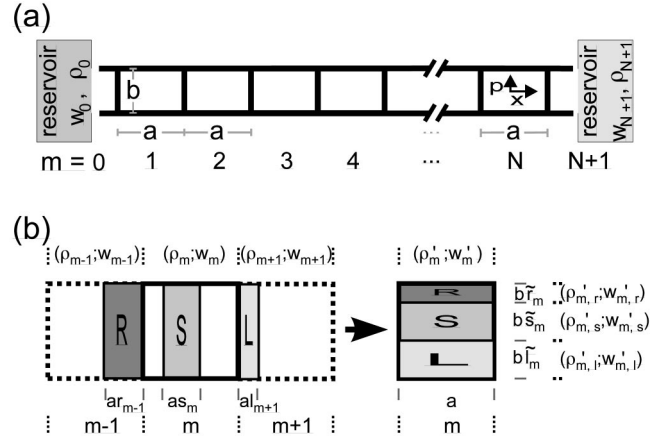

FIG. 2. Graphical illustration of the action of the multibaker map on the phase space (x,p). (a) The mapping is defined on a domain of $N \equiv L/a$ identical rectangular cells of size $a \times b$, with boundary conditions imposed in two additional cells 0 and $N+1$. (b) After every time unit τ each cell is divided into three columns, which are squeezed and stretched to obtain horizontal strips of width a. The average values of the fields $\varrho(x,p)$ and $w(x,p)$ on the cells (strips) [cf. Eqs. (21) and (25)] are given on the margins. Iteration of this rule defines the time evolution.

one of the diffusing materials, and the quantity kD is the thermal diffusion coefficient [36]. Based on this analogy, we consider kD in Eq. (18) as the thermal diffusion coefficient of charged particles in the thermoelectric problem.

III. THE MULTIBAKER MAP

Baker maps are known to be prototypes of strongly chaotic systems [37]. Multibaker maps are a generalization, where a spatially extended system is modeled by a chain of mutually interrelated baker maps, in order to model transport [21,22,24,16–18,31] via the dynamics of the (multibaker) phase-space density ϱ. The single-particle phase space modeled by the multibaker map consists of N identical cells of width a and height b, which are labeled by the index m [Fig. 2(a)]. After each time unit τ every cell is divided into three columns [Fig. 2(b)]. The right (left) column of width ar_m (al_m) is mapped onto a strip of width a and of height $b\widetilde{r_{m+1}}$ $(b\widetilde{l_{m-1}})$ in the right (left) neighboring cell. The middle one preserves its area $\widetilde{s_m} = s_m$. The map is globally phase-space preserving, i.e., $s_m + r_m + l_m = \widetilde{r_m} + \widetilde{l_m} + \widetilde{s_m} = 1$. A formal definition is given in Appendix A. The map mimics the time evolution of a many-particle system with weak interactions in a single-particle phase space [38]. The equilibrium equations of state will turn out to be those of a classical ideal gas.

The (x,p) dynamics of the multibaker map is considered to be a microscopic dynamics in the sense that it is deterministic, chaotic, and mixing. It drives two fields which generate ever refining phase-space structures.

As well as these fields, we also consider coarse-grained densities obtained by averaging over the cells. The cell width a is considered to be the smallest length scale where a thermodynamic description applies. In the spirit of local thermodynamic equilibrium, the local averages of the microscopic variables characterize the thermodynamic state in the cells. The temporal evolution of the coarse-grained versions of ϱ

and w is consequently expected to describe an approach toward a steady state, where the the coarse-grained fields no longer change in time (in contrast to the fully resolved fields, which approach closer and closer toward fractal distributions). To emphasize that coarse graining is taken over the cells, the coarse-grained density will also be called the *cell density*.

The dynamics of earlier multibaker models is the same for all cells. There can be inhomogeneities in the densities, but the evolution equations are kept translation invariant. Here, we relax this constraint by allowing the transfer rates of cell m to depend on the coarse-grained fields in cell m and its neighbors. This dependence mimics the effect of the thermodynamic driving force due, for instance, to a local temperature gradient. It induces an m dependence of the parameters. Since all calculations can be performed without ever referring to the form of these dependencies, we will not yet specify them but start from a map with a general set of space- and time-dependent parameters. Their form will be fixed *a posteriori* by comparison with thermodynamics.

Due to the self-similarity of the multibaker dynamics, the local transport and entropy balance can be worked out by a calculation considering one time step only. A discussion of more general prescriptions for the coarse graining is relegated to Appendix B.

A. Evolution of the phase-space density

Thermodynamic transport equations describe the time evolution of the phase-space density ϱ and the kinetic-energy density w. For explicit calculations of their time evolution we always start with the constant values ϱ_m and w_m in every cell m. This is convenient from a technical point of view, and does not lead to a restriction of the domain of validity of the model, as demonstrated in Appendix B. After one step of iteration the densities will be piecewise constant on the strips $i=R,S,L$ defined in Fig. 2(b). Due to the conservation of the particle number, they are

$$\varrho'_{m,r}=\frac{r_{m-1}}{\widetilde{r_m}}\,\varrho_{m-1},$$

$$\varrho'_{m,s}=\varrho_m,\qquad\qquad(21)$$

$$\varrho'_{m,l}=\frac{l_{m+1}}{\widetilde{l_m}}\,\varrho_{m+1}.$$

The factors $r_{m-1}/\widetilde{r_m}$ and $l_{m+1}/\widetilde{l_m}$ give rise to local contraction or expansion of phase-space volumes.

The coarse-grained density ϱ'_m after one time step is the average of the contributions (21) on the different strips:

$$\varrho'_m=(1-r_m-l_m)\varrho_m+r_{m-1}\varrho_{m-1}+l_{m+1}\varrho_{m+1}.\quad(22)$$

Multiplying the equation by τ^{-1} and introducing the current

$$j_m=\frac{ab}{\tau}(r_m\varrho_m-l_{m+1}\varrho_{m+1})\qquad(23)$$

through the right boundary of cell m, Eq. (22) appears in the form of a continuity equation,

$$\frac{b(\varrho'_m-\varrho_m)}{\tau}=-\frac{j_m-j_{m-1}}{a}.\qquad(24)$$

It can be seen as the discrete counterpart of Eq. (6a). Note that by definition the current through the left boundary of cell m is the same as the current through the right boundary of cell $m-1$. In this paper all types of currents associated with cell m will also be defined as a flow through the right boundary.

B. Evolution of the kinetic-energy density

The (x,p) dynamics does not imply any constraint on w. Its time evolution can be chosen according to physical intuition. In contrast to the particle density, we consider the kinetic energy per unit volume $\varrho_m w_m$ as a nonconserved quantity. In addition to a contribution from the particle flow, the new values $w'_{m,i}$ on the strips $i=R,S,L$ will therefore contain terms characterized by a local source strength q_m, which accounts for a local heating:

$$\varrho'_{m,r}w'_{m,r}=\frac{r_{m-1}}{\widetilde{r_m}}\varrho_{m-1}w_{m-1}(1+\tau q_m),$$

$$\varrho'_{m,s}w'_{m,s}=\varrho_m w_m(1+\tau q_m),\qquad(25)$$

$$\varrho'_{m,l}w'_{m,l}=\frac{l_{m+1}}{\widetilde{l_m}}\varrho_{m+1}w_{m+1}(1+\tau q_m).$$

The source term q_m is taken constant in every cell since more general choices affect only terms that drop out in the macroscopic limit. The particular form of q_m will only be specified later, in order to demonstrate that there is a *unique* choice for q_m, where the time evolution of the kinetic energy can become consistent with thermodynamics. Other choices for the source term q_m lead to a nonvanishing entropy flux $\Phi^{(\text{thermostat})}$, and can be considered to characterize a thermostat in the spirit of nonequilibrium molecular dynamics.

An update of the kinetic-energy density can be calculated similarly to the update of the particle density. In cell m the average value $\varrho'_m w'_m$ after one time step is obtained by averaging the different contributions on the strips in cell m [cf. Eq. (25)], yielding

$$\varrho'_m w'_m=[\varrho_m w_m(1-r_m-l_m)+r_{m-1}\varrho_{m-1}w_{m-1}$$
$$+l_{m+1}\varrho_{m+1}w_{m+1}](1+\tau q_m).\qquad(26)$$

For a fixed set of transition probabilities r_m,s_m,l_m, and $q_m=0$, Eq. (26) amounts to a passive advection of the field w by the deterministic dynamics. The possible dependence of the transition probabilities on differences of the coarse-grained w and the presence of the source q_m, however, make the advection nonpassive.

Equation (26) can also be rewritten in the form of the discrete balance equation

$$\frac{b(\varrho'_m w'_m-\varrho_m w_m)}{\tau}=b\varrho'_m w'_m\frac{q_m}{1+\tau q_m}-\frac{j_m^{(\varrho w)}-j_{m-1}^{(\varrho w)}}{a}.$$
$$(27)$$

The first term on the right-hand side characterizes the source strength of the field $\varrho_m w_m$ per unit time τ, and the second one is the discrete divergence of the ϱw current,

$$j_m^{(\varrho w)} = \frac{ab}{\tau}(r_m \varrho_m w_m - l_{m+1} \varrho_{m+1} w_{m+1}). \quad (28)$$

Since ϱw plays the role of a kinetic energy, we consider $j^{(\varrho w)}$ to be an energy current.

