Entropy Production for Open Dynamical Systems

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The concept of the conditional probability density is used to define a specific entropy for open dynamical systems exhibiting transient chaos. The production of entropy turns out to be proportional to the difference of the escape rate and the sum of all averaged Lyapunov exponents on the saddle governing the dynamics. The single-particle transport properties do not depend on the microscopic details provided the dynamical systems produce the same entropy. The dimension of the unstable foliation of the saddle is shown to be identical in all microscopic single-particle models of the same transport process. [S0031-9007(96)01271-9]

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Irreversible entropy production is a key concept in nonequilibrium thermodynamics [1]. Being the product of the generalized forces and the canonically conjugated fluxes, it is a measure of the decay to thermal equilibrium. In the regime of small perturbations the fluxes are linear functions of the forces, and the entropy production is weak. In the case of electric conductivity, for instance, the entropy production is proportional to the Joule heat, i.e., to field strength times current intensity.

Recent investigations have shown that transport processes can be understood in a *single-particle* picture by means of low-dimensional *chaotic* dynamics [2–9]. This also raises the question of how to define entropy production for classical chaotic dynamical systems.

One type of approach to chaotic transport [2–5] is working with *closed systems* in an external field constrained by periodic boundary conditions. An increase of the kinetic energy of the particle is compensated by introducing *dissipation* (a "Gaussian thermostat" [2]) to ensure energy conservation. This velocity dependent friction force simulates the interaction of the system with a heat bath, and leads to the appearance of a chaotic attractor. No dissipation is needed in another approach [6–9] based on *open Hamiltonian systems* of finite size, which allows for escape of the particles from the system. The escape models the coupling of the system to a particle reservoir. The rate κ describing the escape is directly related to the diffusion and drift coefficients [6,8] and other transport properties [9].

In closed thermostated systems a microscopic mechanism of entropy change was identified [4,5] with the contraction rate of the flow in the phase space, i.e., with the sum of all average Lyapunov exponents. The entropy was defined as the phase-space average of $-\ln \varrho_t(x)$, where, for any time t, the density $\varrho_t(x)$ is the microscopic probability to find the system around the phase-space point x. We will show that this concept of entropy change can be extended to open dynamical systems in a natural way. In such cases particles are allowed to escape to the environment, but can never return to the system. By phase space we understand in the following the phase space associated with the motion *inside* the system; i.e., we do not consider the dynamics of the environment. The support of any density in phase space is then *shrinking* due to escape. As a consequence, the escape rate κ plays the same role in open Hamiltonian systems as the rate of phase-space contraction in closed dissipative systems. Closed thermostated and open Hamiltonian systems are two extremes; we shall also deal with intermediate cases: open invertible systems subject to an external force and a thermostat.

We shall see below that the systems allow for reversible entropy currents into the environment. The change of the total entropy has a contribution due to this effect. The other contribution reflects the contraction of the phase-space volume. This latter term is related to irreversible entropy production caused by a finite resolution of any observation of a physical system. The fractal structure of the underlying invariant chaotic set is connected in both open and closed systems with the entropy production by the fact that it contains an infinite amount of information on arbitrary fine scales which cannot be extracted through any observation.

First we define an entropy and work out its time derivative. Let $\psi_t(x)$ denote a general phase-space density which will be explicitly specified below. It undergoes some time evolution, and we normalize ψ_t by keeping its integral over the phase-space unity. We define the *specific entropy* (i.e., entropy per particle) $s(t)$ at time t with respect to ψ as

$$s(t) = -\int \psi_t(x) \ln \psi_t(x)\, dx\,. \tag{1}$$

As time goes on, the support of ψ_t splits into an increasing number of strips in the phase space. In the course of this, a volume element around a point x is assumed to shrink exponentially like $\exp[-\sigma(x)t]$, where $\sigma(x)$ is a smooth function of the coordinates. The normalized density then increases like $\psi_{t+dt}(x) = \exp[\sigma(x)\,dt]\ \psi_t(x)\ \chi_{t+dt}(x)$, where χ_{t+dt} is the characteristic function of the support at time $t + dt$. The entropy $s(t + dt)$ at time $t + dt$ can be determined by inserting this into Eq. (1),

$$s(t + dt) = -dt \int \sigma(x)\psi_t(x)e^{\sigma(x)\,dt}\chi_{t+dt}(x)\,dx - \int \psi_t(x)\ln\psi_t(x)e^{\sigma(x)\,dt}\chi_{t+dt}(x)\,dx\,. \tag{2}$$

In both integrals the decrease of the support of ψ is counterbalanced by the factor $\exp[\sigma(x)\,dt]$ such that the first integral tends to the phase-space average $\bar{\sigma}$ of $\sigma(x)$ and the second one to the specific entropy $s(t)$ at time t. Hence, it follows that

$$\dot{s} = -\bar{\sigma}\,. \tag{3}$$

After a sufficiently long time, $\dot{s}$ approaches a constant, namely, the average rate $-\bar{\sigma}$ of the phase-space contraction taken with respect to the density ψ.

