Thermostating by Deterministic Scattering: Construction of Nonequilibrium Steady States

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We present a novel approach for constructing nonequilibrium steady states. It is based on a deterministic and time-reversible mechanism for dissipating energy from a subsystem into a thermal reservoir. The key idea is to thermalize a moving particle by appropriately modeling its microscopic collision rules with a boundary mimicking a thermal reservoir with arbitrarily many degrees of freedom. We demonstrate our method for the periodic Lorentz gas with an external electric field. By applying our thermostat we do not find an ergodic breakdown with increasing field strength.

A fundamental problem of nonequilibrium statistical mechanics is the construction and characterization of nonequilibrium steady states (NSS). In recent years, a number of interesting connections between macroscopic statistical properties and the underlying microscopic chaotic dynamics have been put forward [1–4]: One major line of research employs deterministic, time-reversible bulk thermostating schemes, where the change of the internal energy of a fluid caused, e.g., by applying external fields is compensated by introducing a fictitious frictional force into the microscopic equations of motion [1,5]. For this class of systems the measures characterizing NSS are typically singular [5–7]. This is in contrast to systems which have been thermostated by stochastic boundaries leading to smooth nonequilibrium measures [8]. To bridge the gap between these two approaches, shear flow NSS have been created by "Maxwell daemonlike" moving boundaries [9]. Moreover, in the context of bulk thermostating schemes a deterministic generalization of the chaotic hypothesis of Boltzmann has been proposed [10]. An alternative approach to nonequilibrium was initiated by Gaspard, where nonequilibrium is induced by appropriate boundary conditions in spatially extended systems [3,11]. The main difficulty resulting from these different approaches is that the associated NSS exhibit very different statistical dynamical properties. This implies that different answers to fundamental questions of nonequilibrium thermodynamics are obtained. In particular, bulk thermostating schemes have led to the conclusion that there exists an identity between irreversible entropy production and phase space contraction [7,9,12,13]. This identity is at the heart of specific formulas which relate transport coefficients to Lyapunov exponents [6,12,14]. On the other hand, apparently different such relations have emerged from the method of Gaspard [3,11]. Despite efforts to unify the latter two approaches [15], it is still not clear whether relations obtained from a certain mechanism to create NSS are of general validity or just characterize a specific class of models.

In this Letter we propose a novel deterministic, time-reversible thermostat yielding NSS. Our scheme is differ-

ent from bulk thermostats since it does not appeal to fictitious frictional forces. However, it goes beyond the one of Ref. [9] since our scattering rules include an energy transfer between subsystem and thermal reservoir. In particular, it enables one to correctly interpolate between deterministic thermostats and stochastic thermal boundaries. Our approach thus provides a suitable tool to check for the validity of the above-mentioned general relations obtained from the various approaches to nonequilibrium. The aim of our Letter is to systematically construct this thermostat for a simple model system and to characterize the resulting NSS by computer simulations.

We chose the periodic Lorentz gas, a standard model in the field of chaos and transport [2,3,11], where a point particle scatters elastically at hard disks arranged on a triangular lattice. It mimics classical diffusive transport in a crystal but is as well isomorphic to a periodic fluid of two hard disks per unit cell [16]. In the driven case an electric field acts on the moving particle, and a thermostat must be applied to generate NSS [5,6,13,17–21]. We consider one scatterer in an elementary cell with periodic boundary conditions, see Fig. 1(a), and assume unit mass and unit charge for the moving particle. For the spacing between two neighboring disks at disk radius $R = 1$ we choose, following the literature [6,20,21], $w \simeq 0.2361$, ensuring that a particle cannot move collision-free for infinite time. Figure 1(b) defines the relevant variables for the collision
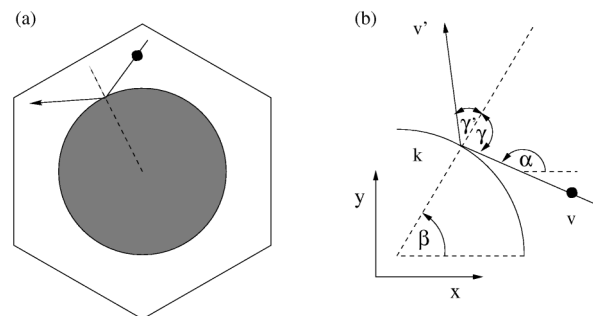