C. Diffusion and drift

The local transition probabilities r_m, s_m, and l_m govern the evolution of the coarse-grained densities ϱ_m and w_m. In view of the master equations (22), the cell-to-cell dynamics of the model is equivalent to the dynamics of random walkers with fixed step length a and local transition probabilities r_m and l_m over time unit τ. Such random walks are characterized [39] by the local drift v_m and diffusion coefficient D:

$$r_m - l_m = \frac{\tau}{a} v_m, \quad (29a)$$

$$r_m + l_m = \frac{2\tau}{a^2} D. \quad (29b)$$

Hence, the transition probabilities r_m and l_m can be expressed as

$$r_m = \frac{\tau D}{a^2}\left(1 + \frac{a v_m}{2D}\right), \quad (30a)$$

$$l_m = \frac{\tau D}{a^2}\left(1 - \frac{a v_m}{2D}\right). \quad (30b)$$

We allow in the present paper only for a location dependence of the drift v_m, but keep the diffusion coefficient spatially homogeneous. The m dependence of the drift should be a consequence of the inhomogeneity of the kinetic-energy (temperature) gradient along the chain.

In spite of the freedom we still have in specifying v_m, these definitions already allow us to write the currents in a form very close to their thermodynamic counterparts. The current for the phase-space density appears in the form

$$j_m = \frac{b}{2}(\varrho_m v_m + \varrho_{m+1} v_{m+1}) - bD\,\frac{\varrho_{m+1} - \varrho_m}{a}, \quad (31a)$$

a discrete version of Eq. (3a). Similarly, for the ϱw current one obtains

$$j_m^{(\varrho w)} = w_m j_m - b\,\varrho_{m+1} D\frac{w_{m+1} - w_m}{a}\left(1 - \frac{a v_{m+1}}{2D}\right), \quad (31b)$$

which comprises an advection of the w fields by the particle current and a contribution from the discrete gradient of the kinetic energy.

D. Parametrizing phase-space contraction

Due to the condition $\widetilde{r}_m + \widetilde{l}_m = r_m + l_m$, one can express $\widetilde{r}_m$ and $\widetilde{l}_m$ in an analogous way to Eq. (30) by introducing an additional parameter ϵ via

$$\widetilde{r}_m = \frac{\tau D}{a^2}\left(1 + \epsilon\frac{a v_m}{2D}\right), \quad (32a)$$

$$\widetilde{l}_m = \frac{\tau D}{a^2}\left(1 - \epsilon\frac{a v_m}{2D}\right). \quad (32b)$$

Using Eqs. (32) and (30) to evaluate $\widetilde{r}_{m+1} - \widetilde{l}_m$, one easily verifies that

$$\epsilon = \frac{\widetilde{r}_{m+1} - \widetilde{l}_m}{r_m - l_{m+1}} \quad (33)$$

is constant along the chain. This number fully characterizes the phase-space contraction of the multibaker map. In harmony with the common use in the dynamical-system literature, we will also say that ϵ characterizes the *dissipation*. It will be kept constant when taking the macroscopic limit.

There are two special values of the parameter ϵ that are worth mentioning. When ϵ takes the value $\epsilon = 1$, the phase-space dynamics is locally area preserving ($\widetilde{r}_{m+1} = r_m, \widetilde{l}_m = l_{m+1}$). For $\epsilon = -1$ ($\widetilde{r}_{m+1} = l_{m+1}, \widetilde{l}_m = r_m$) we call the resulting phase-space dynamics time reversible, since the initial area of any small region is recovered after taking an arbitrary closed path along the chain (at points differing from the initial one, however, the area is in general different from the initial one).

IV. ENTROPIES AND THEIR TIME EVOLUTION

A. Gibbs entropy $S^{(G)}$

For the generalized multibaker map, the Gibbs entropy is defined in terms of the phase-space density $\varrho(x,p)$ and the kinetic-energy density $w(x,p)$ as

$$S^{(G)} = -k_B \int dx\,dp\;\varrho(x,p)\;\ln\frac{\varrho(x,p)}{\varrho^\star(w(x,p))}, \quad (34)$$

where $\varrho^\star(w)$ is a reference density, which depends on w, and, through it, also on the phase-space coordinates (k_B denotes Boltzmann's constant). We write $\varrho^\star(w)$ in the form

$$\varrho^\star(w) = \frac{\varrho^\star}{f(w(x,p))}, \quad (35)$$

where $\varrho^\star$ is a constant reference phase-space density, and f is a dimensionless function. The actual form of $f(w)$ will be determined below by the requirement of consistency with thermodynamics. At the moment we assume only that it is sufficiently smooth to expand it to second order in its argument w.

The Gibbs entropy $S_m^{(G)\prime}$ after one time step can be expressed by making use of Eqs. (21) and (25) for the three columns of cell m:

$$S_m^{(G)\prime} = -k_B ab \left[(1 - r_m - l_m) \varrho_m \ln\left(\frac{\varrho_m}{\varrho^\star} f(w'_{m,s}) \right) \right.$$

$$+ r_{m-1} \varrho_{m-1} \ln\left(\frac{r_{m-1}}{\widetilde{r_m}} \frac{\varrho_{m-1}}{\varrho^\star} f(w'_{m,r}) \right)$$

$$\left. + l_{m+1} \varrho_{m+1} \ln\left(\frac{l_{m+1}}{\widetilde{l_m}} \frac{\varrho_{m+1}}{\varrho^\star} f(w'_{m,l}) \right) \right]. \quad (36)$$

After inserting the update (22) for the phase-space density, subtracting $S_m^{(G)} = -k_B ab \varrho_m \ln[\varrho_m f(w_m)/\varrho^\star]$, and rearranging terms, one finds

$$\frac{S_m^{(G)\prime} - S_m^{(G)}}{a\tau} = -k_B \frac{b}{\tau} \left[(\varrho'_m - \varrho_m) \ln\left(\frac{\varrho_m}{\varrho^\star} f(w_m) \right) \right.$$

$$+ \varrho'_m \ln\left(\frac{f(w'_{m,s})}{f(w_m)} \right)$$

$$+ r_{m-1} \varrho_{m-1} \ln\left(\frac{r_{m-1}}{\widetilde{r_m}} \frac{\varrho_{m-1}}{\varrho_m} \frac{f(w'_{m,r})}{f(w'_{m,s})} \right)$$

$$\left. + l_{m+1} \varrho_{m+1} \ln\left(\frac{l_{m+1}}{\widetilde{l_m}} \frac{\varrho_{m+1}}{\varrho_m} \frac{f(w'_{m,l})}{f(w'_{m,s})} \right) \right]$$

$$\equiv -\frac{j_m^{(s)} - j_{m-1}^{(s)}}{a} + \Phi^{(\text{thermostat})} \equiv \Phi. \quad (37)$$

This can be interpreted as a balance equation for the Gibbs entropy. The temporal change of $S^{(G)}$ comprises two contributions: the divergence of an entropy current

$$j_m^{(s)} \equiv -j_m k_B \ln\left(\frac{\varrho_m}{\varrho^\star} f(w_m) \right)$$

$$+ k_B \frac{ab l_{m+1}}{\tau} \varrho_{m+1} \ln\left(\frac{\varrho_{m+1}}{\varrho_m} \frac{f(w_{m+1})}{f(w_m)} \right) \quad (38a)$$

and a flux into the thermostat

$$\frac{\Phi^{(\text{thermostat})}}{k_B} \equiv -\frac{b}{\tau} \left[\varrho'_m \ln\frac{f(w'_{m,s})}{f(w_m)} \right.$$

$$+ r_{m-1} \varrho_{m-1} \ln\left(\frac{r_{m-1}}{\widetilde{r_m}} \frac{f(w'_{m,r}) f(w_m)}{f(w'_{m,s}) f(w_{m-1})} \right)$$

$$\left. + l_{m+1} \varrho_{m+1} \ln\left(\frac{l_{m+1}}{\widetilde{l_m}} \frac{f(w'_{m,l}) f(w_m)}{f(w'_{m,s}) f(w_{m+1})} \right) \right].$$
$$(38b)$$

In general, this decomposition is not unique. It will turn out that $\Phi^{(\text{thermostat})}$ contains terms that can be combined to a divergence and hence transferred to the entropy current. This freedom can only be removed in the macroscopic limit, where in physically relevant situations the splitting is unique. In any case, the form of the current is close to the thermodynamic one (3b): it contains a contribution proportional to

the current density j and another term that by its dependence on the function $f(w)$ characterizes the local kinetic-energy gradient.

We identify the temporal change of the Gibbs entropy with the flux of the coarse-grained entropy. This is meaningful from an information theoretic point of view. After all, the Gibbs entropy characterizes the information encoded in the *microscopic* time evolution of a system. Consequently, changes of this entropy may only be due to an entropy current and to a coupling to the thermostat, i.e., to terms like those identified in Eq. (37).

