Coarse-grained entropy and information dimension of dynamical systems: The driven Lorentz gas

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We study the resolution dependence of the steady-state saturation values of coarse-grained entropies characterizing general dynamical systems. For dissipative maps they are proportional to the information codimension of the chaotic attractor. Thus, they provide a highly accurate method for determining the information dimension and related characteristics of the dynamical system. This general result is demonstrated for the field-driven Lorentz gas. In the discussion, we take the results on the resolution dependence of the entropy as the starting point to revisit different approaches to define thermodynamic entropy production for transport processes in dynamical systems, and discuss the role of local equilibrium in this enterprise.

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I. INTRODUCTION

The heart of irreversible thermodynamics [1] is to setup an entropy balance for the thermodynamic entropy S [2]. This balance is commonly written in the form

$$\frac{dS(t)}{dt} = \Phi(t) + \Sigma^{(irr)}(t). \tag{1}$$

The temporal change of the entropy is written here as the sum of an external change $\Phi(t)$ and an internal (or *irreversible*) change of entropy $\Sigma^{(irr)}(t)$. The former accounts for an entropy flux Φ out of the considered volume. The latter is due to irreversible entropy production. $\Sigma^{(irr)}$ is nonnegative, while Φ can have any sign. Earlier results [3,4] show that a relation in the form of Eq. (1) can also be found in deterministic systems if a suitably chosen *coarse-grained entropy* is considered. In this paper we study properties of this coarse-grained entropy and show that its steady-state saturation value scales with the linear size of the applied coarse graining. In dissipative maps the saturation value is found to be proportional to the information codimension of the chaotic attractor.

In Sec. II we define the coarse-grained entropy of a general dynamical system and present its most important properties: the tendency to converge to a saturation value and the relation of this value to the information dimension of the chaotic invariant set. In Sec. III the field-driven Lorentz gas is presented as well as the numerical results obtained for the time evolution of the coarse-grained entropy. The saturation value provides a highly accurate method of determining the information dimension, even in systems where the invariant measures only minutely deviate from a smooth distribution. Section IV concludes the paper by taking up recent discussions on analogies of local equilibrium in dynamical-system models for transport.

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II. COARSE-GRAINED ENTROPIES FOR DYNAMICAL SYSTEMS

We treat *invertible* dissipative dynamical systems [5,6] with a closed d-dimensional phase space. The long-time dynamics is then associated with a chaotic attractor [5,6], i.e., with a *fractal* phase-space structure which has no volume with respect to the Liouville measure. The set of average Lyapunov exponents characterizing the associated invariant set will be denoted by $\overline{\lambda}_1 \geqslant \overline{\lambda}_2 \geqslant \cdots \geqslant \overline{\lambda}_d$, and the location dependent eigenvalues of the linearized dynamics are accordingly $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_d$. A key ingredient of dynamical-system models for irreversible processes are ever refining phase-space structures related to the convergence towards a fractal measure. It is impossible to describe the asymptotic states by smooth stationary densities in phase space. Instead, we consider a *coarse-grained* description that approximates the ever refining structures in phase space with a finite resolution. Comparing the time evolution in this coarse-grained description with the exact one gives insight in the dynamics. For illustrational purposes, we confine ourselves to discuss only the simplest possible coarse graining. It consists in dividing the adimensionalized phase space into identical boxes of linear size ε much smaller than unity ($\varepsilon \ll 1$). The phase-space volume of the boxes is then ε^d.

A. Exact and coarse-grained densities

We use two different phase-space densities [4] characterizing the evolution of the same smooth initial condition: (1) $\varrho(x,t)$, the *exact phase-space density* at phase-space location x and time t, (2) $\varrho_\varepsilon(i,t)$, the *coarse-grained density* of box i at time t, specifying the average value of $\varrho(x,t)$ in box i. The density $\varrho(x,t)$ is normalized to unity $\int dx \varrho(x,t) = 1$, on the phase space accessible to the system, and accordingly $\Sigma_i \varrho_\varepsilon \varepsilon^d = 1$ for the coarse-grained density. The averaging on the set of boxes defines the coarse graining.

After a long time there is a qualitative difference between the exact and the coarse-grained densities: the exact density keeps developing finer and finer structures and has no time-independent limit. It becomes undefined as a density such

that the asymptotic distribution can only be described by a natural invariant measure μ [5]. On the other hand, the coarse-grained density converges to a (piecewise constant) *stationary distribution* $\overline{\varrho}_\varepsilon(i)$, such that the measure $\mu_i(\varepsilon)$ of box i equals $\overline{\varrho}_\varepsilon(i)\varepsilon^d$. For points x on the attractor of the dynamical system the asymptotic temporal dependence of $\varrho(x,t)$ can be written, in the spirit of large deviation theorems, as

$$\varrho(x,t)\sim e^{\sigma(x)t}, \tag{2a}$$

while

$$\varrho_\varepsilon(i,t)\sim\overline{\varrho}_\varepsilon(i). \tag{2b}$$

Here $\sigma(x)$ is the local phase-space contraction rate [7–9] at point x. Equation (2a) follows from the fact that the phase-space volume around x is behaving like $\exp[-\sigma(x)t]$ and the measure of a given volume is not changing in time due to the conservation of probability. The phase-space contraction rate is the negative sum of all local eigenvalues [7]