In closed dissipative systems with cyclic boundary conditions the entropy is defined with respect to the natural density ϱ [4,5], i.e., $\psi = \varrho$. Under time evolution the dissipation causes the density to concentrate more and more around a chaotic attractor. Because of the boundary condition the chaotic attractor forms a complicated manifold on a torus, and transport is due to the motion along the unstable manifold of the attractor. After a sufficiently long time the density will concentrate in narrow bands along the attractor, and the contraction rate is given by the sum of the local expansion rates (local Lyapunov exponents, cf. [10]), $\zeta(x) \equiv -\sum_i \lambda_i(x)$; thus, $\sigma = \zeta$. The averages have to be taken with respect to the natural density, and we recover $\dot{s} = \sum_i \bar{\lambda}_i$: after a sufficiently long time, the time derivative of the specific entropy is the sum of the average Lyapunov exponents on the *attractor* [5]. This sum is negative due to dissipation.

Turning now to open systems, we consider a broad class of systems, called *hyperbolic*, for which the escaping process is exponential [10]. When an ensemble of N_0 particles is distributed initially in the whole phase space, the number $N(t)$ of particles still staying inside the system after a sufficiently long time t decays as $N(t) = N_0\exp(-\kappa t)$, where the constant κ is the escape rate of the system. Particles escape from the phase space along the *unstable foliation* of an invariant chaotic saddle governing transport and diffusion in the system [6,8]. One can define the *conditional* density $\tilde{\varrho}_t(x)$ at time t to be the probability that a particle is around x under the condition that it has not yet escaped from the system. Thus, $\int \tilde{\varrho}_t(x)\,dx$ is constant. As time goes on, the density $\tilde{\varrho}_t(x)$ concentrates more and more around the unstable manifold. In the limit $t \to \infty$ the density $\tilde{\varrho}_t(x)$ approaches a *stationary* distribution stabilized along the unstable manifold, namely, the *conditionally invariant measure* [11] of the open system.

In the spirit of these arguments it is natural to consider the specific entropy for those particles that *have not yet escaped* by time t. To that end we define the entropy s in (1) with respect to the conditional density, i.e., with $\psi = \tilde{\varrho}$.

In *open Hamiltonian* systems there is no phase-space contraction due to dissipation. The support of the conditional density, however, shrinks because of the escape of particles through the open boundaries. Under time evolution a typical initial density $\tilde{\varrho}_0(x)$ concentrates in narrow bands along the unstable manifold inside the phase space: its support shrinks after a long time t by a factor $\exp(-\kappa t)$, and the conditional density increases as $\exp(\kappa t)$. Consequently, the rate σ in Eq. (2) tends to the escape rate κ, and from the general relation (3) we obtain $\dot{s} = -\kappa$. No phase-space average appears in this case since κ is independent of the coordinates. For long times, $\dot{s}$ approaches a constant, which is nothing but the negative escape rate.

In *open dissipative* systems, both mechanisms mentioned above are present: phase-space contraction and escape. Because of the latter, the natural density does not remain normalized. Therefore, we have to consider again the specific entropy taken with respect to the conditional density: $\psi = \tilde{\varrho}$. Thus, the phase-space contraction consists of two terms: a contraction with rate $\zeta(x) \equiv -\sum_i \lambda_i(x)$ due to dissipation, and an additional term with rate κ due to normalizing $\tilde{\varrho}$ in order to compensate escape. The asymptotic mean contraction rate is thus $\bar{\sigma} = \bar{\zeta} + \kappa$. Accordingly, Eq. (3) implies that

$$\dot{s} = \sum_i \bar{\lambda}_i - \kappa\,. \tag{4}$$

Here, the $\bar{\lambda}_i$ denote the average Lyapunov exponents on the *chaotic saddle.* They have to be computed by means of the conditionally invariant measure [11,12]. The equation can be shown to be valid for discrete-time dynamical systems (i.e., mappings), too, with all quantities measured in the time units of the map.

Equation (4) is our central result. We find two mechanisms changing the specific entropy: dissipation and escape. In both closed and open dynamical systems the decrease of the specific entropy is due to the fact that during time evolution the particles staying inside the system become more and more localized along the unstable manifold.