B. Coarse-grained entropy S

The coarse-grained entropy S_m of cell m is defined in an analogous way to the Gibbs entropy (34), but using now the cell density ϱ_m and the cell's kinetic-energy density w_m,

$$S_m = -k_B ab \varrho_m \ln\left(\frac{\varrho_m}{\varrho^\star} f(w_m) \right). \quad (39)$$

The coarse-grained entropy of cell m after one time step is

$$S'_m = -k_B ab \varrho'_m \ln\left(\frac{\varrho'_m}{\varrho^\star} f(w'_m) \right). \quad (40)$$

It depends on the updated values of the coarse-grained quantities.

In order to find the balance equation for the coarse-grained entropy, we make use of the argument of the previous subsection that the change in the Gibbs entropy may be interpreted as the macroscopic entropy flux. This allows us to rewrite the temporal change of the coarse-grained entropy as

$$\frac{\Delta S_m}{\tau} \equiv \frac{S'_m - S_m}{\tau} = \frac{S_m^{(G)\prime} - S_m^{(G)}}{\tau} + \frac{(S'_m - S_m^{(G)\prime}) - (S_m - S_m^{(G)})}{\tau}.$$
$$(41)$$

The first term on the right-hand side is the entropy flux $\Delta_e S_m / \tau$ through cell m, and the second one represents an irreversible entropy production $\Delta_i S_m / \tau$. Hence, Eq. (41) constitutes a discrete entropy balance in the form

$$\Delta S_m = \Delta_e S_m + \Delta_i S_m \quad (42)$$

with

$$\Delta_e S_m = S_m^{(G)\prime} - S_m^{(G)}, \quad (43a)$$

$$\Delta_i S_m = (S'_m - S_m^{(G)\prime}) - (S_m - S_m^{(G)}). \quad (43b)$$

In the information theoretic interpretation of entropies, the difference $S_m - S_m^{(G)}$ measures the information of a microscopic system which cannot be resolved by a coarse-grained description. Hence, $\Delta_i S_m$ is the increase per time unit τ of the information which cannot be resolved when characterizing the state of the system by coarse-grained densities. It is positive by construction, and, except for a transient behavior obtained for certain initial conditions (which will not be considered here), it can only increase.

Note that the entropy S_m and the difference $S_m - S_m^{(G)}$ might depend in general on details of the coarse graining. This dependence drops out in the macroscopic limit, when calculating temporal changes (cf. Appendix B). All quantities appearing in the entropy balance (42) will turn out to be thermodynamically well-defined observables.

As a last step, we discuss the explicit form of the the rate of irreversible entropy production. The initial condition that the system is prepared with uniform densities in every cell implies $S_m = S_m^{(G)}$. The irreversible entropy change during one time step is therefore the difference between the Gibbs and the coarse-grained entropies taken after one time step $\Delta_i S_m = S_m' - S_m^{(G)'}$. It can be split into two parts, an f-independent part, which comprises contributions due to the particle current, and another one, which is related to inhomogeneities in the kinetic-energy density, and hence in temperature. We write

$$\Delta_i S_m = \Delta_i S_m^{(particle)} + \Delta_i S_m^{(heat)}, \tag{44}$$

where

$$\Delta_i S_m^{(particle)} = k_B a b \left[-\varrho_m' \ln \frac{\varrho_m'}{\varrho_m} \right.$$

$$+ r_{m-1} \varrho_{m-1} \ln \left(\frac{r_{m-1}}{\tilde{r}_m} \frac{\varrho_{m-1}}{\varrho_m} \right)$$

$$\left. + l_{m+1} \varrho_{m+1} \ln \left(\frac{l_{m+1}}{\tilde{l}_m} \frac{\varrho_{m+1}}{\varrho_m} \right) \right] \tag{45a}$$

and

$$\Delta_i S_m^{(heat)} = k_B a b \left(-\varrho_m' \ln \frac{f(w_m')}{f(w_{m,s}')} \right.$$

$$+ r_{m-1} \varrho_{m-1} \ln \frac{f(w_{m,r}')}{f(w_{m,s}')}$$

$$\left. + l_{m+1} \varrho_{m+1} \ln \frac{f(w_{m,l}')}{f(w_{m,s}')} \right). \tag{45b}$$

All terms appearing in Eqs. (45) have a proper physical meaning. The first one in each equation characterizes the change of entropy due to the time evolution of the coarse-grained fields. The others amount to an entropy of mixing of regions in phase space with different phase-space or kinetic-energy densities. Note that contributions from phase-space contraction appear only in $\Delta_i S_m^{(particle)}$.

V. THE MACROSCOPIC LIMIT

A. Definition of the limit

The macroscopic limit implies that $a \ll L$, $N \gg 1$, and τ is much smaller than typical macroscopic time scales (for instance, L^2/D). Formally it is defined as

$$a, \tau \to 0 \tag{46}$$

such that the spatial coordinate

$$x \equiv a m \tag{47}$$

is finite. The phase-space density ϱ_m integrated over the momentumlike variable p becomes the local particle density $n(x)$. Since ϱ_m is independent of p, the integration corresponds to a multiplication with the vertical cell size b. As mentioned earlier, the field w is assumed to go over into the local temperature $T(x)$ in the macroscopic limit. Thus we have

$$b \varrho_m \to n(x), \tag{48a}$$

$$w_m \to CT(x), \tag{48b}$$

where C is a constant of dimension 1 over temperature. Moreover, the local drift, diffusion, and source strength q are kept finite while taking the limit

$$D \to D, \tag{49a}$$

$$v_m \to v(E, T, \partial_x T), \tag{49b}$$

$$q_m \to q(x). \tag{49c}$$

E denotes the external field. In the following we do not write out the x dependence of the fields, the drift, and the source term explicitly.

B. Number and kinetic-energy density

We first notice that under the assumption of smoothness the spatial dependence of the two fields can be expressed as

$$b \varrho_{m \pm 1} \to n \pm a \partial_x n + \frac{a^2}{2} \partial_x^2 n,$$

$$w_{m \pm 1} \to CT \pm a \partial_x (CT) + \frac{a^2}{2} \partial_x^2 (CT). \tag{50}$$

In order to calculate the macroscopic limit of the particle current (31a) we use Eqs. (30) and (49), to obtain

$$j = v n - D \partial_x n. \tag{51}$$

From Eq. (24), the time evolution of the density n can be obtained as

$$\partial_t n = -\partial_x (n v) + D \partial_x^2 n. \tag{52}$$

Similarly, we have for the time evolution of nT [cf. Eqs. (27) and (31b)]

$$\partial_t (nT) = -\partial_x j^{(nT)} + nTq \tag{53}$$

with the nT current

$$j^{(nT)} = Tj - nD \ \partial_x T. \tag{54}$$

C. Irreversible entropy production

For the contribution (45a) of the particle current to the irreversible entropy production we obtain (cf. the analogous calculation in [17,18] for details)

$$\frac{\Delta_i S_m^{(particle)}}{k_B a \tau} = \frac{j_\epsilon^2}{nD}, \tag{55a}$$

where

$$j_\epsilon \equiv j - \frac{1+\epsilon}{2} \; nv = \frac{1-\epsilon}{2} \; nv - D\partial_x n \qquad (55b)$$

agrees with the particle current (51) up to the dissipation-dependent term $(1-\epsilon)/2$.

The other contribution (45b) to the irreversible entropy production comprises the explicit dependence on the kinetic-energy field. It can be evaluated in a straightforward manner by Taylor expanding the function f and the logarithms to quadratic order around $w'_{m,s}$. The terms linear in $f'(w'_{m,s})/f(w'_{m,s})$ exactly cancel. [Here $f'(z)$ denotes the derivative of $f(z)$ with respect to z]. In nonvanishing order the macroscopic limit is therefore

$$\frac{\Delta_i S_m^{(\text{heat})}}{k_B a \tau} = nD(\partial_x CT)^2 \left[\frac{f''(CT)}{f(CT)} - \left(\frac{f'(CT)}{f(CT)} \right)^2 \right]. \qquad (55c)$$

Note that the square bracket can also be written as the second derivative of $\ln f$.

D. Entropy flux

By expanding $f(w_{m\pm1})$ to linear order around w_m, one finds for the macroscopic limit of the entropy current (38a)

$$\frac{j^{(s)}}{k_B} = -j \; \ln \frac{nf(CT)}{n^\star} + D\partial_x n + nD\partial_x(CT)\frac{f'(CT)}{f(CT)}, \qquad (56a)$$

where $n^* \equiv b\varrho^*$ is a reference particle density, which is constant in space and time.

