Heat Conductivity and Dynamical Instability

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We present a series of numerical and analytical computations on heat conduction for a strongly chaotic system—the Lorentz gas. Heat conduction is characterized by nontrivial features: While the heat conductivity is well defined in the thermodynamic limit, a linear gradient appears only for quite small temperature differences. The key dynamical feature inducing such a behavior is recognized as deterministic diffusion (along transport direction) which is usually associated to full hyperbolicity. [S0031-9007(99)08614-7]

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What are the dynamical properties needed to have normal transport in a given system? This is a nontrivial question and for many years has been addressed according to different perspectives. It concerns, on one hand, the foundations of nonequilibrium statistical mechanics and, on the other hand, the practical issue of constructing microscopic models which agree with the macroscopic equations which describe transport. The latter set of "hydrodynamic" equations has a phenomenological character, is based on conservation laws (either local or global), and is derived without appealing to the microscopic structure of matter. This body of knowledge has been very successful, and still today it represents a very important branch of science with applications in physics, engineering, biology, and other fields. The hydrodynamic description emphasizes the role played by transport coefficients, such as diffusion constant, viscosity, and heat conductivity: establishing their existence starting at a mechanical level is quite a different task (see [1–4] as regards diffusion and [5] for viscosity).

Recently, a number of authors have proposed a novel approach to nonequilibrium statistical mechanics starting from microscopic dynamics: For instance, a full Liouvillian description for diffusion without appealing to the Boltzmann equation [3] has been proposed for particular models. More generally, for a class of hyperbolic systems (transitive Anosov) a guiding principle has been proposed (the so-called *chaotic hypothesis* [6]) as a prescription for extending equilibrium methods to nonequilibrium situations. We remark that in these works the randomness needed to obtain a consistent description of the *irreversible* macroscopic phenomena comes from the exponential instability of the microscopic chaotic dynamics.

According to these observations, it seems natural to investigate the problem of heat conduction as related to dynamical instability, and indeed a number of models have been investigated along such lines: In the case of the Lorentz gas with a random configuration of scatterers, it has been shown that the heat transport is normal in the Boltzmann-Grad limit [7], in which the Boltzmann equation is satisfied. Another group of studies (in which no Markovian limit is involved) have been devoted to one dimensional chains of nonlinearly coupled oscillators. There are strong numerical evidence [8] (see [9,10] for recent developments) for the validity of the Fourier heat conduction law in the so-called "ding-a-ling" (where oscillators exchange energy via intermediate hard spheres), while the situation is considerably more complicated in the Fermi-Pasta-Ulam chain (where oscillators are coupled by third and fourth order nonlinear terms) where, even above the chaoticity threshold, heat conductivity seems abnormal [11]. Both systems exhibit exponential instability in numerical simulations, thus positivity of the Lyapunov exponent cannot presumably be a sufficient condition to induce normal transport properties. While establishing a complete connection between ergodic properties and macroscopic transport features is still beyond reach, our will is to point out how deterministic diffusion may play an important role. In the model we investigate, mass and energy transport are directly related; however, we believe that our considerations may be applied to more general settings.

The model we consider is a two dimensional billiard, a Lorentz channel (LC) (see Fig. 1). It consists of two parallel lines of length L at distance h, that we take to be unity, and a series of semicircles of radius R placed in a triangular lattice along the channel. By construction no particle can move along the horizontal direction without colliding with the disks. The dynamics in the LC is mixing and all trajectories with nonzero projection on the x direction are of hyperbolic type; further it has positive Kolmogorov-Sinai entropy, and a well defined diffusion constant [2].