$$\sigma(x)=-\sum_{j=1}^{d}\lambda_j(x). \tag{3}$$

The emergence of differences between the coarse-grained and the exact density depends on the type of initial conditions. In what follows we always consider smooth initial conditions. The difference between the densities is then initially on the order of the box size ε, and therefore negligible for sufficiently small ε. Strong deviations develop after a crossover time t_ε, after which the contraction due to the negative Lyapunov exponents makes the support of the density in the stable direction of the same order as the box size. An upper limit to this time scale is

$$t_\varepsilon\approx-\frac{1}{|\overline{\lambda}_-|}\ln\varepsilon, \tag{4}$$

where $\overline{\lambda}_-$ is the largest negative average Lyapunov exponent (the smallest one in modulus). For typical dynamical systems this Lyapunov exponent is of the order unity in a dimensionless description. Thus, the crossover time is on the order of the characteristic time (iteration unit) of the dynamical system. It depends only logarithmically on the box size.

The qualitative difference between the behavior of the exact and the coarse-grained densities [cf. Fig. (2a) and (2b)] is a *hallmark of irreversibility*. Every macroscopic description of transport is based on coarse-grained densities, i.e., (coarse-grained) averages of smoothly varying functions in phase-spacelike particle numbers or the (kinetic) energy [10]. Hence, such a description, even if applied to dynamical systems, cannot resolve *all* information on the fine details of the system's phase-space dynamics.

B. Gibbs and coarse-grained entropies

A natural choice for the entropy characterizing the state of a general dynamical system at time t is the information-theoretic entropy taken with respect to a phase-space density at that time. Since we consider the time evolution of the exact and the coarse-grained densities, two entropies are defined: (1) The entropy $S^{(G)}$ evaluated with respect to the exact density

$$S^{(G)}(t)\equiv-\int d^dx\,\varrho(x,t)\ln\left(\frac{\varrho(x,t)}{\varrho^*}\right), \tag{5a}$$

where ϱ^* is a constant reference density. $S^{(G)}$ is commonly referred to as the *Gibbs entropy*. (2) The coarse-grained entropy S_ε is defined in an analogous way as a sum over boxes of size ε

$$S_\varepsilon(t)\equiv-\sum_i\varrho_\varepsilon(i,t)\varepsilon^d\ln\left(\frac{\varrho_\varepsilon(i,t)}{\varrho^*}\right). \tag{5b}$$

The notation S_ε expresses that the coarse-grained entropy explicitly depends on the box size ε.

In the choice of the normalization ϱ^* of the density under the logarithms we follow Green [11], even though other choices have also been adopted recently (cf. for instance, Ref. [8]). The expressions for differences of the *same* entropy evaluated at different times agree, however, for all these choices. For convenience we identify the reference density ϱ^* with the average density in the system. This amounts to a choice of the entropy scale where the entropies vanish for a uniform density distribution in phase space, i.e., for $\varrho(x,t)\equiv\varrho_\varepsilon(i,t)\equiv\varrho^*$.

The entropies (5) are defined irrespective of the notion of local thermodynamic equilibrium. In Eq. (12) even the splitting (1) of the entropy changes into a ''flux'' and an ''irreversible'' part is done without referring to that notion. The relation of the formal splitting of the entropy to concepts of irreversible thermodynamics will be addressed in the discussion.

The time evolution of the entropies immediately follows from that of the densities. For smooth initial conditions, $S^{(G)}$ and S_ε nearly coincide until the crossover time t_ε is reached. Typically, they both decrease since the distributions start approaching the one on the invariant set and hence the information content is increasing. This tendency does not change for $S^{(G)}$, which keeps decreasing after t_ε. Based on Eqs. (5a) and (2a) one immediately verifies that $S^{(G)}=-\sigma(t)\,t+\text{const}$, where $\sigma(t)$ is the average of the phase-space contraction rate [defined by Eq. (2a)] taken with $\varrho(x,t)$ at time t. The asymptotic behavior is a linear decay

$$S^{(G)}\to-\overline{\sigma}t \tag{6}$$

with $\overline{\sigma}$ as the long-time average of the phase-space contraction rate taken with respect to the natural invariant measure.

The coarse-grained entropy, on the other hand, levels off around t_ε, since with the given resolution the invariant set does not change any longer after this time. Asymptotically, the coarse-grained entropy tends to the constant value $\overline{S_\varepsilon}$ (see Fig. 1), which depends on the box size but is *independent* of the initial condition

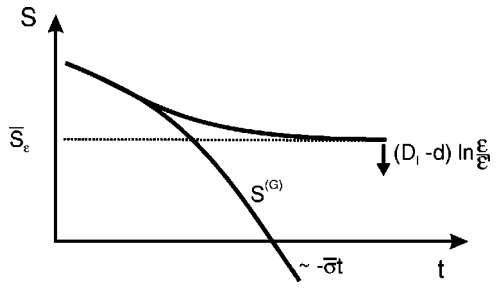

FIG. 1. Time evolution of the Gibbs entropy $S^{(G)}$ and the coarse-grained entropy S_ε in d-dimensional dissipative systems relaxing towards a steady state described by a chaotic attractor. ε denotes the coarse-graining grid size and $\overline{S_\varepsilon}$ stands for the steady-state coarse-grained entropy. The arrow represents the shift of the coarse-grained entropy curve when changing the resolution from ε to $\varepsilon' < \varepsilon$, and D_I stands for the information dimension of the attractor.

$$S_\varepsilon(t) \to \overline{S_\varepsilon}. \tag{7}$$

The saturation expresses the convergence of the coarse-grained density to a stationary value.