The macroscopic limit of the entropy flux into the thermostat [Eq. (38b)] is found to be

$$\frac{\Phi^{(\text{thermostat})}}{k_B} = -nCT\frac{f'(CT)}{f(CT)}q - \frac{v}{D}\left(\frac{(1-\epsilon)^2}{4}nv + \epsilon D\partial_x n \right)$$
$$+ \partial_x(nv). \qquad (56b)$$

It contains the spatial derivative $\partial_x(nv)$, which underpins our earlier statement that the splitting of the entropy flux into the divergence of a current and a flux going directly into a thermostat is not unique. It is natural to remove the derivative from $\Phi^{(\text{thermostat})}$, which leads to the entropy current

$$\frac{j_1^{(s)}}{k_B} = -j\left(1 + \ln\frac{nf(CT)}{n^\star} \right) + nD\partial_x(CT)\frac{f'(CT)}{f(CT)}, \qquad (57a)$$

and to the flux

$$\frac{\Phi_1^{(\text{thermostat})}}{k_B} = -nCT\frac{f'(CT)}{f(CT)}q - \frac{v}{D}\left(\frac{(1-\epsilon)^2}{4}nv + \epsilon D\partial_x n \right). \qquad (57b)$$

However, there are other ϵ-dependent splittings, too. For instance, by adding $(1+\epsilon)nv/2$ to the entropy current one obtains

$$\frac{j_2^{(s)}}{k_B} = -j\ln\frac{nf(CT)}{n^\star} - j_\epsilon + nD\partial_x(CT)\frac{f'(CT)}{f(CT)} \qquad (58a)$$

and

$$\frac{\Phi_2^{(\text{thermostat})}}{k_B} = -nCT\frac{f'(CT)}{f(CT)}q - \frac{1-\epsilon}{2}\frac{v}{D}j_\epsilon + \frac{1+\epsilon}{2}n\partial_x v. \qquad (58b)$$

This shows that the splitting of the total entropy flux into a divergence of an entropy current and a flux $\Phi^{(\text{thermostat})}$ is in general not unique for arbitrary values of ϵ, not even in the macroscopic limit.

VI. CONSISTENCY WITH THERMODYNAMICS

Having found the general expressions for the macroscopic limit of the particle and entropy fluxes, and of the irreversible entropy production, we are now in a position to make specific choices for the parameter ϵ, for the yet undetermined functions $q(x)$ and $f(w)$, and for the functional $v(E,T,\partial_x T)$.

Comparing Eq. (51) with the thermodynamic particle current (17), we find that the drift $v(E,T,\partial_x T)$ must take the form

$$v = v_{el} - k\frac{D}{T}\partial_x T. \qquad (59)$$

Since earlier we have not found any necessity to fix v, this choice is obviously consistent with thermodynamics. It remains to be seen, however if the other constraints can be fulfilled.

The form of f can be fixed by observing that the term $(\partial_x T/T)^2$ appears in the irreversible entropy production (2a) with the *same* coefficient as the $-\partial_x T/T$ term in the entropy current (3b). Comparing the f-dependent parts in Eqs. (55c) and (56a) [or Eqs. (57a) or (58a)] we find that this can only happen if

$$z(\ln f(z))'' = -(\ln f(z))'. \qquad (60)$$

The solution of this differential equation is a power law,

$$f(z) = z^{-\gamma} \qquad (61)$$

with γ as a free constant parameter. A constant prefactor can be absorbed into the definition (35) of $\varrho^\star$.

Concerning the value of ϵ, there are several constraints, which all lead to the same unique choice. (i) The requirement to have the same coefficient in front of the $v_{el}n$ and the $-D\partial_x n$ terms in the entropy current (19) fixes the value of ϵ to be -1 [cf. $j_2^{(s)}$ given by Eq. (58a)]. (ii) A natural splitting of the entropy flux into the negative divergence of the entropy current and a flux into the thermostat holds for $\epsilon = -1$, too. In particular, we then have $j_1^{(s)} = j_2^{(s)}$ and $\Phi_1^{(\text{thermostat})} = \Phi_2^{(\text{thermostat})}$. (iii) The particle flux into the thermostat Eq. (57b) [or Eq. (58b)] has a well-defined meaning only when its second term contains the full particle current j. For all these reasons the only dynamics that leads to physically acceptable results corresponds to the choice $\epsilon = -1$, which was connected to a time-reversible dissipation mechanism in Sec. III D. For this choice also the particle-current-

dependent part of the entropy production (55a) contains the full square of j as required for consistency with the corresponding thermodynamic contribution (2a).

With these choices

$$\frac{j^{(s)}}{k_B} = -j\left(1+\ln\frac{n(CT)^{-\gamma}}{n^\star}\right) - nD\gamma\ \frac{\partial_x T}{T}. \qquad (62)$$

In view of Eq. (3b), we identify the thermal conductivity λ and the Peltier coefficient Π as

$$\lambda = k_B nD\gamma, \qquad (63a)$$

$$\frac{\Pi}{T} = \frac{k_B}{e}\left[-1-\ln\left(\frac{n}{n^\star}(CT)^{-\gamma}\right)\right]. \qquad (63b)$$

Through this, the transport coefficients could be expressed by system parameters. It is remarkable that finite values were found for λ and Π although only the finiteness of v and D was assumed in the course of the macroscopic limit.

Similarly, for the flux into the thermostat one obtains

$$\frac{\Phi^{(\text{thermostat})}}{k_B} = \gamma nq - \frac{vj}{D}. \qquad (64)$$

It contains a term vj/D corresponding to the change of entropy associated with Joule's heating due to the drift v of the particles. In thermodynamics $\Phi^{(\text{thermostat})}$ vanishes in the bulk, so that the source term q takes the form

$$\frac{q^*}{k_B} = \frac{vj}{\lambda}. \qquad (65)$$

It describes the increase of the local kinetic energy due to dissipative heating. The heat thus deposited in the system will be transported to the boundaries by a heat current.

The entropy density obtained as the macroscopic limit of Eq. (39) is

$$s = -k_B n\ln\left(\frac{n}{n^\star}(CT)^{-\gamma}\right). \qquad (66)$$

This implies that, up to an additive constant, $e\Pi/T$ is the entropy per particle s/n.

Since the multibaker map describes a system of weakly interacting particles [38], it is natural to assume that not only its entropy function (66) but also its chemical potential corresponds to that of a classical ideal gas. We take

$$\mu_c \equiv k_B T(1+\gamma) - T\frac{s}{n}. \qquad (67)$$

From these two equations of state γ follows as the specific heat at constant volume, measured in units k_B.

By substituting the chemical potential (67) into the thermodynamic expression of the Peltier coefficient (20) and comparing it with the particular form obtained for Π/T in Eq. (63b), one immediately sees that the coefficient k of Eq. (59) has to vanish. Hence, $\mathrm{s}=e\alpha$ from Eq. (18), and from Eq. (16b) one recovers the Onsager relation $\Pi=T\alpha$. The

fact that k turns out to be zero seems to be a special feature of the baker model with three strips. In this version temperature cannot move without an explicit particle motion, and hence no thermal diffusion is expected.

Next, we consider the heat current $j^{(\text{heat})}$, i.e., the energy current from which the potential energy of the external field is excluded,

$$j^{(\text{heat})} \equiv Tj^{(s)} + \mu_c j. \qquad (68)$$

Inserting the explicit form of currents j and $j^{(s)}$ [cf. Eqs. (51) and (62)] into Eq. (9a), this yields

$$j^{(\text{heat})} = -\lambda\partial_x T + k_B T\ \gamma j. \qquad (69)$$

This form is indeed consistent with thermodynamics, and also with the macroscopic limit of the nT current (54). Multiplying the latter by $k_B\gamma$, we recover Eq. (69).

It is worth pointing out that due to the definition (16a) of the diffusion coefficient and the particular form of the chemical potential (67), we find that

$$\sigma_{el}k_B T = e^2 Dn. \qquad (70)$$

Consequently, Einstein's relation holds in the multibaker map. One can thus express the electric conductivity by the diffusion coefficient D in all formulas. In particular, we find

$$\sigma^{(\text{irr})} = \lambda\left(\frac{\nabla T}{T}\right)^2 + \frac{k_B j^2}{nD}, \qquad (71)$$

a formula which in the case of constant temperature has already been derived in earlier versions of the multibaker map [17,18].

As further consequences of Einstein's relation, we mention the following. (i) The electric drift v_{el} (4) is proportional to E/T,

$$v_{el} = \frac{eD}{k_B}\frac{E}{T}, \qquad (72)$$

since the diffusion coefficient is assumed to be constant. (ii) Comparing the heat and electric conductivities (63a) and (70), we find

$$\frac{\lambda}{\sigma_{el}T} = \gamma\left(\frac{k_B}{e}\right)^2, \qquad (73)$$

which implies that this ratio is independent of thermodynamic state variables. Thus, the Wiedemann-Franz law [40] proves to hold for the multibaker model. (iii) the elementary Drude theory [40] of metallic conduction predicts the Seebeck coefficient $\alpha=\Pi/T$ to be proportional to k_B/e, i.e., to be independent of temperature or density, which contradicts observation. Such a term is indeed present in Eq. (63b), but its second term also predicts a specific state dependence. Thus, the present model turns out to describe certain features of transport more realistically than the classical Drude model, although it cannot be expected to give a microscopically realistic theory of thermoelectric phenomena (which contain essential quantum effects due to the strong degeneracy of the fermionic electron gas) [41].

