Steady-State Conduction in Self-Similar Billiards

Felipe Barra[1] and Thomas Gilbert[2]

[1]*Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Casilla 487-3, Santiago, Chile*
[2]*Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, CP 231, Campus Plaine, B-1050 Brussels, Belgium*

(Received 4 October 2006; published 28 March 2007)

The self-similar Lorentz billiard channel is a spatially extended deterministic dynamical system which consists of an infinite one-dimensional sequence of cells whose sizes increase monotonically according to their indices. This special geometry induces a nonequilibrium stationary state with particles flowing steadily from the small to the large scales. The corresponding invariant measure has fractal properties reflected by the phase-space contraction rate of the dynamics restricted to a single cell with appropriate boundary conditions. In the near-equilibrium limit, we find numerical agreement between this quantity and the entropy production rate as specified by thermodynamics.

DOI: 10.1103/PhysRevLett.98.130601 PACS numbers: 05.70.Ln, 05.45.−a, 05.60.−k

Over the last two decades, the nonequilibrium statistical mechanics of chaotic dynamical systems has received a great deal of attention, in particular, regarding the positivity of entropy production and its connection to dynamical properties characteristic of chaos, such as the Lyapunov exponents [1–4].

Of particular interest is the two-dimensional periodic Lorentz gas with external forcing and a Gaussian isokinetic thermostat (GIKLG) [1]. This is an elementary model of electronic conduction under a nonequilibrium constraint. The thermostat is actually a mechanical constraint and acts so as to remove the energy input from the external forcing [2]. Under the action of this thermostat, the kinetic energy remains constant and thus fixes the temperature of the system; no interaction with a hypothetical environment is needed in order to achieve thermalization. Rather, dissipation occurs in the bulk. As shown in [5], this model enjoys strong chaotic properties. Its natural invariant measure is fractal, with one positive and one negative Lyapunov exponent, whose sum is negative, and identified as minus the entropy production rate [6]. The comparison with the corresponding phenomenological expression provides a relation between the phase-space contraction rate and conductivity.

The GIK dynamics can actually be given a Hamiltonian formulation [7]. This result is contained in a more general formalism [8], by which one identifies the GIK trajectories with the geodesics of a torsion free connection, called the Weyl connection. In this formalism, one shows the GIKLG is equivalent, by a conformal transformation, to a distorted billiard whose trajectories are straight lines, referred to as W flow. In this geometry, the cells are stretched and trajectories accelerated in the direction of the external field. A detailed analysis of the W flow [9] reveals that the cells' stretching is the essential mechanism to driving the nonequilibrium stationary state.

In this Letter, we investigate the connection between the chaotic dynamics and nonequilibrium thermodynamics of a self-similar billiard chain, such as defined in [10]. This billiard chain can be thought of as a simplified version of W flow described above; we retain the stretched geometry of the cells, but get rid of the bulk dissipation.

A self-similar billiard is thus a one-dimensional spatially extended system such as shown in Fig. 1. It consists of an infinite collection of two-dimensional cells, identical in shapes, but differing in sizes, which are scaled and glued together along a horizontal axis. Each cell consists of convex obstacles upon which point particles collide elastically, independently of one another. The left and right borders of every cell are open and scaled by a constant ratio which we denote by μ. The system is so constructed that $\mu = 1$ corresponds to the Lorentz channel [3], which exhibits diffusion, but no bias. When $\mu \neq 1$, the system sustains a nonequilibrium stationary state, characterized by a steady density current from the smaller to the larger scales.

Strictly speaking, this self-similar billiard channel is different from the W flow, constructed along the lines of [8]. However, the two systems have in common the scaling property between the left and right borders of every cell. An important difference concerns the dynamics between collisions. Here we assume free propagation of point particles between collision events, which amounts to suppressing the thermostating mechanism of the GIK dynamics. Another example of a billiard with a similar scaling mechanism was considered in [11]. Other systems

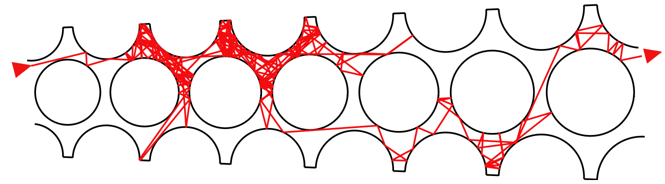

FIG. 1 (color online). The self-similar Lorentz channel billiard and a trajectory.

which bear similarities with this one are the multibaker maps with energy [12]. Both systems are area preserving and energy conserving, with an external driving force (here in the form of a geometric constraint) that induces a macroscopic current, without the necessity of a thermostating mechanism.