It is worth briefly discussing the dependence of the entropy on the resolution ε. To this end, we rewrite the coarse-grained entropy (5b) in the form

$$S_\varepsilon(t) = -\sum_i \varrho_\varepsilon(i,t)\varepsilon^d \ln\frac{\varrho_\varepsilon(i,t)}{\varrho^*} = -\sum_i \varrho_\varepsilon(i,t)\varepsilon^d \ln\frac{\varrho_\varepsilon(i,t)\varepsilon^d}{\varrho^*\varepsilon^d}. \tag{8}$$

The measure of the full phase space is, by definition, unity. For a partitioning of this domain in cells of linear size ε the product $\varrho^*\varepsilon^d$ is the average measure of the boxes. It is an increasing function of the linear size ε (ϱ^* does not depend on ε). The measure of a given box i at the time instant t is denoted by $\mu_\varepsilon(i,t) = \varrho_\varepsilon(i,t)\varepsilon^d$. The corresponding average measure of the boxes is $\overline{\mu_\varepsilon} \equiv \varrho^*\varepsilon^d$. Using these notations, one obtains for the coarse-grained entropy

$$S_\varepsilon(t) = -\sum_i \mu_\varepsilon(i,t)\ln\frac{\mu_\varepsilon(i,t)}{\overline{\mu_\varepsilon}}. \tag{9}$$

The ε dependence of the asymptotic ($t \to \infty$) coarse-grained entropy can be expressed by a number: the information dimension D_I of the coarse-grained steady-state distribution, i.e., the dimension of the natural invariant measure $\overline{\mu}$ on the attractor. This quantity has been introduced in the context of the multifractal characterization of chaotic attractors, and of other fractal distributions [12–14]. For every stationary measure characterized by boxes of very small (but finite) linear size ε, which carry probabilities $\mu_\varepsilon(i)$, the information dimension is defined by the relation $-\Sigma_i \mu_\varepsilon(i)\ln\mu_\varepsilon(i) \sim -D_I \ln\varepsilon$ for $\varepsilon \ll 1$. In view of this, the dependence of $\overline{S_\varepsilon}$ on ε for fine enough resolutions is

$$\overline{S_\varepsilon} = (d - D_I)\ln\varepsilon. \tag{10}$$

Refining the box size from ε to $\varepsilon' < \varepsilon$ the saturation value is shifted downward by $(d - D_I)\ln(\varepsilon/\varepsilon')$ (Fig. 1). This shift is proportional to the codimension $(d - D_I)$. At the same time the initial value of the entropy characterizing the uniform initial condition is unchanged (it remains zero). Consequently, for a higher resolution (smaller ε) the steady-state distribution will be reached at later times, as already stated by Eq. (4).

Finally, we point out that even for general dynamical systems there is an analog of the thermodynamical relation (1). Since the difference $S_\varepsilon(t) - S^{(G)}(t)$ between the coarse-grained and the Gibbs entropy measures the loss of information on the exact state, one can identify [4,15,16] the time derivative

$$\Sigma_\varepsilon^{(irr)}(t) \equiv \frac{d}{dt}[S_\varepsilon(t) - S^{(G)}(t)] \tag{11}$$

with the rate of irreversible entropy production of the dynamical system due to a coarse graining with resolution ε. The dependence of $\Sigma_\varepsilon^{(irr)}$ on ε is weak, and it disappears latest upon reaching the steady state of the coarse-grained entropy. By writing $S_\varepsilon = S^{(G)} + (S_\varepsilon - S^{(G)})$ and taking the time derivative, we obtain in view of Eq. (11)

$$\frac{dS_\varepsilon(t)}{dt} = \Phi(t) + \Sigma_\varepsilon^{(irr)}(t), \tag{12}$$

where the entropy flux is $\Phi(t) \equiv dS^{(G)}/dt$. By this an entropy balance [cf. Eq. (1)] has been established for dynamical systems. It is based on a simultaneous knowledge of both the coarse-grained and the Gibbs entropies. By considering only one of them, no balance equation can be derived with a meaningful distinction of flux and entropy production.

In a general investigation of the entropy of nonequilibrium steady states, Evans and Rondoni [17] came to similar conclusions based on a different form of coarse graining. They considered the Gibbs entropy for a many particle system. For noninteracting particles it diverges in a nonequilibrium steady state, while otherwise the lower-order terms ($n = 1,2,3$) of a perturbation series involving n body terms converge in time towards a finite value, which according to these authors might be related to the thermodynamic entropy. Interpreting the truncated expansion as a coarse-grained entropy, one observed then that also in this setting the entropies for systems subjected to an electric field are very close to the one characterizing the field-free case.