FIG. 1. (a) Elementary cell of the periodic Lorentz gas on a triangular lattice. (b) Definition of the relevant variables to describe the collision process.

process, where we express the velocity v of the particle in local polar coordinates (γ, v) with γ as the angle of incidence and v as the absolute value of the velocity. The dashed variables indicate the respective values after the collision. We also introduce the angle β, which determines the position of the colliding particle at the disk. In contrast to an elastic collision $(\gamma, v) = (\gamma', v')$, we propose to include an energy transfer between particle and disk. We do this by introducing an additional velocity variable k associated with the disk and by allowing that $\gamma \neq \gamma'$. We require that the total energy E of the system is conserved at the collision, $v^2 + k^2 = v'^2 + k'^2 = 2E$. Thus, the collision process in velocity space is still effectively defined by the dynamics of two variables for which we take (γ, v). One possible implementation of this setup would be when the disk rotates with k as an angular velocity. By

keeping v perpendicular to the disk fixed and allowing the exchange of energy via only the tangent component, the collision process effectively reduces to one of two colliding masses on a line. Requiring energy and momentum conservation yields for the scattering rules a two-dimensional piecewise linear map. As a drastic simplification of such a model, but keeping important dynamical properties as time reversibility, a deterministic dynamics, and the dynamical instability induced by the disk geometry, we choose here our collision rules according to a simple baker's map [3,4]. We apply it on the respective Birkhoff coordinate of the ingoing angle, $\sin|\gamma|$, as its x coordinate and on $v/\sqrt{2E}$ in the range of $0 \leq v \leq \sqrt{2E}$ as its y coordinate. To ensure that the system is time reversible, the forward baker acts if $0 \leq \gamma \leq \pi/2$, and its inverse if $-\pi/2 \leq \gamma < 0$. The angle γ' always goes to the respective other side of the normal, as shown in Fig. 1(b). For $\gamma \geq 0$ this gives

$$M(\sin|\gamma|, v/\sqrt{2E}) = \begin{cases} (2\sin|\gamma|, v/\sqrt{8E}) & \sin|\gamma| \leq 0.5 \\ [2\sin|\gamma| - 1, (v/\sqrt{2E} + 1)/2], & \sin|\gamma| > 0.5 \end{cases} \tag{1}$$

and *vice versa* for $\gamma < 0$. As for k', it is obtained from energy conservation. To avoid any symmetry breaking induced by this combination of forward and backward baker, we alternate their application in γ with respect to the position β of the colliding particle on the circumference [22].

The above setting leads to a well-defined scattering system with three degrees of freedom. As it stands, however, it does not satisfy the microcanonical distribution in the absence of a field, since the energy is not equipartitioned between all degrees of freedom. We incorporate this essential feature by amending the microscopic scattering rules, as given by the baker, in the most straightforward way. As a starting point, we calculate the projection of the microcanonical density $\rho(v_x, v_y, k) = c\delta(2E - v_x^2 - v_y^2 - k^2)$ onto v, where c is a constant to be fixed by normalization yielding $\rho(v) = v/\sqrt{2E(2E - v^2)}$. To achieve this long-time limiting density in our model we proceed as follows: Let $\rho_{\mathrm{map}}(v)$ be the probability density for v at the moment of the collision corresponding to a respective Poincaré surface of section, in contrast to the probability density of the time-continuous system $\rho_{\mathrm{cont}}(v)$. During the free flight the particle cannot change its velocity, and thus $\rho_{\mathrm{map}}(v)$ and $\rho_{\mathrm{cont}}(v)$ are simply related via the average time the particle travels between two collisions with velocity v. This average time plays the role of a weighting factor leading to