In order to specify the stationary properties of the system, we resort to the special flow of the billiard [13], thus substituting the real time dynamics by a discrete mapping from one collision event to the next. This is a usual procedure for the study of ergodic properties of billiards, which allows us to replace the volume-preserving dynamics on the extended system by a phase-space contracting mapping on a periodic cell. This feature is also common to multibaker maps with energy, which can be reduced to dissipative baker maps such as studied in [14], see [12]. Moreover, the invariant measure has fractal properties much like that of the GIKLG [15].

Following [6], we identify the phase-space contraction rate with the entropy production rate, and take the limit $\mu \to 1$ so as to compare this expression to its thermodynamic counterpart. We thus infer a relation between the current of the near-equilibrium system ($\mu \neq 1$) and the diffusion coefficient of the equilibrium system ($\mu = 1$), much like a fluctuation-dissipation theorem. This result is confirmed by our numerical computations.

Going back to the definition of the model, the reference cell, with index $i = 0$, is represented in Fig. 2(a). It is a region defined by the exterior of five disks, four of which are centered at the corners of the cell, and one located at the center. The dissymmetry between the left- and the right-hand sides depends on the scaling parameter μ. The other tunable parameter is the ratio R/d between the center disk's radius R and the cell's horizontal width d. The radii of the outer disks are fixed to $R/\sqrt{\mu}$ (to the left) and $R\sqrt{\mu}$ (to the right). The vertical separations between the outer disks are taken to be $d\sqrt{3/\mu}$ to the left and $d\sqrt{3\mu}$ to the right, so that the usual Lorentz channel is retrieved for $\mu = 1$. We note that restrictions must be imposed on the range of permitted values of the parameters for the self-similar billiard to share the hyperbolicity of the Lorentz channel. The details can be found in [10]. We assume these conditions to be met in the sequel.

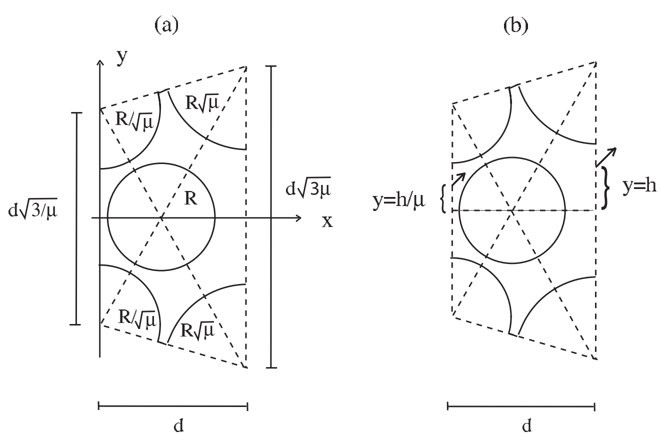

FIG. 2. (a) Geometry of the reference cell. (b) Sketch of the boundary conditions in the periodic cell, as given by Eqs. (1) and (2).

The whole chain is constructed by adding a cell to the right of the reference cell, with index $i = 1$, identical in shape but with all its lengths multiplied by μ, and another one to the left, with index $i = -1$, with all the lengths divided by μ. We repeat this construction in such a way that in the ith cell, $i \in \mathbb{Z}$, all the lengths are multiplied by μ^i. The resulting billiard chain is so constructed that the mirror symmetry with respect to the transformation $\mu \to 1/\mu$ remains.

Consider a particle moving inside the billiard with velocity $\vec{v}$. Figure 1 shows such a trajectory. As the particle moves from one cell to a neighboring one, the length scales change by a factor μ. Equivalently we can rescale the velocity by a factor $1/\mu$ and keep the length scales unchanged. For both transformations the characteristic time between successive collisions with the walls changes by a factor μ.