III. THE FIELD-DRIVEN LORENTZ GAS

A. The Lorentz gas dynamics

In this section the above considerations are explicitly worked out for the field-driven Lorentz gas, i.e., for a billiard, where particles are scattered elastically from a periodic array of circular scatterers (Fig. 2). To avoid technical difficulties arising from trajectories which travel infinitely far between collisions (i.e., moving in an array of scatters with

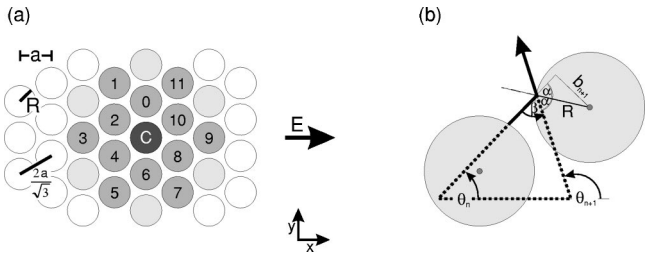

FIG. 2. Dynamics of the Lorentz gas. (a) Arrangement of the scatters on a triangular lattice; a denotes the lattice spacing, R the radius of scatterers, and E an external field parallel to the x axis. The numbers $0,\ldots,11$ inside the scatterers denote the values of the symbols s of those disks which can be hit immediately after leaving the one in the center. For $E\neq 0$, in addition to these also the light shaded disks can be reached. (b) The dependence of b_{n+1} on θ_n. The center of the scatterer is indicated by gray bullets; all other symbols are explained in the text.

an *infinite horizon*) we choose a triangular arrangement of scatterers and fix the lattice constant a to be twice the radius of the scatterers $R=a/2$. In other words we fix a to the largest value where the horizon is finite. Moreover, we set the mass of the particle to be one and use $R\equiv 1$ as length.

The motion of particles in response to an applied external field E has extensively been discussed for the Lorentz gas. In order to avoid an unbounded growth of the energy, the system is typically subjected to a thermostat fixing the energy, which can for instance be achieved by means of a Lagrange multiplier. The dimensionless equations of motion are in that case

$$\dot{x}=p_x, \tag{13a}$$

$$\dot{y}=p_y, \tag{13b}$$

$$\dot{p}_x=E-\zeta p_x, \tag{13c}$$

$$\dot{p}_y=-\zeta p_y, \tag{13d}$$

where $\zeta=Ep_x$ assures conservation of kinetic energy $\partial_t p^2=0$. Since the momentum p of the particles does not change its modulus during the motion its value can also taken to be unity.

The equations (13) describe the trajectory segments in between collisions. Since they can be solved in closed analytic form [18], it is sufficient to follow the time evolution only by specifying the new initial conditions after each collision [19]. The coordinates of the mapping are a position and a conjugate quantity, and it is convenient to specify the latter in terms of the the angular momentum b of the trajectory with respect to the scatterer hit at the last collision (since the momentum is set to one, b is the impact parameter at the collision) and the angle θ of the trajectory with the y axis (cf. Fig. 2b). We specify the scatterer hit in collision $n+1$ by $s_n=0,\ldots,11$ [cf. Fig. 2(a)].

The impact parameter, and hence also the angular momentum measured with respect to the center of the respective disk, is preserved in a collision. Moreover, observing that