$$\rho_{\mathrm{cont}}(v) = \frac{c}{v} \rho_{\mathrm{map}}(v). \tag{2}$$

We want that the map which determines the collision rules generates an invariant velocity distribution $\rho^*_{\mathrm{cont}}(v) \equiv \rho(v)$. This leads to

$$\rho^*_{\mathrm{map}}(v) = \frac{2v^2}{\pi E \sqrt{2E - v^2}}. \tag{3}$$

However, the invariant density of the baker's map is simply $\rho^*(x_B, y_B) = 1$. Therefore, we define a conjugate map which produces the desired density by including a transformation $y_B = Y(v)$, where y_B is the actual baker variable. This transformation must be continuous and invertible, as defined by conservation of probability,

$$\rho^*(y_B)|dy_B| = \rho_{\mathrm{map}}(v)|dv|. \tag{4}$$

$Y(v)$ can then be computed to

$$Y(v) = -\frac{v}{\pi E}\sqrt{2E - v^2} + \frac{2}{\pi} \arcsin \frac{v}{\sqrt{2E}}, \tag{5}$$

with $0 \leq v \leq \sqrt{2E}, 0 \leq Y(v) \leq 1$. If we write $x_B = X(\gamma) = \sin|\gamma|$, the full collision rules read

$$(\gamma', v') = (X^{-1}, Y^{-1}) \circ M \circ (X, Y). \tag{6}$$

Computer simulations carried out along the lines of Refs. [6,20] confirm that a Lorentz gas with these collision rules is microcanonical in both its position and momentum coordinates in phase space.

We now inquire how the above ideas can be used to mimic the interaction of a moving particle with a thermal reservoir. For this purpose we associate arbitrarily many degrees of freedom to the disk which could be related, e.g., to different lattice modes in a crystal as mechanisms for dissipating energy from a colliding particle. For the sake of simplicity we do not distinguish here between all the individual velocities in the reservoir. Instead, we pretend that the particle interacts instantaneously with *all* $(d - 2)$ velocity components k_j of the reservoir via an absolute reservoir velocity $k = \sqrt{k_1^2 + k_2^2 + \cdots + k_{d-2}^2}$ to

which we identify the disk velocity. To ensure that the projected densities of the accessible variables (v_x, v_y, k) be generated from the microcanonical distribution of the full d-dimensional system, we need the projection of the microcanonical distribution $\rho_d(v_x, v_y, k_1, k_2, \ldots, k_{d-2}) = c\delta(2E - v_x^2 - v_y^2 - \sum_{j=1}^{d-2} k_j^2)$ onto $\rho_d(v)$, which can be calculated for $d > 2$ to

$$\rho_d(v) = (d-2)(2E)^{-(d-2)/2} v (2E - v^2)^{(d-4)/2}. \quad (7)$$

Using the equipartition theorem $E/d = T/2$ with temperature T and Boltzmann constant $k_B = 1$, and taking the limit $d \rightarrow \infty$, this expression reduces to the Maxwellian distribution $\rho_\infty(v) = v/T \exp[-v^2/(2T)]$. Choosing $\rho^*_{\text{cont},d}(v) \equiv \rho_d(v)$ according to Eq. (7) and using Eq. (2) determines the corresponding density $\rho^*_{\text{map},d}(v)$ of the Poincaré section. The transformation $Y_d(v)$ which yields $\rho^*_{\text{map},d}(v)$ can then be calculated from Eq. (4). In the limit of $d \rightarrow \infty$, $Y_\infty(v)$ reads

$$Y_\infty(v) = -\sqrt{\frac{2}{\pi T}} v e^{-v^2/(2T)} + \text{erf}\left(\frac{v}{\sqrt{2T}}\right), \quad (8)$$

with $0 \leq v \leq \infty, 0 \leq Y(v) \leq 1$. Computer simulations confirm that a periodic Lorentz gas with these collision rules approaches projected densities in (v_x, v_y, k) which are identical to the ones obtained from a uniform distribution on the energy shell in $(v_x, v_y, k_1, k_2, \ldots, k_{d-2})$. The temperature T of the equilibrium system is unambiguously defined via equipartitioning of energy as it enters into Eq. (8). In Ref. [23] it is shown how these scattering rules can alternatively be derived from stochastic boundary conditions.