To induce transport of heat we place the LC between two heat reservoirs, which are modeled by stochastic

FIG. 1. Geometry of the model. The fundamental domain is indicated as well as the two heat reservoirs at different temperatures. The x coordinate goes along the channel and the y coordinate is perpendicular to it. The transport of heat goes along the x coordinate.

kernels of Gaussian type,

$$\mathcal{P}(v) = \pm\frac{|v|}{T}\exp\frac{-v^2}{2T}, \tag{1}$$

where v stands for the horizontal component of the velocity at the collision with the heat bath, and the signs are conveniently taken to eject back the particle to the scatterer after a collision with the heat baths. We set Boltzmann's constant equal to one. Transport takes place in the x direction, which is the transport coordinate. The channel consists of n replicas of a single fundamental cell (of length l, thus yielding a total length $L = ln$), so the thermodynamic limit is obtained upon taking larger and larger values of n and keeping the density (number of particles/n) fixed. As particles do not interact, this is equivalent to running long trajectories of a *single* particle and rescaling the flux of a factor n (if we consider unit density). In our simulations we have taken n to be 1, 5, 9, 13, and 17. We fix the temperature of one of the reservoirs T_0 and the temperature of the other heat bath is taken as $T_1 = T_0 + \Delta T$.

To compute the temperature field at the stationary state, we evaluate time averages as follows; we divide the configuration space in a set of boxes $\{C_i\}$. The time spent within a box in the jth visit is denoted by t_j and the total number of crossings of a box C_j during the simulation is N. We compute the kinetic energy $E_j(C_i)$ at the jth crossing of the box C_i and define the temperature field as

$$T_{C_i} = \langle E\rangle_{C_i} = \frac{\sum_{j=1}^{N} t_j E_j(C_i)}{\sum_{j=1}^{N} t_j}. \tag{2}$$

This defines the temperature field as a two coordinate (coarse grained) field $T(x, y)$. As transport is along the x coordinate, we will focus on the projection of T on the x-$T(x, y)$ plane.

The other quantity of relevance is heat flux, especially in the stationary state. Within the channel energy is conserved; it changes only at collisions with heat baths. Let $(\Delta E)_k$ denote the change of energy at the kth collision with a reservoir,

$$(\Delta E)_k = E_{\text{in}} - E_{\text{out}}. \tag{3}$$

Summing over N such events taking place during a time t_N, we have the following definition for heat flux:

$$j_N = \frac{1}{t_N}\sum_{j=1}^{N}(\Delta E)_j. \tag{4}$$

For large enough N we expect that heat flux to reach a stationary value, and this is indeed verified in our simulations.

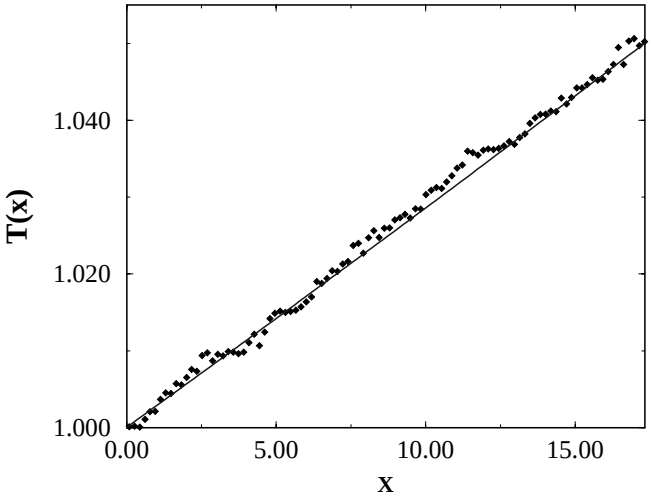

FIG. 2. Horizontal temperature field for $\Delta T = 0.05$. Diamonds were obtained by numerical simulation and are compared with Eq. (7), full line. The agreement is good. The number of fundamental cells in this simulation is $n = 5$, a typical single particle simulation involves millions of collisions with the reservoirs.

For small temperature differences ΔT the profile of local temperatures is linear, but when the temperatures of the two heat reservoirs are appreciably different then the profile has a nontrivial shape (see Figs. 2 and 3). In fact, to a high degree of accuracy, it is a nonlinear, rational function of the position x. We will give an analytical argument for this in the final part of the paper: From a numerical point of view this can be understood by noting that expression (2) is defined by a ratio. When separately plotting the numerator and the denominator, we observe that both are linear functions, with slopes of opposite sign (see Fig. 4).