In order to connect the decrease of specific entropy with more conventional concepts, let us consider the entropy $S(t)$ of *all* the particles staying in the phase space: $S(t) = N(t)s(t)$ where $s(t)$ is taken with respect to the conditional density, and $N(t) = N_0\exp(-\kappa t)$. For simplicity, we assume that the rate of contraction of phase-space volume is constant, and that the initial distribution $\tilde{\varrho}_0 \equiv 1$ in the phase space. Then, the conditional density increases in time as $\tilde{\varrho}_t = 1/\Gamma(t)$ where $\Gamma(t) = \exp(\sigma t)$ and $\sigma = \kappa - \sum_i \bar{\lambda}_i$. Consequently, $S(t) = N(t)\ln\Gamma(t)$, and we can write the time derivative of the total entropy as

$$\dot{S} = \frac{\partial S}{\partial N}\dot{N} + \frac{\partial S}{\partial \Gamma}\dot{\Gamma} = -\kappa S - \sigma N . \qquad (5)$$

The first term, $-\kappa S$, corresponds to the entropy flow out of the system due to escape. The more interesting second term is due to the contraction of phase-space volume. The time derivative of the specific entropy $d(S/N)/dt \equiv \dot{s} = -\sigma$ contains only this contribution.

We now discuss *irreversible* entropy production that arises by taking into consideration the effect of coarse graining. There is always a smallest scale of resolution $\epsilon \ll 1$ for the observer. Let us define a coarse grained specific entropy $s_{\mathrm{cg}}(t)$ with the conditional density washed out on a grid of resolution ϵ. When starting with a smooth initial distribution, this coarse grained entropy will initially coincide with s (up to an error of order ϵ). Sooner or later, however, the fine filamentation of the support of the phase-space density reaches the resolution scale. From this time on, $s_{\mathrm{cg}}(t)$ will be nearly constant; in the limit $t \to \infty$ it tends to a stationary value which is determined by the coarse grained conditionally invariant measure. On the other hand, $s(t)$ continues to decrease linearly in time [cf. Eq. (4)]. Thus, $s_{\mathrm{cg}}(t) - s(t)$ is a measure of the lack of information caused by the unavoidable finite resolution. Its change in time can be considered to be the irreversible specific entropy production $\dot{s}_{\mathrm{irr}}$. Since the coarse grained entropy s_{cg} becomes stationary for large t, $\dot{s}_{\mathrm{irr}}$ tends towards $-\dot{s}$, and for $t \to \infty$

$$\dot{s}_{\mathrm{irr}} = -\dot{s} = \bar{\sigma} = -\sum_i \bar{\lambda}_i + \kappa > 0 . \qquad (6)$$

The sources of irreversible entropy given in Eq. (6) are additive. They correspond to the contact with different types of surroundings: the term $-\sum_i \bar{\lambda}_i$ is due to the interaction with a heat bath, while κ is due to the coupling with a particle reservoir. In order to see the consistency of Eq. (6) with classical results, we mention that for one-particle open Hamiltonian systems of linear size L compatible with a Fokker-Planck description, the escape rate is [8] $\kappa = j^2/(2D) + O(L^{-2})$. Here, j is the particle current and D the diffusion coefficient. Thus, for large systems, $\dot{s}_{\mathrm{irr}} = j^2/(2D)$ in accordance with linear irreversible thermodynamics [1].

An important consequence of the concepts exposed above is that different single-particle microscopic pictures (closed and dissipative, open and Hamiltonian, or open and dissipative) used to model relaxation mechanisms for a given physical situation might lead to identical transport (e.g., diffusion) coefficients. The condition for this is that, at a fixed current, the irreversible entropy production per particle

$$\kappa - \sum_i \bar{\lambda}_i = \text{const} \qquad (7)$$

is the same in the large system limit. We shall see below that these models also share certain fractal properties.

The irreversible specific entropy production $\dot{s}$ is also related to the Kolmogorov-Sinai (KS) entropy h_{KS} [10]. The latter can be expressed in invertible systems by means of the chaotic saddle's characteristics [12]

$$h_{\mathrm{KS}} = \sum_{\lambda_i>0} \bar{\lambda}_i D_1^{(i)} = -\sum_{\lambda_i<0} \bar{\lambda}_i D_1^{(i)} = \sum_{\lambda_i>0} \bar{\lambda}_i - \kappa , \qquad (8)$$

where $D_1^{(i)}$ stands for the partial information dimension of the saddle along direction i (note that the sum of the partial information dimensions yields the information dimension of the saddle: $\sum_i D_1^{(i)} = D_1$). Inserting Eq. (8) into Eq. (6) one obtains