We can therefore analyze the dynamics on the extended self-similar billiard in terms of the dynamics in a periodic cell by applying proper boundary conditions and rescaling the vertical coordinate and velocity, as the particle exits either

$$\text{to the right:} \begin{cases} \vec{r} = (d, h) & \to (0, h/\mu), \\ \vec{v} = (v_x, v_y) & \to (v_x/\mu, v_y/\mu), \end{cases} \tag{1}$$

$$\text{or to the left:} \begin{cases} \vec{r} = (0, h) & \to (d, h\mu), \\ \vec{v} = (v_x, v_y) & \to (v_x\mu, v_y\mu). \end{cases} \tag{2}$$

Here h is the y coordinate of the trajectory as it crosses the cell's left or right boundaries. An example is depicted in Fig. 2(b). These conditions are analogous to periodic boundary conditions for the usual Lorentz channel billiard but for the self-similar structure parametrized by μ.

Billiards are instances of so-called special flows [13], which is to say their time evolutions can be specified by the mapping of the coordinates between successive collision events, together with the time interval between them. This kind of representation is particularly useful to the evolution of self-similar billiards, where the absence of an overall time scale in the extended system poses difficulties in the definition of proper time averages. Indeed, point particles typically move towards the direction of increasing cell sizes, thereby decreasing their collision frequency. Such ambiguities become irrelevant when the evolution is considered from one collision event to the next.

The particle's coordinates from one collision with the walls to the next are specified by the Birkhoff map [3] $\xi_n \equiv (s, v, \varpi)_n \mapsto \xi_{n+1} \equiv \phi(\xi_n)$. Here the variable s represents the arclength along the unit cell boundary (including the open sides), v is the modulus of the particle's velocity, and ϖ is the sine of the angle between the outgoing velocity and the normal to the cell's boundary. This map, together with Eqs. (1) and (2), provide the map for the specification of a trajectory.

In order to keep track of the correspondence between the dynamics on the periodic cell and that on the extended lattice, we introduce a new variable I_n, which takes integer values and labels the cell where the particle is located after n iterations of the map. This variable changes according to $I_{n+1} = I_n + a(\xi_n)$, where we introduced the jump function, $a(\xi_n)$, which takes the values $a(\xi_n) = 1$ (respectively -1) if $\phi(\xi_n)$ has the spatial coordinate s_{n+1} on the right (respectively left) open side of the cell, otherwise $a(\xi_n) = 0$.

The time it takes a trajectory at a (phase-space) point ξ on the boundary to intersect again with the boundary of the billiard depends on the speed v as

$$T(\xi) = \frac{L(\xi)}{v}, \qquad (3)$$

where $L(\xi)$ is the length of the trajectory between intersections at ξ and $\phi(\xi)$ of the trajectory with the boundary of the unit cell. A complete characterization of the continuous time flow is thus given by the variables (ξ, τ) in the unit cell, with $0 < \tau < T(\xi)$, a new variable that restores the position between collisions. The equivalence between the continuous time flow on the extended lattice and the Birkhoff map with the extra variable τ is further discussed in [10].

A remarkable property of the Birkhoff map defined above is that it does not preserve phase-space volumes. Indeed, as the particle exits to the right and reenters to the left or vice versa, both s and v coordinates are rescaled by μ^{-1} (respectively μ). Accordingly, probability measures evolve under iteration of the density evolution operator associated to the Birkhoff map towards a unique invariant measure (i.e., a probability measure invariant under this operator) with fractal properties, characteristic of a nonequilibrium stationary state. This measure has three Lyapunov exponents, two negative and one positive, $\lambda_1 > 0 \geq \lambda_2 > \lambda_3$, and such that the phase-space contraction rate $\sigma \equiv -(\lambda_1 + \lambda_2 + \lambda_3) > 0$.

The second Lyapunov exponent, λ_2, is specific to the self-similar geometry of the billiard; it is due to the contraction of the v coordinate as the particle moves around the cell:

$$\lambda_2 = -\lim_{n\to\infty} \frac{\Delta I_n}{n} \log\mu \leq 0, \qquad (4)$$

where $\Delta I_n = I_n - I_0$ is the lattice displacement vector after n iterations or winding number. If $\mu > 1$, the particle moves preferentially to the right, corresponding to $\Delta I_n/n > 0$ and the other way around if $\mu < 1$. The symmetric case $\mu = 1$ is the usual Lorentz channel with only two nontrivial Lyapuonv exponents, i.e., $\lambda_2 = 0$. We therefore see that the stationary value of v under the Birkhoff map is trivially $v_n \to v_\infty = 0$, which is to say particles ever move towards the larger lattice scales, where times between collisions keep increasing and collisions become seldom.