In all cases, the temperature profile has a regular scaling under variations of the length of the chain. Let $T_{[0,1]}(x)$

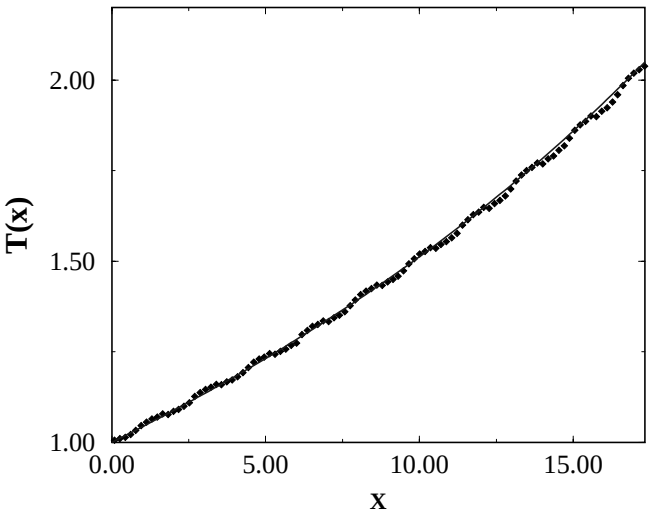

FIG. 3. As in Fig. 3 for the case $\Delta T = 1.05$; again the agreement with Eq. (7) (full line) is excellent.

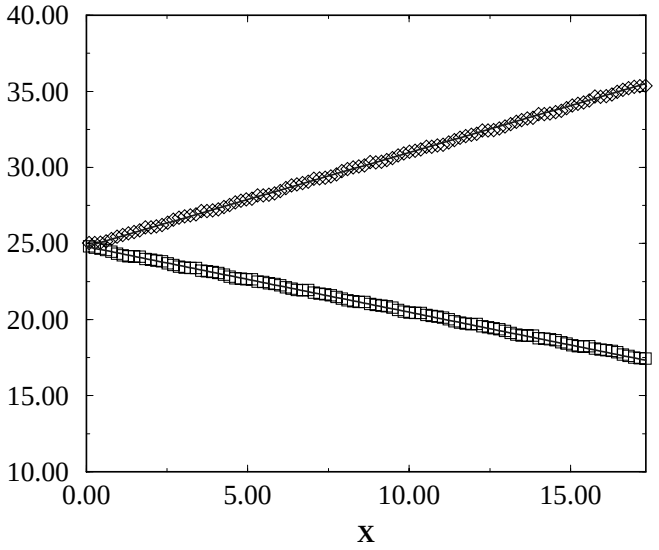

FIG. 4. Behavior of the numerator (diamonds) and denominator (squares) of Eq. (2). The temperature difference is $\Delta T = 1.05$. We can see that at the stationary state both fields are linear in transport direction X. The predictions of Eq. (7) are represented by full lines, the agreement is excellent. We remark that in this case the temperature field is not linear (see Fig. 3).

and $T_{[0,L]}(x)$ be the temperature fields of systems of size 1 and L, respectively, then we have

$$T_{[0,1]}(x) = T_{[0,L]}(x/L)\,. \tag{5}$$

In the case of linear behavior the temperature gradient is given by

$$\nabla T = \frac{T_1 - T_0}{L} = \frac{T_1 - T_0}{nl}\,, \tag{6}$$

which means that it scales as $1/n$.

To verify whether heat conductivity is normal, we have then to look at the way heat flux scales with length: For a single particle simulation we compute a flux $j_{(1)}(n)$. A correct implementation of the thermodynamic limit then consists in considering the flux corresponding to larger and larger systems with a constant density; that is, we have to look at the scaling of $j_{(n)}(n) = nj_{(1)}(n)$ (for a density of one particle per cell). We find that $j_{(n)}(n) \approx \alpha n^{-\beta}$, where our numerical values for $\beta \approx 0.98$–0.99 are very close to one (Fig. 5): The heat conductivity ($\kappa \approx \frac{j_{(n)}(n)}{\nabla T}$) is thus normal and the Fourier law is satisfied, in the regime of small temperature differences.