We are now ready to set up a nonequilibrium situation by taking the system as defined in equilibrium for $d \rightarrow \infty$ and by switching on an electric field parallel to the x axis. This field affects the velocity of the moving particle. However, since the particle is a small subsystem in a large reservoir, and since we have built in a mechanism of equipartitioning of energy, one expects that the particle is still getting thermalized by our scattering rules at a temperature determined by the temperature T of the reservoir, thereby approaching NSS with kinetic energy and conductivity fluctuating around constant mean values. This is fully confirmed by computer simulations. That such NSS exist according to our scattering mechanism is the central result of our Letter.

In the following, we illustrate some important characteristics of this state as deduced from computer simulations. Figure 2 demonstrates that for small enough field strength and high enough temperature the energy of the system is still approximately equipartitioned between $(\langle v^2 \rangle - \langle v_x \rangle^2)$ and the reservoir. Figure 3 depicts the conductivity $\sigma(\varepsilon) = \langle v_x \rangle / \varepsilon$ with respect to the field strength ε. The strong decrease of $\sigma(\varepsilon)$ indicates that the system is in a highly nonlinear regime. Ohm's law may be suspected to hold only at very small field strengths $\varepsilon \ll 0.1$ [13]; however, in this regime reliable numerical results are diffi-
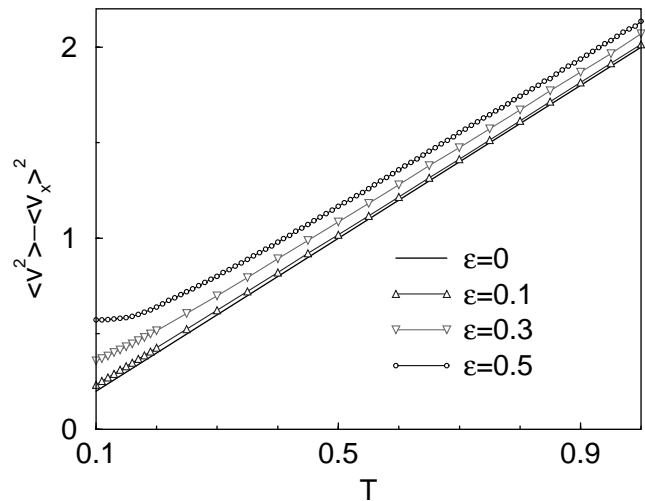

FIG. 2.   Relation between average velocity squared in the frame moving with the current, $\langle v^2 \rangle - \langle v_x \rangle^2$, and temperature T for the infinite dimensional model. Equipartitioning of energy would imply $\langle v^2 \rangle - \langle v_x \rangle^2 = 2T$. The numerical error is less than the size of the symbols.