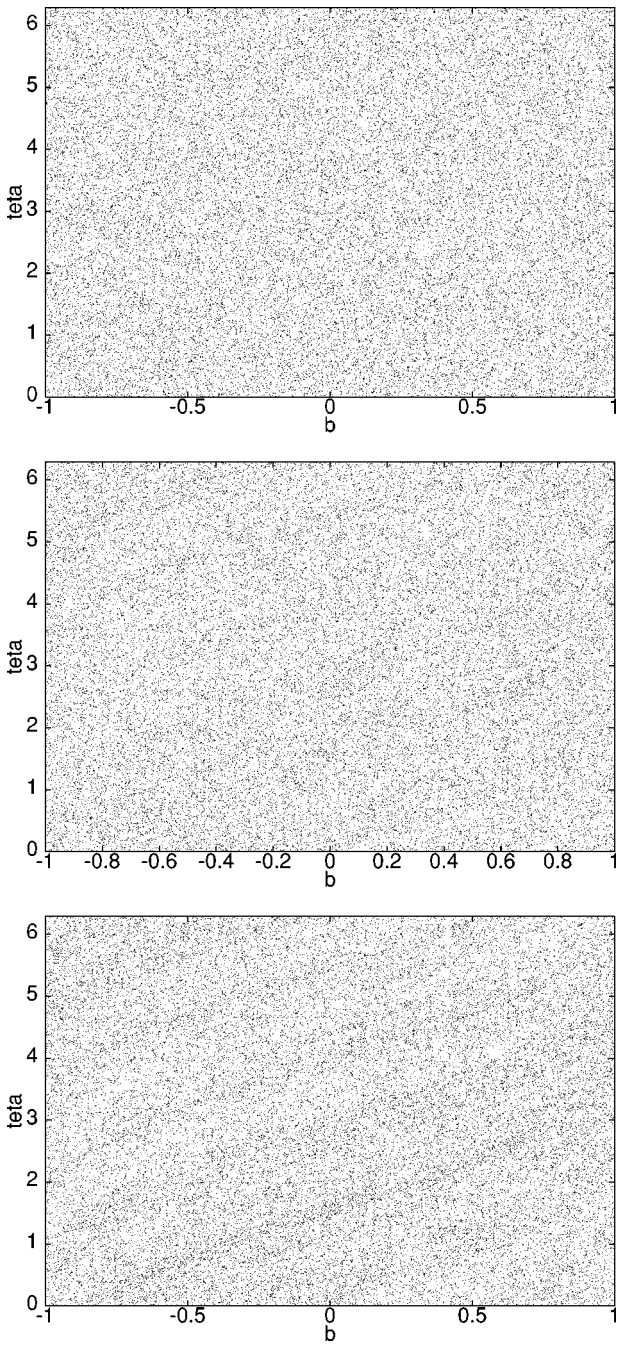

FIG. 3. Chaotic sets of the Lorentz gas for (a) $E=0$, (b) $E=0.1$, and (c) $E=0.2$ ($p=1$, $R=1$). The dots in the figures give an impression on the respective invariant densities by showing about 50 000 iterations of the initial condition $(b,\theta)=(0,0.1457\pi)$.

$\sin\alpha=b_{n+1}$ and $\beta=\pi-2\alpha$, as well as elementary trigonometry (cf. Fig. 2), one immediately finds for the angle θ_{n+1},

$$\theta_{n+1}=\theta_n+\pi+2\arcsin b_{n+1}. \tag{14}$$

By definition $b\in[-1,1]$ and θ can be taken in $[0,2\pi]$ such that the resulting mapping $\mathcal{M}$ defining the time evolution is defined on the *fundamental domain* $[-1,1]\times[0,2\pi]$. It is periodic in its coordinate θ and remains one-to-one on its domain (cf. Fig. 3) as long as the field is not very strong ($E<2.2$) [20].

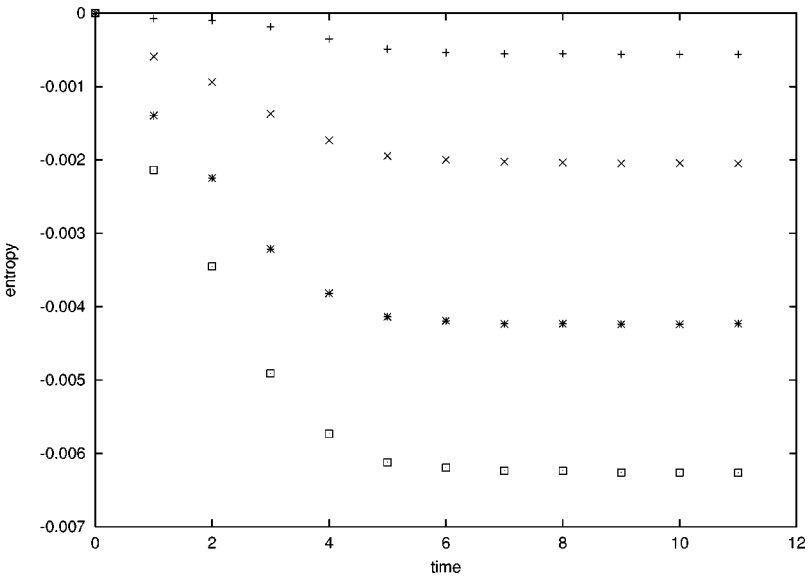

FIG. 4. The time dependence of the coarse-grained entropy for different electric fields: $E=0.00$ (+), 0.05 (×), 0.08 (*), and 0.10 (□). The horizontal time axis marks the number of collisions n. The nonvanishing asymptotic value of the coarse-grained entropy for $E=0$ is caused by fluctuations due to the finite number of points used in simulations.

B. Numerical integration of evolution equations

For numerical studies Eqs. (13) are solved by a fourth order Runge-Kutta method [21] (RK4), with periodic boundary conditions based on a unit cell containing (in the notation of Fig. 2) the area between the central disk C and the disks labeled by 6, 8, and 10.

At a field $E=0.1$ the average momentum in the direction of the external field is found to be $\overline{p_x}=0.025\pm0.001$. Since $\overline{\sigma}=\overline{\zeta}=E\,\overline{p_x}$ (remember $p^2=1$), the average phase-space contraction is

$$\overline{\sigma}(E=0.1)=\overline{\zeta}(E=0.1)=(2.5\pm0.1)\times10^{-3}. \qquad (15)$$

Comparing the divergence of closeby trajectories one finds for the largest Lyapunov exponent of the Lorentz gas at $E=0.1$ that $\overline{\lambda_1}=1.73\pm0.02$. Combining this result with Eq. (15) allows us to calculate the fractal dimension of the attractor in phase space. To this end we write the Kaplan-Yorke formula $D_I=1-\overline{\lambda_1}/\overline{\lambda_2}$ for the information dimension D_I as

$$D_I=2-\frac{\overline{\lambda_1}+\overline{\lambda_2}}{\overline{\lambda_2}}=2-\frac{\overline{\sigma}}{\overline{\lambda_2}}, \qquad (16)$$

where the average phase-space contraction rate is $\overline{\sigma}=-\overline{\lambda_1}-\overline{\lambda_2}$. For an external field $E=0.1$ we thus obtain for the codimension

$$2-D_I(E=0.1)=\frac{\overline{\sigma}}{\overline{\sigma}+\overline{\lambda_1}}=(1.44\pm0.07)\times10^{-3}. \qquad (17)$$

This value is of the same order of magnitude as the one obtained by Dellago *et al.* [22] by means of a completely different method, for a slightly different geometry and field strength.