λ_2 accounts for one half of the total phase-space contraction rate. The contraction of the vertical coordinate in Eqs. (1) and (2) accounts for the other half, due to λ_1 and λ_3,

$$\lambda_1 + \lambda_3 = \lambda_2 < 0. \qquad (5)$$

These two Lyapunov exponents are related to the components s and ϖ of ξ.

The invariant measure therefore has a product structure, $d^3m(\xi) = d^2m_1(s, \varpi)dm_2(v)$. When $\mu \neq 1$, we have $dm_2(v) = \delta(v)dv$ on the one hand, where δ is the Dirac delta function, and, on the other hand, since $\lambda_1 > 0$ and $\lambda_3 < 0$, m_1 is a fractal , whose Lyapunov dimension, here defined by $1 + \lambda_1/|\lambda_3|$, is somewhere between 1 and 2.

The entropy production per collision can be defined dynamically as the phase-space contraction rate [6], $\sigma = -(\lambda_1 + \lambda_2 + \lambda_3) = -2\lambda_2$, which can be computed in terms of the winding number, as in Eq. (4).

The winding number can furthermore easily be connected to the average drift of particles on the extended system. As we showed in [10], the average of the spatial coordinate X on the extended system evolves linearly in time, with a slope V which defines the drift velocity, $\langle X\rangle_t = Vt$. The winding number and drift velocity are equal up to dimensional factors:

$$\lim_{n\to\infty} \frac{\Delta I_n}{n} = \frac{T_\mu}{d} V, \qquad (6)$$

where d is the reference cell's width and T_μ the average time between collisions measured in that same cell. The phase-space contraction rate can therefore be expressed directly in terms of the average drift velocity: $\sigma = \frac{2T_\mu V}{d} \times \log\mu$. This expression can be transposed to a phase-space contraction rate per unit time in the limit $\mu \to 1$. In this limit, V and $\log\mu$ both scale like $\mu - 1$, so that the lowest order contribution to σ is $\mathcal{O}(\mu - 1)^2$, with $T_{\mu=1}$. Dividing σ by the latter defines the (dynamical) entropy production per unit time,

$$\frac{\sigma}{T_{\mu=1}} = \frac{2V}{d}(\mu - 1) + \mathcal{O}(\mu - 1)^3. \qquad (7)$$

As we showed in [10], the phenomenology of self-similar systems such as this one is characterized on the one hand by a constant drift from the small to the large scales and, on the other, by a mean square displacement which undergoes a transition from diffusive to ballistic behavior at a crossover time which scales like $\mu^{3/2}/(\mu - 1)$. Therefore, as $\mu \to 1$, self-similar systems can be considered as diffusive systems with constant drift, such as modeled by a Smoluchowski type equation for the proba-

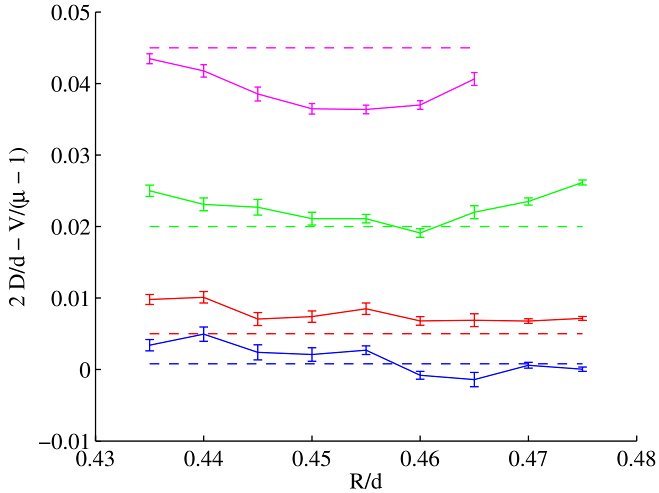

FIG. 3 (color online). The difference $2\mathcal{D}/d - V/(\mu - 1)$ vs R/d is $\mathcal{O}(\mu - 1)^2$, as expected from Eq. (8). Here shown are the values $\mu = 1.02$, 1.05, 1.10, 1.15 from bottom to top. The straight lines show $2(\mu - 1)^2$. Here V is computed as the slope of $\langle X \rangle_t$ vs t, where the average is computed out of many random initial conditions.

bility density W, $\partial_t W = \mathcal{D}\partial_x^2 W - V\partial_x W$. In the stationary state, the phenomenological entropy production rate is given [14] by the drift velocity V squared, a term quadratic in $\mu - 1$, divided by the diffusion coefficient $\mathcal{D}$, here computed at $\mu = 1$.