Finally, we consider the temperature equation following from Eq. (53). It takes the form

$$\partial_t T = qT + \frac{\partial_x(\lambda \partial_x T)}{k_B \gamma n} - j\frac{\partial_x T}{n}, \qquad (74)$$

which can be shown to be consistent with the general relation [cf. Eq. XIII.(85) of [33]] expressing the entropy's local time derivative as

$$\partial_t s = \frac{\partial_x(\lambda \partial_x T)}{T} - \partial_x \left(\frac{e\Pi j}{T} \right) + \frac{ej^2}{\sigma_{el} T}. \qquad (75)$$

Here, the respective terms are contributions due to heat conduction, the Peltier and Joule heating. Using Eq. (66) and the form of Peltier coefficient Eq. (63b), one finds that Eq. (75) becomes an identity if and only if the thermodynamic choice Eq. (65) is taken for the source term.

VII. THERMOSTATING

After having identified the condition for full consistency with thermodynamics in the form of $\Phi^{(\text{thermostat})} = 0$ or $q = q^*$, we turn to a short discussion of cases where there can be an entropy flux into the thermostat. In the thermostating algorithm of nonequilibrium molecular dynamics [4], heat is taken out of the system in order to keep the temperature constant in a spatially homogeneous steady state, and to avoid overheating due to the permanent acceleration produced by en electric field. In our setting this corresponds to a case with $\partial_x T = 0$. Such a uniform temperature field is stationary for $q = 0$ only, as follows from the temperature equation (74), such that $\Phi^{(\text{thermostat})} = -k_B v j/D$. It is indeed a kind of Joule's heat, which is let into the thermostat. Note, however, that classical thermodynamics does not admit a stationary homogeneous state $\partial_x T = 0$ to be steady, since the temperature increases in the bulk due to Joule's heating. This indicates that thermostating is a tool by which one can turn a preselected temperature profile into a steady state. After all, for every density profile consistent with given boundary conditions and a preselected fixed temperature profile $T(x)$ there is a source term distribution $q(x)$, such that the temperature does not change in time [cf. Eq. (74) with $\partial_t T = 0$]. In all these cases $\Phi^{(\text{thermostat})} = k_B(\gamma nq - v j/D)$ is different from zero. This shows that the algorithm for thermostating can be maintained even for complicated temperature profiles. Since the source q appears neither in the currents, nor in the irreversible entropy production, nor in the constraint for the Onsager relation to hold, nor in the transport coefficients, the local entropy balance is consistent with every choice of q or $\Phi^{(\text{thermostat})}$ provided the entropy flux appears in the form of Eq. (5). In general, the divergence of the entropy current $j^{(s)}$ contributes to the entropy flux Φ, and the remaining part of the reversible change of the entropy is transferred to the thermostat.

We conclude that, although thermostating is a deviation from classical thermodynamics, it seems to be the *weakest* possible deviation in the sense that except for the form of the entropy flux it leaves all *local* thermodynamic relations invariant. It can thus be seen as an idealization of a physical thermostat (which can in reality only be attached to the boundaries of a system), where heat need not be transported spatially (to the boundaries), but can be released directly into the surroundings. This gives rise to a nonthermodynamic contribution to the entropy flux in the local entropy-balance equation in a generalization of nonequilibrium thermodynamics [cf. Eqs. (5) and (1)]. This generalization of the local balance equation, however, does not imply at all a similarity of *global* transport properties, which in general depend on the spatial dependence of the fields. It is clear from Eq. (74) that a state which is steady with a given $q(x)$ will not be steady with the thermodynamic choice $q^*(x)$. It will not even have similar density profiles. Therefore, thermodynamics and thermostated descriptions might lead to very different results on the global level.

VIII. DISCUSSION

We have extended multibaker models by augmenting the density field ϱ of these models with a temperaturelike field variable w. This allowed us to address problems like thermoelectric cross effects requiring two independent thermodynamic driving fields. The model has the following features.

(a) The evolution equation of w requires source terms reflecting the local irreversible heating of the system in the presence of transport.

(b) The temperature enters the entropy through a kinetic-energy-dependent normalization of the (phase-space) density.

(c) Consistency with the thermodynamic description of transport is achieved for densities that are coarse grained in regions of small spatial extension.

(d) Comparing the coarse-grained description with the microscopic one allows us to identify all contributions to the *local* entropy balance.

(e) The time evolution of the system can be interpreted as that of weakly interacting particles, whose motion may only be coupled through a mean-field-like dependence of the evolution equations on the coarse-grained field variables. In accordance with this, the resulting ''multibaker'' gas obeys the classical ideal-gas equation of state. The Onsager relation, the Wiedemann-Franz law, and the Einstein relation can be derived, and expressions are found for the Peltier and Seebeck coefficients.

(f) The local entropy balance of nonequilibrium thermodynamics can be generalized by introducing at every location an instantaneous flow of entropy (i.e., of heat) into a thermostat. When time reversibility is maintained, the dynamics becomes closely reminiscent of numerical algorithms related to Gaussian thermostats.

(g) Dissipation and thermostating play different roles in dynamical-system models for transport. The condition $\epsilon = -1$, for time reversibility, was found independently of the choice of $\Phi^{(\text{thermostat})}$. With this dissipation we can describe both thermostated and nonthermostated systems.

It is remarkable that agreement with thermodynamics could be achieved by this comparatively simple model. Indeed, strong restrictions on the choice of its parameters were needed. The free functions (drift v, source strength of heat q, and normalization of densities f) had to be chosen appropriately, and a free dissipation-related parameter (ϵ) had to be fixed to a given value leading to a time-reversible dissipative dynamics (even a Hamiltonian, volume-preserving dynamics is excluded). With the given choices, however, we do not find any restriction to weak gradients. This might be caused

by the strong chaoticity and the Markovian property of the dynamics, which is based on the baker map's piecewise-linear character and the fact that this family of maps admits no pruning.

We have used a generalized concept of dynamical systems to model open boundaries where transport can be induced by appropriately chosen boundary conditions. The time evolution of a macroscopically large number of independent ''particles'' is considered. Consequently, not even in steady states is the natural measure of the multibaker map relevant to calculate physical observables. After all, this measure is defined only if the map is closed by periodic boundary conditions. Rather, another measure, the one *forced* on the system by the open boundary conditions, plays the central role. Such measures were first investigated by Gaspard and co-workers [3,21,22].

Finally, we draw attention to the fact that the present model differs in important features from other models of transport by low-dimensional dynamical systems. The transition probabilities (which are closely related to the drift and diffusion coefficients) may depend on the coarse-grained fields. This dependence leads to a dynamical system with many degrees of freedom. Consequently, the full time evolution of the (x,p) dynamics together with the time dependence of the parameters can be interpreted as a peculiar coupled map lattice designed to closely follow transport equations. In a steady state, however, the parameters take time-independent values such that the time evolution of the particles is described by a two-dimensional dynamical system, a map acting on (x,p), which in general lacks translation invariance.

It is worth emphasizing that a further reduction of the dimension is impossible. By neglecting the p variable (i.e., when projecting the baker map to obtain a one-dimensional map describing the transport of particles along the x direction) one finds full consistency with macroscopic transport equations, but all drift-dependent terms disappear from the entropy balance, which therefore deviates from its thermodynamic form [Eqs. (1) and (2)]. Hence, modeling only the transport processes via dynamical systems is a much easier enterprise than aiming also for a proper description of entropies. From the point of view of a correct entropy balance, the existence of a phase-space variable orthogonal to the transport direction is essential. Only in this case can the fractal structures in the microscopic densities be followed, whose unresolvability leads to entropy production. It is an open question at present, however, if a dissipative dynamics is needed for this, since a variation of the cell size in the sense of [31] might convert contributions to the entropy production due to local phase-space contraction into those of mixing.

The suggested method for modeling thermoelectric cross effects can be considered as a combination of a dynamical-system and a hydrodynamic description. In addition to the appearance of a source term of the kinetic energy, the strong *mixing* character of the chaotic dynamics is essential, which leads to fractal phase-space patterns in the forced measure considered. By that it ensures that irreversibility, and thus consistency with thermodynamics, can be reached in a description based on a low-dimensional dynamical system.

APPENDIX A: RIGOROUS DEFINITION OF THE MAP AND OF THE TIME EVOLUTION OF DENSITIES

Every point (x,p) with $x \in [a, a(N+1)]$, $1 \leq m \leq N$, and $y \in [0,b]$ is mapped by the multibaker map B as follows:

$$B(x,p) = \begin{cases} \left(\dfrac{x-am}{l_m} + a(m-1), & \widetilde{l_{m-1}}p \right) & \text{for} \quad 0 < \dfrac{x-am}{a} < l_m \\[2ex] \left(\dfrac{x-a(m+l_m)}{s_m} + am, & b\widetilde{l_m} + \widetilde{s_m}p \right) & \text{for} \quad l_m < \dfrac{x-am}{a} < l_m + s_m \\[2ex] \left(\dfrac{x-a(m+l_m+s_m)}{r_m} + a(m+1), & b(\widetilde{l_{m+1}} + \widetilde{s_{m+1}} + \widetilde{r_{m+1}}p) \right) & \text{for} \quad l_m + s_m < \dfrac{x-am}{a} < 1. \end{cases} \quad (A1)$$

The dynamics of the phase-space density $\varrho(x,p;t)$ can be interpreted as the time evolution of a typical set of points distributed in phase space. It is governed by the Frobenius-Perron equation

$$\varrho(z;t+\tau) = \int dz' \, \delta(z - B(z')) \varrho(z';t), \quad (A2)$$

where z denotes points (x,p) in the phase space of the multibaker chain.