cult to get. The broadest fluctuations on smaller scales are beyond numerical uncertainties and may be reminiscent of strong irregularities as they occur in the conductivity of the Gaussian Lorentz gas [6,18–21]. Figures 4(a) and 4(b) show Poincaré plots of $(\beta, \sin \gamma)$ at the collisions. In Fig. 4(b) the deterministic baker has been replaced by a random number generator thus mimicking stochastic boundaries. Figure 4(a) indicates the existence of a fractal attractor, analogous to the one found in the Gaussian Lorentz gas [6,17,20], whereas in Fig. 4(b) the fractal structure is lost due to the stochasticity of the boundary conditions. Figure 4(c) should be compared to the analogous diagram obtained from the Lorentz gas with a Gaussian thermostat [5,19]. In the case of our model,
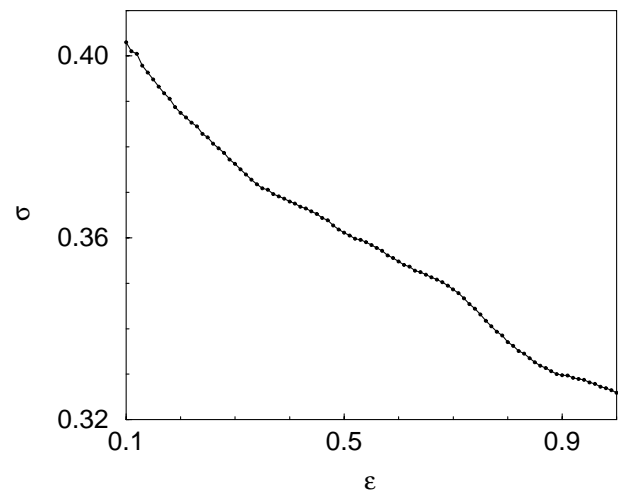

FIG. 3.   Conductivity $\sigma(\varepsilon)$ as it varies with field strength ε. The curve consists of 90 data points; the numerical error is equal to the size of the symbols.
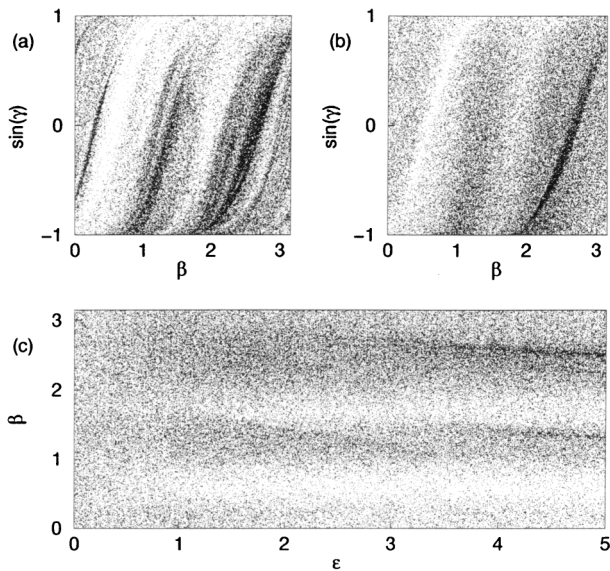
FIG. 4. (a),(b) Poincaré section of $(\beta, \sin\gamma)$ defined in Fig. 1 at the moment of the collision for field strength $\varepsilon = 1$. In (a) a baker's map has been used for defining the collisions; in (b) the baker's has been replaced by a random number generator. (c) Poincaré section of β at the moment of the collision for varying field strength ε.

there is no indication of a pruning-induced "bifurcation scenario" or an ergodic breakdown as in the Gaussian version. The same holds for other choices of Poincaré sections in phase space.

Having the novel thermostating mechanism at hand described in this Letter, one can elaborate on further principal features of NSS like entropy production and Lyapunov exponents. In particular, one can inquire about the universality of relations between these quantities as found for specific thermostats. On the basis of this Letter, these issues have been studied in recent work [23–26]: For a system of hard disks under temperature gradient and shear thermostated by our method, Ref. [23] shows that, in general, no identity between phase space contraction and entropy production exists. As a consequence, there is no general relation between transport coefficients and Lyapunov exponents. Furthermore, no conjugate pairing rule between Lyapunov exponents holds for systems thermostated by deterministic scattering [26]. A detailed comparison of our thermostat to different types of Nosé-Hoover thermostats in the driven periodic Lorentz gas revealed different kinds of bifurcation scenarios depending on the specific way of thermostating [24,25]. To obtain universal characterizations of NSS generated by different thermostating schemes thus remains an open question.

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