C. Information codimensions

According to Eq. 10 the information codimension can also be calculated based on the resolution (i.e., ε) dependence of the levels of saturation of the coarse-grained entropy S_ε. Using Eq. (9), this entropy is calculated by partitioning the fundamental domain ($[-R,R]\times[0,2\,\pi]$) into boxes of size $\varepsilon\times\varepsilon$ and estimating the respective measures of the boxes as the ratio of the number of points found in box i (at time t), and the total number of points [23]. Choosing for instance a partitioning of 2^6 parts in both the vertical and the horizontal direction, one considers $2^{11}\times2^{11}$ uniformly spread initial conditions in such a way that in every box there is a number of $2^5\times2^5$ starting points. These points mimic a uniform initial density, where the average measure of each cell is $\mu_\varepsilon=1/(\text{number of boxes})=1/(2^6\times2^6)$. The initial measure $\mu_\varepsilon(i,t=0)$ coincides with $\overline{\mu_\varepsilon}$ such that $S_\varepsilon(t=0)=0$ since the number of points in each box is *exactly* the same.

Figure 4 shows the time evolution of the coarse-grained entropy S_ε at different electric fields [24]. Starting from the initial condition $S_\varepsilon=0$, the distribution changes, and the coarse-grained entropy becomes negative for $t>0$. Its saturation value increases in modulus at increasing electric field. Due to the finite number of points used to approximate the temporal evolution of the measures, however, the entropy takes a nonvanishing value even in the absence of the electric field, which is immediately related to the variance of (randomly) distributed points in the respective boxes. When both the number of boxes and the number of points in each box (N_{box}) are sufficiently large, a simple estimate of the entropy yields a proportionality of S_ε to $1/N_{\text{box}}$, which is consistent with the asymptotic value of the data (+) in Fig. 4 belonging to $E=0$. This deviation from zero (the expected value for $E=0$) can be taken as an estimate for the systematic errors of the calculation of S_ε based on a finite number of particles. In principle the offset can be eliminated by using increasingly higher number of points N and working out the scaling of the entropy for $N^{-1}\to0$. For the present study this is not

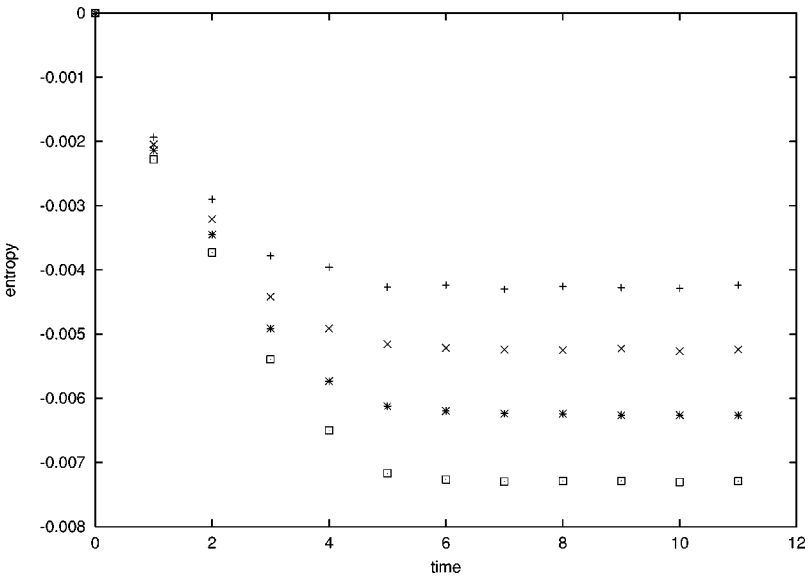

FIG. 5. The ε dependence of the time evolution of the coarse-grained entropy S_ε for $E=0.1$. Time is specified in terms of the number of collisions, and the different symbols refer to $\varepsilon=2^{-6}$ (+), 2^{-7} (×), 2^{-8} (*), and 2^{-9} (□). Note that the difference between neighboring saturation levels does not depend on ε.

necessary, however, since we are interested in *differences* of the saturation levels for increasing resolution ε. The systematic displacement then drops out when the number of points per cell is maintained. We choose $2^{n+5}\times 2^{n+5}$ points for a $2^n\times 2^n$ partitioning, i.e., for instance $2^{12}\times 2^{12}$ initial conditions for the partition into $2^7\times 2^7$ boxes.