The boundary conditions are that $\varrho(z;t)$ is fixed to ϱ_0 and ϱ_{N+1} in the cells $m=0$ and $m=N+1$, respectively. They are taken into account by the choice

$$\varrho(z;t+\tau) = \begin{cases} \varrho_0 & \text{for } \mathcal{B}^{-1}(z) \text{ in cell } 0 \\ \varrho_{N+1} & \text{for } \mathcal{B}^{-1}(z) \text{ in cell } N+1, \end{cases} \quad (A3)$$

for points z whose preimages $\mathcal{B}^{-1}(z)$ lie in cell 0 $(N+1)$.

Due to the chaoticity of the map and the difference in the boundary conditions, the density $\varrho(z;t)$ becomes more and more irregular as time goes on (at least for any smooth initial distribution). Therefore, asymptotically the concept of density is not well defined. For $t \rightarrow \infty$ one assigns the measure $\mu(A) \equiv \lim_{t \rightarrow \infty} \int_A dz \, \varrho(z;t)$ to any phase-space region A.

Similarly to the phase-space density $\varrho(z;t)$, the time evolution of the kinetic-energy density

$$\omega \equiv \varrho w \tag{A4}$$

is described by the integral equation

$$\omega(z;t+\tau) = [1 + \tau q(z)] \int dz' \, \delta(z - B(z')) \omega(z';t). \tag{A5}$$

In generalization of the Frobenius-Perron equation (A2), however, a source term $q(x)$ is included now, which is piecewise constant in the cells. The corresponding boundary conditions for $w(z;t)$ are

$$\omega(z;t+\tau) = \varrho_{0(N+1)} w_{0(N+1)} [1 + \tau q(z)] \tag{A6}$$

for points whose preimages are in cell 0 or $N+1$, respectively.

In this case, also $w(z;t)$ is no longer well defined asymptotically. Instead, the stationary kinetic-energy distribution should be considered as an invariant measure ν, different from μ, which assigns the weight $\nu(A) \equiv \lim_{t \rightarrow \infty} \int_A dz \, \omega(z;t)$ to every region A in phase space.

APPENDIX B: STRUCTURAL STABILITY OF MACROSCOPIC RESULTS

In this appendix we generalize the results of Vollmer *et al.* [17] and of Gilbert and Dorfman [20] who considered thermostated multibakers describing conduction without cross effects. We demonstrate that, after taking the macroscopic limit, our results are independent of the detailed prescription of coarse graining. One part of such a demonstration should be that the same results are obtained when coarse graining is applied to any number m_c of successive cells after every time step. In this case all previous results for quantities of unit volume remain unchanged in the macroscopic limit for any fixed m_c, since both the length of the investigated region and the differences of the values of the coarse-grained fields become multiplied by a factor m_c, and thus the macroscopic gradients do not change.

We therefore concentrate on the more involved case of coarse graining on the cells only after every n time steps. From a density that is constant in each cell, the dynamics generates structure on the nth level of the refining partition obtained by the nth images of the cells. Structural stability is demonstrated by showing that the total entropy production can be decomposed into a sum of contributions from coarse graining on the different levels (starting with the finest structures) and that all these contributions are the same in the macroscopic limit. This is equivalent to showing that coarse graining may also be applied to a finer partitioning within the cells, without affecting the resulting thermodynamic relations. For the sake of conciseness we immediately explore
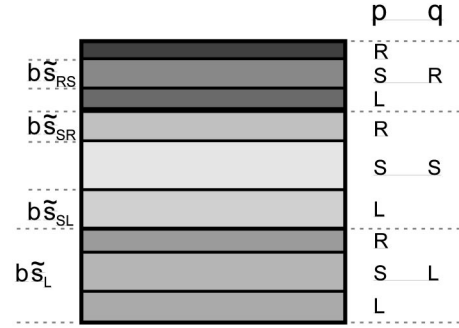

FIG. 3. Notation used to define the level-2 partitioning of a cell after two applications of the map. Every strip is labeled by a two-letter sequence p,q, where $p,q \in \{L,S,R\}$ label the level-2 strips. (p stands for the level-2 strips within level-1 strips selected by the label q.) To illustrate the use of these labels, the heights of a few strips are indicated at the left side of the cell.

the physically relevant case $f(z) = z^{-\gamma}$ [cf. Eq. (61)], suppress the normalization constant $\varrho^\star$ of the density and Boltzmann's constant k_B, and only work out the case $n=2$. Although this corresponds to just the simplest possibility, it indicates the strategy to be followed when discussing further refinements [42].

1. Preliminaries

We first extend our notation in order to describe densities, entropies, and fluxes defined on the different levels of coarse graining. To this end we consider the level-2 partitioning (cf. Fig. 3) of the cells two time steps after the initial coarse graining. Again primes denote quantities evaluated after the first application of the mapping. Similarly, double primes are used for the values after two iterations. Note that the transition probabilities r_m, s_m, and l_m and the widths and heights of the corresponding columns and strips also receive primes now, due to their possible dependence on ϱ_m and w_m (which evolve in time).

In every cell m there are 3^2 strips labeled by a pair of symbols (p,q) with $p,q \in \{L,S,R\}$; p indicates the strip (L,S,R) of Fig. 2(b) in which the point is located after one time step (irrespective of the cell index), and q specifies its position in the strip (L,S,R) after the second time step. The strips (p,q) have height $b\widetilde{s}_{p,q} = b\widetilde{s}_{m,q}' \, \widetilde{s}_{m_q,p}$, and carry densities $\varrho_m''(p,q)$ and $w_m''(p,q)$. Here,

$$\widetilde{s}_{m,q} = \begin{cases} \widetilde{r}_m & \text{for } q=R \\ \widetilde{s}_m & \text{for } q=S \\ \widetilde{l}_m & \text{for } q=L \end{cases} \tag{B1}$$

is a shorthand notation for the height after one time step, and the subscript

$$m_q = \begin{cases} m+1 & \text{for } q=L \\ m & \text{for } q=S \\ m-1 & \text{for } q=R \end{cases} \tag{B2}$$

is used as a book-keeping device to indicate the cell from which come the points in a given strip. An analogous definition holds for the quantities $s_{m,q}$ without tildes.

We call $\varrho''_m(p,q)$, $\varrho''_m(q)$, and ϱ''_m [$\varrho''_m(p,q)w''_m(p,q)$, $\varrho''_m(q)w''_m(q)$, and $\varrho''_m w''_m$] the level-2, level-1, and level-0 densities [kinetic-energy densities] after two time steps, respectively. By construction, the level-0 densities coincide with the cell densities considered in preceding sections. The densities defined on different levels are related to each other since coarse graining preserves their average value in each cell:

$$\varrho''_m = \sum_q \widetilde{s_{m,q}}{}' \, \varrho''_m(q) = \sum_q \widetilde{s_{m,q}}{}' \sum_p \widetilde{s_{m_q,p}} \, \varrho''_m(p,q),$$

$$\text{(B3a)}$$

$$\varrho''_m w''_m = \sum_q \widetilde{s_{m,q}}{}' \, \varrho''_m(q)w''_m(q)$$

$$= \sum_q \widetilde{s_{m,q}}{}' \sum_p \widetilde{s_{m_q,p}} \, \varrho''_m(p,q)w''_m(p,q).$$

$$\text{(B3b)}$$

Based on the time evolution of the fields, relations between densities at different instants of time can be calculated. Taking into account the respective actions (21) and (25) of the mapping on the densities ϱ and w, we obtain

$$\varrho''_m(p,q) = \frac{s'_{m_q,q}}{\widetilde{s_{m,q}}{}'} \, \varrho'_{m_q}(p) = \frac{s'_{m_q,q}}{\widetilde{s_{m,q}}{}'} \frac{s_{m_{q,p},p}}{\widetilde{s_{m_q,p}}} \, \varrho_{m_{q,p}},$$

$$\text{(B4a)}$$

$$w''_m(p,q) = w'_{m_q}(p)(1+\tau q'_m) = w_{m_{q,p}}(1+\tau q_{m_q})(1+\tau q'_m).$$

$$\text{(B4b)}$$

Here $m_{p,q}$ denotes the action of Eq. (B2) applied to m_p: $m_{p,q}=(m_p)_q$. In order to follow the time evolution of the entropies, we consider coarse-grained entropies defined with respect to densities of different resolution. The level-i entropy $S_m^{(i)}$ is defined with respect to the level-i densities. Thus, $S_m^{(0)} \equiv S_m = -ab\,\varrho_m \ln(\varrho_m w_m^{-\gamma})$, while the level-1 and level-2 entropies at time τ and 2τ take the forms

$$S_m^{(1)\prime} = -ab \sum_p \widetilde{s_{m,p}} \varrho'_m(p)\ln[\varrho'_m(p)w'_m{}^{-\gamma}(p)]$$

$$\text{(B5a)}$$

and

$$S_m^{(2)\prime\prime} = -ab \sum_{p,q} \widetilde{s_{m,q}}{}' \, \widetilde{s_{m_q,p}} \, \varrho''_m(p,q)$$

$$\times \ln[\varrho''_m(p,q)w''_m{}^{-\gamma}(p,q)],$$

$$\text{(B5b)}$$

respectively.