$$\dot{s} = \sum_{\lambda_i<0} \bar{\lambda}_i + h_{\mathrm{KS}} . \qquad (9)$$

This formula, too, is valid for *both* Hamiltonian and dissipative systems. The first term is the decrease of the entropy due to the convergence towards the invariant set, the second is the increase of the entropy due to the chaos of the dynamics. Because the negative Lyapunov exponents are typically of the order of unity in modulus, the formula also means that a *weak* entropy production typically requires the dynamics of the subsystem to be *strongly* chaotic: h_{KS} should be of the same order as the sum of the negative Lyapunov exponents. The general expressions (8) imply that the irreversible specific entropy production $-\dot{s}$ is the *escape rate of the time reversed dynamics.*

We turn now to the question of how the fractal properties of the unstable manifold of the underlying invariant sets are connected with the specific entropy production. To this end, we consider a single particle dynamics with a three-dimensional phase space. On a Poincaré map, i.e., on a plane transverse to the flow, the chaotic saddle is the direct product of two Cantor sets with partial dimensions [10,12] $D_1^{(u)} = 1 - \kappa/\bar{\lambda}_1$ and $D_1^{(s)} = -D_1^{(u)}\bar{\lambda}_1/\bar{\lambda}_2$, along the unstable and stable directions, respectively; $\bar{\lambda}_1 > 0$ and $\bar{\lambda}_2 < 0$ are the two average Lyapunov exponents of the map on the chaotic saddle. The unstable manifold is the direct product of the Cantor set along the stable direction and a line [13]. Given that in the flow the invariant manifolds have an additional smooth direction, the information dimension of the full unstable manifold can be expressed as

$$D_1 = 2 + D_1^{(s)} = 3 - \frac{\kappa - (\bar{\lambda}_1 + \bar{\lambda}_2)}{|\bar{\lambda}_2|} . \qquad (10)$$

Note that the numerator of the quantity subtracted from 3 is just the irreversible entropy production, i.e.,

$$D_1 = 3 - |\dot{s}|/|\bar{\lambda}_2| \approx 3 - |\dot{s}|/\bar{\lambda}_{1,0} , \qquad (11)$$

where $\bar{\lambda}_{1,0}$ is the positive Lyapunov exponent in the closed Hamiltonian system limit. The approximate equality holds if the entropy production is small relative to $|\bar{\lambda}_2|$, i.e., if the system is sufficiently close to thermal equilibrium and therefore $|\bar{\lambda}_2|$ can be replaced by $|\bar{\lambda}_{2,0}| = \lambda_{1,0}$. Rearranging Eq. (11) we obtain

$$|\dot{s}| = (1 - D_1^{(s)})\,|\bar{\lambda}_2| \approx (1 - D_1^{(s)})\,\bar{\lambda}_{1,0}\,. \qquad (12)$$

This states that the irreversible specific entropy production is proportional to the deviation from unity of the partial information dimension of the stable manifold.

In conclusion, we have shown how the concept of entropy production can be understood in the framework of open dynamical systems. Since the present approach does not make use of the concept of temperature, it avoids problems which might arise in a single-particle picture (cf. [5]). It unifies previous approaches based on the escape-rate formalism and on thermostated systems with an external thermostat. The essential effect leading to entropy production is the contraction of the phase-space volume in an ever refining fractal manner. We pointed out that the specific entropy defined with respect to the conditional density in the phase space is an appropriate tool for characterizing the increase of information connected with this effect. Because of a finite resolution, the refinement of the phase-space structure cannot be followed forever. Using the convergence of the coarse grained density to a stationary one, we showed that in dynamical systems the irreversible entropy production caused by the lack of information due to coarse graining is given by the difference of two terms: the escape rate from the system, which characterizes the contact with a particle reservoir, and the sum of all average Lyapunov exponents, which measures the strength of dissipation.

We close with a remark concerning the relation with stationary nonequilibrium ensembles recently proposed for thermostated systems [14–17]. They provide a basis for solving the so-called paradox of irreversibility. The present connection between the thermostated approach for closed systems and the Hamiltonian approach for open systems based on the concept of conditional density contributes to establish a class of stationary nonequilibrium ensembles for Hamiltonian systems. The latter can be considered as an ensemble with constant energy in contact with a particle reservoir, while the thermostated approach [17] is the analog of the canonical ensemble.

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Note added.—After submitting this paper, we became aware of independent work of Ruelle [18] who rigorously proves that for axiom A systems the contraction of phase-space volume is given by the right-hand side of Eq. (4). However, he does not discuss the role of coarse graining to identify its relation to irreversible entropy production.

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