Figure 5 shows the time evolution S_ε and its saturation values at an external field $E=0.1$ for different resolutions $\varepsilon=2^{-6}$, 2^{-7}, 2^{-8}, and 2^{-9}. For smaller ε (increasing resolution), the saturation occurs later, and its level is shifted downwards by $S_\varepsilon - S_{2\varepsilon}=(d-D_I)\ln 2$ relative to the previous one. The slope of the initial decay before saturation is expected to follow the Gibbs entropy (cf. Fig. 1), i.e., it should amount to the phase-space contraction rate. A reasonable estimate can be obtained after the decay of correlations ($n>2$), and sufficiently far from the saturation region. There are only few data fulfilling these conflicting constraints, but in the highest resolution case ($\varepsilon=2^{-9}$) the line that goes through points $n=2$ and $n=3$ has a slope, 2×10^{-3}, a value close to the result $\overline{\sigma}=(2.5\pm 0.1)\times 10^{-3}$ reported in Sec. III B.

The difference between different saturation values is $\Delta=(1.00\pm 0.04)\times 10^{-3}$, from which we obtain the following estimate of the codimension

$$d-D_I=\Delta/\ln 2=(1.44\pm 0.05)\times 10^{-3} \qquad (18)$$

as compared to the value $2-D_I=(1.44\pm 0.07)\times 10^{-3}$ obtained in Eq. (17) from the Kaplan-Yorke formula.

This analysis was also done for the electric field $E=0.2$. In this case the information codimension evaluated from the saturation values of the entropies is $d-D_I=(5.26\pm 0.31)\times 10^{-3}$, which agrees well with the codimension $(5.30\pm 0.22)\times 10^{-3}$ obtained by the Kaplan-Yorke method [22]. Altogether the numerical results are therefore consistent with a quadratic increase of the codimension with electric field.

IV. CONCLUSION

Equation (10) provides a, highly accurate method for calculating the information dimension of a chaotic attractor. It is based on the observation that the difference between the saturation values of the coarse-grained entropies of different resolution is a numerically very robust quantity to calculate, which makes accurate predictions even for systems with information codimension of the invariant measures of less than a few promille. The data were used to test the relation (17) between the information codimension of two-dimensional maps, their phase-space contraction and the largest Lyapunov exponent. Such relations and their numerical tests have received considerable attention in the recent literature due to suggested relations between the thermodynamic entropy production and the phase-space contraction towards invariant measures characterizing the (long-time) dynamics [7,15].

In the remaining part of this discussion we revisit this relation from the point of view of the present results. For a general dynamical system the coarse-grained entropy S_ε is—to our understanding—the closest analog of the thermodynamical entropy. This does not imply, however, that the analogy is very close. In irreversible thermodynamics after all the change of the entropy is related to the fluxes of macroscopic thermodynamic variables. On the level of a global balance the requirements for such an agreement are not known, yet. On the other hand, for certain classes of spatially extended systems the (much more restrictive) conditions for the agreement of a *local* entropy balance with the requirements of irreversible thermodynamics were worked out [8,4,25]. To that end, (cf. Refs. [15,26]) the system has to admit a decomposition into small spatial domains representing regions characterized by a local thermodynamic equilibrium [27]. The unit cells of the periodic Lorentz gas [cf. Fig. 2(a)] are an appropriate choice of such regions. Local equilibrium corresponds in this system to a constant velocity of particles and uniform distribution in angles [28]. Its basic characteristics is the density of particles in the cell obtained by integrating over all the momenta and the spatial coordi-

nates of the cell. After all, in the absence of external fields, every initial condition will relax to a state with a uniform distribution of the particles in each cell. Local equilibrium implies the assumption that for each cell the macroscopically relevant averages taken with respect to the true nonequilibrium distribution are indistinguishable from those taken with respect to the uniform (equilibrium) distribution (Sec. 3 of Ref. [29]). The unit cells may be characterized by different equilibrium densities, which are updated in time by *solely* considering the constraints implied by conservation laws. This approach is valid for the Lorentz gas if (and only if) the channels between the disks are very narrow so that a particle will have many collisions inside a cell before progressing to a neighboring one [28,30]. Since irreversible thermodynamics is based on local-equilibrium densities, there cannot be an *a priori* relation between the coarse-grained entropies S_ε of dynamical systems, which are defined in Sec. II irrespective of local equilibrium, and the entropy functional characterizing thermodynamic transport processes. Consequently, it is overambitious [31–33] to identify the phase-space contraction rate in thermostated models with the thermodynamic entropy production.

It is also interesting to investigate the notion of a stationary nonequilibrium state from the present perspective. Approaches based on dynamical systems [7,31–35] often relate these states to the natural invariant measures of the underlying chaotic dynamics. It was repeatedly pointed out that a key difference between equilibrium and typical nonequilibrium steady states is the observation that the natural measures of the former obey smooth densities while the latter are only defined in the sense of fractal distributions. Let us now consider a dynamical system where at time $t=0$ a driving force is switched on, which will eventually force the system into a nonequilibrium steady state. For diffusive relaxation in a system of linear spatial extension L this will roughly happen after a time $t \approx L^2/D$; or—if external forces induce a drift v—the somewhat shorter, but still macroscopic, time scale L/v. In the course of this relaxation the phase-space distribution describing the associated chaotic dynamics contracts exponentially like $\exp(-|\overline{\lambda_2}|t)$ towards a fractal phase-space structure, were $\overline{\lambda_2}$ is the average negative Lyapunov exponent. On the macroscopic time scales this contraction reaches length scales $\epsilon \approx \exp(-|\overline{\lambda_2}|L^2/D)$ or $\epsilon \approx \exp(-|\overline{\lambda_2}|L/v)$, which are unphysically small because the exponents contain the ratios of a macroscopic and a microscopic time. This causes conceptual problems in the interpretation of approaches like the one of Ref. [8,25], while it clearly supports our preference [16,15] to relate entropy production to the mixing properties taking place on the scale of the cells used to define local equilibrium, rather than concentrating on miniscule structures in phase space.