2. Entropy balance on level-1 strips

In order to obtain the entropy balance on level-1 strips, we relate $S_m^{(2)\prime\prime}$ to $S_m^{(1)\prime}$. Making use of Eqs. (B1), (B2), (B4), and (B5b), the level-2 entropy after two time steps $S_m^{(2)\prime\prime}$ of cell m can be worked out as

$$S_m^{(2)\prime\prime} = -ab \sum_{p,q} \widetilde{s_{m,q}}{}' \, \widetilde{s_{m_q,p}} \, \varrho''_m(p,q)\ln[\varrho''_m(p,q)w''{}^{-}\gamma_m(p,q)]$$

$$= -ab \sum_q s'_{m_q,q}\varrho'_{m_q}\ln\frac{s'_{m_q,q}}{\widetilde{s_{m,q}}{}'} - ab \sum_{p,q} s'_{m_q,q}s_{m_{q,p},p}\varrho_{m_{q,p}}\ln[\varrho'_{m_q}(p)w'_{m_q}(p)^{-\gamma}(1+\tau q'_m)^{-\gamma}] \quad \text{(B6)}$$

where $\varrho'_{m_q} = \Sigma_p \widetilde{s_{m_q,p}} \varrho'_{m_q}(p)$.

By using Eq. (B5a), $S_m^{(2)\prime\prime}$ takes the form

$$S_m^{(2)\prime\prime} = -ab \sum_q s'_{m_q,q}\varrho'_{m_q}\ln\frac{s'_{m_q,q}}{\widetilde{s_{m,q}}{}'} + \sum_q s'_{m_q,q}S_{m_q}^{(1)\prime} + ab\,\gamma\sum_q s'_{m_q,q}\varrho'_{m_q}\ln(1+\tau q'_m), \quad \text{(B7)}$$

which, after carrying out the summation over q, leads to the level-1 generalization of the the entropy flux,

$$\Delta_e S_m^{(1)\prime} \equiv S_m^{(2)\prime\prime} - S_m^{(1)\prime}$$

$$= -ab\,r'_{m-1}\sum_p \widetilde{s_{m-1,p}}\varrho'_{m-1}(p)\ln\left(\varrho'_{m-1}(p)w'_{m-1}{}^{-\gamma}(p)\frac{r_{m-1}}{\widetilde{r_m}}\right)$$

$$-ab\,l'_{m+1}\sum_p \widetilde{s_{m+1,p}}\varrho'_{m+1}(p)\ln\left(\varrho'_{m+1}(p)w'_{m+1}{}^{-\gamma}(p)\frac{l_{m+1}}{\widetilde{l_m}}\right)$$

$$+ab\,(r'_m+l'_m)\sum_p \widetilde{s_{m,p}}\varrho'_m(p)\ln[\varrho'_m(p)w'_m{}^{-\gamma}(p)] + ab\,\gamma\sum_q s'_{m_q,q}\varrho'_{m_q}\ln(1+\tau q'_m). \quad \text{(B8)}$$

The entropy balance for the level-1 strips then reads

$$\Delta S_m^{(1)'} \equiv S_m^{(1)''} - S_m^{(1)'} \equiv \Delta_i S_m^{(1)'} + \Delta_e S_m^{(1)'} \qquad (B9)$$

with the level-1 irreversible entropy production

$$\Delta_i S_m^{(1)'} = S_m^{(1)''} - S_m^{(2)''}. \qquad (B10)$$

Again it is related to the loss of information on the microscopic state of the system when applying a coarse-grained description.

If the densities ϱ'_{m_q} are uniform in the respective cells m_q, i.e., they do not depend on the partitioning label p, the above relations coincide with Eqs. (37) and (45) [in which ϱ'_m is eliminated via Eq. (22)]. Typically, however, there is a nonvanishing difference

$$\delta \Delta_i S_m^{(1)'} \equiv \Delta_i S_m^{(1)'} - \Delta_i S_m^{(0)}, \qquad (B11)$$

which disappears only in the macroscopic limit, as shown below after the discussion of the entropy balance for coarse graining after every second time step.

3. Entropy balance for coarse graining after every second time step

In order to denote temporal changes taken with a time lag 2τ, we assign the superscript $^{(2)}$ to Δ. A direct consequence of Eq. (B8) is that the entropy flux $\Delta_e^{(2)} S_m^{(0)}$ after two time steps is

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

$$\equiv \Delta_e S_m^{(0)} + \Delta_e S_m^{(1)'}. \qquad (B12)$$

This flux is the two-time-step generalization of the entropy flux $\Delta_e S_m$.

In order to establish the entropy balance, the change of the coarse-grained entropy $\Delta^{(2)} S_m^{(0)}$ is considered (without coarse graining after the first step),

$$\Delta^{(2)} S_m^{(0)} \equiv S_m^{(0)''} - S_m^{(0)} = S_m^{(0)''} - S_m^{(2)''} + S_m^{(2)''} - S_m^{(0)}$$

$$= S_m^{(0)''} - S_m^{(2)''} + \Delta_e^{(2)} S_m^{(0)}. \qquad (B13)$$

Thus, the two-step irreversible entropy change $\Delta_i^{(2)} S_m^{(0)}$ takes the form

$$\Delta_i^{(2)} S_m^{(0)} \equiv \Delta^{(2)} S_m^{(0)} - \Delta_e^{(2)} S_m^{(0)} = S_m^{(0)''} - S_m^{(2)''}. \qquad (B14)$$

Again it is identified as the loss of information caused by coarse graining.

Note that this rate of entropy production can be expressed as

$$\Delta_i^{(2)} S_m^{(0)} = \Delta_i S_m^{(0)'} + \Delta_i S_m^{(1)'} \qquad (B15)$$

where $\Delta_i S_m^{(j)} = S_m^{(j)'} - S_m^{(j+1)'}$ $(j=0,1)$. When coarse graining is applied after each time step, the entropy production is $\Delta_i S_m^{(0)} + \Delta_i S_m^{(0)'}$. Thus, $\delta \Delta_i S_m^{(1)'}$ also amounts to the difference between the irreversible entropy production of the cases, where coarse graining is applied after each and after every second time step.

4. Evaluation of $\delta \Delta_i S_m^{(1)'}$

We recall that $\varrho''_m(q)$ and $w''_m(q)$ denote the fields after two time steps, when coarse graining is applied on the level-1 partition. The level-1 entropy after two time steps is

$$S_m^{(1)''} = -ab \sum_q \widetilde{s_{m,q}}' \, \varrho''_m(q) \ln[\varrho''_m(q) w''_m(q)^{-\gamma}]$$

$$= -ab \sum_q s'_{m_q,q} \varrho'_{m_q} \ln \frac{s'_{m_q,q}}{\widetilde{s_{m,q}'}} + \sum_q s'_{m_q,q}$$

$$\times \{-ab \, \varrho'_{m_q} \ln[\varrho'_{m_q} w'^{-\gamma}_{m_q}(1+\tau q_m)^{-\gamma}]\}. \qquad (B16)$$

Using the form (40) of the coarse-grained entropy, we obtain

$$S_m^{(1)''} = -ab \sum_q s'_{m_q,q} \varrho'_{m_q} \ln \frac{s'_{m_q,q}}{\widetilde{s_{m,q}'}} + \sum_q s'_{m_q,q} S_{m_q}^{(0)'}$$

$$+ ab \, \gamma \sum_q s'_{m_q,q} \varrho'_{m_q} \ln(1+\tau q_m), \qquad (B17)$$

where $S_{m_q}^{(0)'}$ is the coarse-grained entropy of cell m_q evaluated after one time step. This form of level-1 entropy can straightforwardly be compared with the level-2 entropy (B7), leading to

$$\Delta_i S_m^{(1)'} = S_m^{(1)''} - S_m^{(2)''} = \sum_q s'_{m_q,q}(S_{m_q}^{(0)'} - S_{m_q}^{(1)'})$$

$$\equiv s_m \Delta_i S_m^{(0)} + r_{m-1} \Delta_i S_{m-1}^{(0)} + l_{m+1} \Delta_i S_{m+1}^{(0)}$$

$$= \Delta_i S_m^{(0)} - r_m(\Delta_i S_m^{(0)} - \Delta_i S_{m-1}^{(0)}) - l_m(\Delta_i S_m^{(0)} - \Delta_i S_{m+1}^{(0)}) + (r'_{m-1} - r_m)\Delta_i S_{m-1}^{(0)} + (l'_{m+1} - l_m)\Delta_i S_{m+1}^{(0)}, \qquad (B18)$$

where we have used that $s_m = 1 - r_m - l_m$. Expressing r_m and l_m in terms of driving forces and transport parameters (30) and keeping only leading order terms in a, one obtains

$$\delta \Delta_i S = \tau D \partial_x^2 (\Delta_i S^{(0)}) - \tau v \, \partial_x (\Delta_i S^{(0)}) - \tau (\partial_x v) \Delta_i S^{(0)}$$
$$+ \mathcal{O}(\tau^2, a). \qquad (B19)$$

After division by $a\tau$, the right-hand side of Eq. (B19) contains the rate of irreversible entropy production $\Delta_i S^{(0)}/a\tau$ and its spatial derivatives, because $\Delta_i S^{(0)}/a\tau$ has a finite macroscopic limit. Consequently, the difference in the entropy production $\delta \Delta_i S/(a\tau)$ vanishes in the macroscopic limit, when $\tau \to 0$.