Equating Eq. (7) with the expression of the thermodynamic entropy production rate at $\mathcal{O}(\mu - 1)^2$, we infer the following relationship between the velocity drift and diffusion coefficient:

$$\lim_{\mu \to 1} \frac{V}{\mu - 1} = \frac{2\mathcal{D}}{d}, \tag{8}$$

which can be viewed as a definition of the mobility, the external field being given by $2(\mu - 1)$, and therefore establishes the equivalent of a fluctuation-dissipation theorem. This relationship is confirmed by the numerical results presented in Fig. 3, which were carried out for different choices of R/d and four different values of μ close to 1. Equation (6) was also verified in the numerical scheme.

To conclude, self-similar billiards are simple mechanical models of conduction in spatially extended systems with volume-preserving dynamics, whereby a geometric constraint induces a steady current. As in the conformal transformation of the GIKLG [9], or the multibaker maps with energy [12], the essential ingredient for this behavior is the rapid increase of phase-space volumes, whose rate is here given by μ.

These models lend themselves to further exploring the connections between the chaotic properties of nonequilibrium dynamical systems and phenomenological thermodynamics. The dynamical properties are conveniently analyzed by the means of the Birkhoff map on the periodic cell, which specifies the evolution of phase points from one collision to the next, here on a three-dimensional space.

Whereas the dynamics on the extended system preserves phase-space volumes, the Birkhoff map on the periodic cell contracts phase-space volumes, with an invariant measure whose fractal dimension is between 1 and 2. A similar mechanism of contraction of phase-space volumes at the periodic boundaries occurs with the W flow. The phase-space contraction rate can furthermore easily be computed in terms of the map's winding number, which bears a simple connection to the average velocity drift associated to the macroscopic current. The comparison between phase-space contraction rate and phenomenological entropy production yields an expression of the velocity drift near the equilibrium regime.

The authors are grateful to N. I. Chernov and C. Liverani for helpful comments. F. B. acknowledges financial support from Fondecyt Project No. 1060820 and FONDAP No. 11980002. T. G. is financially supported by the Fonds National de la Recherche Scientifique. This collaboration was supported through grant ACT 15 (Anillo en Ciencia y Tecnologia).

[1] W. G. Hoover, *Time Reversibility, Computer Simulation, and Chaos* (World Scientific, Singapore, 2001).
[2] D. J. Evans and G. P. Morriss, *Statistical Mechanics of Non-Equilibrium Fluids* (Academic, New York, 1990).
[3] P. Gaspard, *Chaos, Scattering and Statistical Mechanics* (Cambridge University Press, Cambridge, England, 1998).
[4] J. R. Dorfman, *An Introduction to Chaos in Nonequilibrium Statistical Mechanics* (Cambridge University Press, Cambridge, England, 1999).
[5] 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).
[6] D. Ruelle, J. Stat. Phys. **85**, 1 (1996); Proc. Natl. Acad. Sci. U.S.A. **100**, 3054 (2003); Phys. Today **57**, No. 5, 48 (2004).
[7] C. P. Dettmann and G. P. Morriss, Phys. Rev. E **54**, 2495 (1996); G. P. Morriss and C. P. Dettmann, Chaos **8**, 321 (1998).
[8] M. P. Wojtkowski, J. Math. Pures Appl. **79**, 953 (2000).
[9] F. Barra and T. Gilbert, J. Stat. Mech. (2007) L01003.
[10] F. Barra, T. Gilbert, and M. Romo, Phys. Rev. E **73**, 026211 (2006).
[11] G. Benettin and L. Rondoni, Mathematical Physics Electronic Journal **7**, 3 (2001).
[12] S. Tasaki and P. Gaspard, Theor. Chem. Acc. **102**, 385 (1999); J. Stat. Phys. **101**, 125 (2000).
[13] I. P. Cornfeld, S. V. Fomin, and Ya. G. Sinai, *Ergodic Theory* (Springer-Verlag, Berlin, 1982).
[14] J. Vollmer, T. Tél, and W. Breymann, Phys. Rev. Lett. **79**, 2759 (1997); Phys. Rev. E **58**, 1672 (1998); Chaos **8**, 396 (1998).
[15] G. P. Morriss, C. P. Dettmann, and L. Rondoni, Physica (Amsterdam) **240A**, 84 (1997).