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[1] S.R. de Groot and P. Mazur, *Nonequilibrium Thermodynamics* (North Holland, Amsterdam, 1962).
[2] We refer here to the entropy of the full system.
[3] W. Breymann, T. Tél, and J. Vollmer, Phys. Rev. Lett. **77**, 2945 (1996).
[4] T. Tél and J. Vollmer, in Hard Ball Systems and the Lorentz Gas, edited by D. Szász (Springer, Berlin, 2000).
[5] J.P. Eckmann and D. Ruelle, Rev. Mod. Phys. **57**, 617 (1985).
[6] E. Ott, *Chaos in Dynamical Systems* (Cambridge University Press, Cambridge, 1993).
[7] 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).
[8] P. Gaspard *Scattering, Chaos, and Nonequilibrium Statistical Mechanics* (Cambridge University Press, Cambridge, 1998).
[9] J.R. Dorfman, *An Introduction to Chaos and Nonequilibrium Statistical Mechanics* (Cambridge University Press, Cambridge, 1999).
[10] R.C. Tolman, *The Principles of Statistical Mechanics* (Oxford University Press, Oxford, 1938).
[11] M.S. Green, J. Chem. Phys. **20**, 1281 (1952).
[12] J.D. Farmer, E. Ott, and J.A. Yorke, Physica D **7**, 153 (1983).
[13] P. Grassberger and I. Procaccia, Physica D **13**, 34 (1984).
[14] C. Beck and Schlögl, *Thermodynamic Formalism* (Cambridge University Press, Cambridge, 1993).
[15] J. Vollmer, Phys. Rep. **372**, 131 (2002).
[16] J. Vollmer, T. Tél, and W. Breymann, Phys. Rev. Lett. **79**, 2759 (1997); Phys. Rev. E **58**, 1672 (1998); W. Breymann, T. Tél, and J. Vollmer, Chaos **8**, 396 (1998).
[17] D.J. Evans and L. Rondoni, J. Stat. Phys. **109**, 895 (2002).
[18] W.G. Hoover, *Molecular Dynamics*, (Springer-Verlag, Berlin 1986); C.P. Dettmann, in *Hard Ball Systems and the Lorentz Gas*, edited by D. Szász (Springer, Berlin, 2000).
[19] From the point of view of the dynamical system this constitutes a Poincaré map.
[20] G.P. Morriss and C.P. Dettmann, Chaos **8**, 321 (1998).
[21] The time step of the method is sufficiently small to ensure that the coarse-grained entropy reaches its saturation much before the numerical errors in the trajectories become comparable to the resolution of the partitioning (i.e., the size of the cells).
[22] C. Dellago, L. Glatz, and H.A. Posch, Phys. Rev. E **52**, 4817 (1995).
[23] In the general definition of the entropy we use coarse graining by means of squares in units of the size of the total phase space. For the Lorentz gas this means that the lengths of the

respective sides of a *cell of size* ε are a fraction ε of those of the full domain ($[-1,1]\times[0,2\pi]$). The cells are thus rectangles of size $2\varepsilon\times 2\pi\varepsilon$. From the point of view of the coarse-grained entropy this does not matter, because only the measure of boxes appears in Eq. (9).

[24] L. Mátyás, Ph.D. thesis, ELTE Budapest 2001 (unpublished).

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

[26] L. Rondoni and E.G.D. Cohen, Nonlinearity **13**, 1905 (2000).

[27] Common discussions of transport processes from the point of view of kinetic theory of gases characterize local equilibrium by the *sufficient*, even though *not necessary*, condition of a Maxwellian velocity distribution of the particles. In contrast, we adopt the definition of de Groot and Mazur [1] [Chapter III, Section 2], which is more general than the one in kinetic theory: ''Although the total system is not in equilibrium, there exists within small mass elements a state of ''local'' equilibrium, for which the local entropy is the same function [of the macroscopic thermodynamic variables] as in real equilibrium. [. . .] This hypothesis of local equilibrium can, from a macroscopic point of view, only be justified by virtue of the conclusions derived from it.''

[28] J. Machta and R. Zwanzig, Phys. Rev. Lett. **50**, 1959 (1983).

[29] H. Grad, in *Delaware Seminar in the Foundations of Physics*, edited by M. Bunge (Springer, Berlin, 1967).

[30] R. Klages and C. Dellago, J. Stat. Phys. **101**, 145 (2000).

[31] D. Ruelle, J. Stat. Phys. **95**, 392 (1999).

[32] D. Ruelle, J. Stat. Phys. **85**, 1 (1996).

[33] G. Gallavotti and E.G.D. Cohen, Phys. Rev. Lett. **74**, 2694 (1995); J. Stat. Phys. **80**, 931 (1995); G. Gallavotti, Chaos **8**, 384 (1998).

[34] 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).

[35] E.G.D. Cohen, Physica A **240**, 43 (1997).