Since the temporal change of the level-0 coarse-grained entropy is (by definition) unaltered by changes of the prescription for coarse graining,

$$\Delta^{(2)} S_m^{(0)} = S_m^{(0)''} - S_m^{(0)} = S_m^{(0)''} - S_m^{(0)'} + S_m^{(0)'} - S_m^{(0)}$$
$$= \Delta S_m^{(0)'} + \Delta S_m^{(0)}, \qquad (B20)$$

the entropy flux, i.e., the difference between the changes of the coarse-grained entropy and the irreversible entropy production, also takes the same macroscopic limit, regardless of the procedure for coarse graining.

Note that the calculations given in this Appendix can be generalized in a straightforward manner to account for averaging only after every n time steps on any finite level κ of the partitioning of the cells [42]. All these approaches differ only by terms that can be expressed as a product of τ and spatial derivatives of the macroscopic rate of irreversible entropy production. For larger n and κ, more and higher derivatives appear.

---

[1] J.R. Dorfman, *An Introduction to Chaos in Non-Equilibrium Statistical Mechanics* (Cambridge University Press, Cambridge, 1999).

[2] *Chaos and Irreversibility*, focus issue of Chaos **8**, 309 (1998).

[3] P. Gaspard, *Chaos, Scattering and Statistical Mechanics* (Cambridge University Press, Cambridge, 1998).

[4] D.J. Evans and G.P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic Press, London, 1990); W.G. Hoover, *Computational Statistical Mechanics* (Elsevier, Amsterdam, 1991).

[5] W.N. Vance, Phys. Rev. Lett. **69**, 1356 (1992).

[6] N.I. Chernov, G.L. Eyink, J.L. Lebowitz, and Ya.G. Sinai, Phys. Rev. Lett. **70**, 2209 (1993); Commun. Math. Phys. **154**, 569 (1993).

[7] D.J. Evans, E.G.D. Cohen, and G.P. Morriss, Phys. Rev. Lett. **71**, 2401 (1993).

[8] G. Gallavotti and E.G.D. Cohen, Phys. Rev. Lett. **74**, 2694 (1995); J. Stat. Phys. **80**, 931 (1995); G. Gallavotti, Phys. Rev. Lett. **77**, 4334 (1996); J. Stat. Phys. **86**, 907 (1997).

[9] E.G.D. Cohen, Physica A **213**, 293 (1995); **240**, 43 (1997).

[10] G.P. Morriss and L. Rondoni, J. Stat. Phys. **75**, 553 (1994); L. Rondoni and G.P. Morriss, Physica A **233**, 767 (1996); Phys. Rep. **290**, 173 (1997).

[11] N.I. Chernov and J.L. Lebowitz, Phys. Rev. Lett. **75**, 2831 (1995); J. Stat. Phys. **86**, 953 (1997); Ch. Dellago and H.A. Posch, *ibid.* **88**, 825 (1997).

[12] D. Ruelle, J. Stat. Phys. **85**, 1 (1996); **86**, 935 (1997).

[13] W. Breymann, T. Tél, and J. Vollmer, Phys. Rev. Lett. **77**, 2945 (1996).

[14] G. Nicolis and D. Daems, J. Chem. Phys. **1000**, 19 187 (1996); D. Daems and G. Nicolis, Phys. Rev. E **59**, 4000 (1999).

[15] P. Gaspard, Physica A **240**, 54 (1997); J. Stat. Phys. **88**, 1215 (1997).

[16] J. Vollmer, T. Tél, and W. Breymann, Phys. Rev. Lett. **79**, 2759 (1997).

[17] J. Vollmer, T. Tél, and W. Breymann, Phys. Rev. E **58**, 1672 (1998).

[18] W. Breymann, T. Tél, and J. Vollmer, Chaos **8**, 396 (1998).

[19] T. Gilbert, C.D. Ferguson, and J.R. Dorfman, Phys. Rev. E **59**, 364 (1999).

[20] T. Gilbert and J.R. Dorfman, J. Stat. Phys. **96**, 225 (1999).

[21] P. Gaspard, J. Stat. Phys. **68**, 673 (1992).

[22] S. Tasaki and P. Gaspard, J. Stat. Phys. **81**, 935 (1995).

[23] P. Gaspard and G. Nicolis, Phys. Rev. Lett. **65**, 1693 (1990); P. Gaspard and F. Baras, Phys. Rev. E **51**, 5332 (1995); J.R. Dorfman and P. Gaspard, *ibid.* **51**, 28 (1995); **52**, 3525 (1995); H. van Beijeren and J.R. Dorfman, Phys. Rev. Lett. **74**, 4412 (1995).

[24] T. Tél, J. Vollmer, and W. Breymann, Europhys. Lett. **35**, 659 (1996).

[25] R. Klages and J.R. Dorfman, Phys. Rev. Lett. **74**, 387 (1995); G. Radons, *ibid.* **77**, 4748 (1996).

[26] Z. Kaufmann, Phys. Rev. E **59**, 6552 (1999); Z. Kaufmann, A. Nemeth, and P. Szépfalusy, *ibid.* **61**, 2543 (2000); Z. Kaufmann and P. Szépfalusy, J. Stat. Phys. (to be published).

[27] J.L. Lebowitz and H. Spohn, J. Stat. Phys. **19**, 633 (1978); G. Casati, J. Ford, F. Vivaldi, and W.M. Visscher, Phys. Rev. Lett. **52**, 1861 (1984); L.A. Bunimovich and H. Spohn, Commun. Math. Phys. **176**, 661 (1996).

[28] A. Krámli, N. Simányi, and D. Szász, J. Stat. Phys. **46**, 303 (1984); S. Lepri, R. Livi, and A. Politi, Phys. Rev. Lett. **78**, 1896 (1997); H.A. Posch and Wm.G. Hoover, Phys. Rev. E **55**, 6803 (1997); D. Alonso, R. Artuso, G. Casati, and I. Guarneri, Phys. Rev. Lett. **82**, 1859 (1999); C. Wagner, R. Klages, and G. Nicolis, Phys. Rev. E **60**, 1401 (1999); K. Rateitschak, R. Klages and G. Nicolis, J. Stat. Phys. (to be published).

[29] D.J. Evans and P.T. Cummings, Mol. Phys. **72**, 893 (1991); S. Sarman and D.J. Evans, Phys. Rev. A **45**, 2370 (1992); G. Gallavotti, J. Stat. Phys. **84**, 899 (1996).

[30] L. Mátyás, T. Tél, and J. Vollmer, Phys. Rev. E **61**, R3295 (2000).

[31] S. Tasaki and P. Gaspard, Theor. Chem. Acc. **102**, 385 (1999).

[32] In kinetic theory the fields are related by the square of the momentum variable. Here we show that consistency with thermodynamics can be achieved without referring to this relation.

[33] S.R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (Elsevier, Amsterdam, 1962) (reprinted by Dover, New York, 1984).

[34] D. Landau and E.M. Lifshitz, *Electrodynamics of Continuous Media* (Pergamon Press, London 1960).

[35] I. Prigogine, *Non-Equilibrium Thermodynamics* (John Wiley & Sons, New York, 1961).

[36] D. Landau and E.M. Lifshitz, *Fluid Mechanics* (Pergamon Press, London, 1963).

[37] E. Ott, *Chaos in Dynamical Systems* (Cambridge University Press, Cambridge, 1993).

[38] We say that the particles represented by the multibaker interact weakly, since they are all mapped by the *same* map at every instant of time. There is only a possibility for an indirect, mean-field-type interaction due to the dependence of the parameters of the map on the local coarse-grained densities and their (discrete) gradients.

[39] F. Reif, *Fundamentals of Statistical and Thermal Physics* (McGraw-Hill, New York, 1965), Sec. 1.9.

[40] N.W. Ashcroft and N.D. Mermin, *Solid State Physics* (Holt, Rinehart and Winston, Saunders College, Philadelphia, 1976).

[41] A closer inspection reveals that the multibaker model mimics certain features of the Boltzmann equation approach in the relaxation-time approximation. There $v_{el} = eE\tau_{\mathrm{relax}}/m$, where m is the mass of the particles, and τ_{relax} stands for the relaxation time. This shows that the finiteness of the diffusion coefficient and the conductivity in our approach corresponds to the finiteness of the relaxation time in kinetic theory.

[42] An extension in this spirit for the case of thermostated systems with constant temperature can be found in [20].