Finally, we give a simple argument, based on the use of macroscopic diffusion equations, that captures most of the details of our numerical findings. Let $n_0(x, E; t)$ be the density of particles of energy E whose last collision with a reservoir was with the left-hand one (at T_0), and let $n_1(x, E; t)$ be the corresponding quantity for the right reservoir (at temperature T_1). The reservoirs' properties are included by imposing

$$n_0(0, E; t) = \tilde{n}_0 \frac{1}{T_0}\, e^{-E/T_0},$$

and

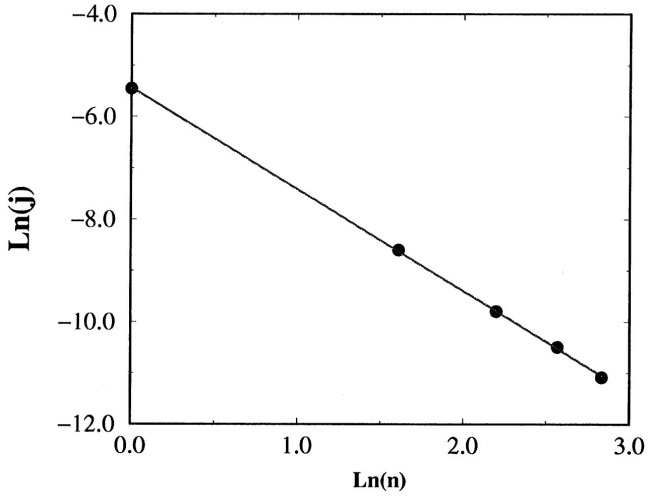

FIG. 5. Typical scaling behavior of the stationary heat flux $j_{(1)}(n)$ (for one particle) with the number of fundamental cells. The least-squares slope in the picture is -1.98, very close to 2 (see text).

$$n_1(L, E; t) = \tilde{n}_1 \frac{1}{T_1}\, e^{-E/T_1},$$

where L is the length of the channel. When a particle of one type hits the other reservoir it is absorbed. Now we suppose each n satisfies a diffusion equation (in the x variable), with a diffusion constant $D = D(E)$ (independent of the position). The stationary solutions are linear functions of the position and have to satisfy the following boundary conditions; $n_0(L, D) = 0$ and $n_1(0, D) = 0$. So the stationary solutions are

$$n_0(x, E) = \tilde{n}_0 \frac{1}{LT_0}\, e^{-E/T_0}(L - x)\,,$$

and

$$n_1(x, E) = \tilde{n}_1 \frac{1}{LT_1}\, e^{-E/T_1} x\,.$$

If we further impose that the total mass flux is zero (as in our numerical simulations), then

$$J = \int dE\, \frac{D(E)}{L} \left(\frac{\tilde{n}_0}{T_0}\, e^{-E/T_0} - \frac{\tilde{n}_1}{T_1}\, e^{-E/T_1} \right) = 0\,.$$

If we assume that $D(E) \sim E^{1/2}$ (to reproduce the correct scaling behavior of the Lorentz gas), we get

$$\sqrt{T_0}\,\tilde{n}_0 = \sqrt{T_1}\,\tilde{n}_1\,.$$

We can now compute the temperature field, by writing

$$T(x) = \frac{\int dE\, E[n_0(x, E) + n_1(x, E)]}{\int dE\, [n_0(x, E) + n_1(x, E)]}\,,$$

which yields

$$T(x) = \frac{T_1^{1/2} T_0 (L - x) + T_0^{1/2} T_1 x}{T_1^{1/2} T_0 (L - x) + T_0^{1/2} x}\,. \tag{7}$$

In Figs. 2 and 3, we plot the temperature field along the x direction obtained from the numerical simulations

together with the estimates from Eq. (7); the agreement is quite good. Further from Eq. (7), we can see that for a fixed temperature gradient the temperature field is a rational function on the transport coordinate, and when the gradient of temperature is small $T(x)$ is well approximated by a straight line. It is also evident that the temperature field scales with L, as expressed in Eq. (5). This simple model takes into account the main features of the numerical simulations and explains the data obtained in a satisfactory manner. The heat flux can also be computed and it depends on the temperatures in agreement with numerical results.

In conclusion, we have shown that the heat conductivity is finite and transport of heat is normal in a dynamical system, the Lorentz channel, for which the Kolmogorov-Sinai entropy is positive, and the orbits that are not fully contained in the y direction are hyperbolic. Most of our argument lies on the fact that the system exhibits normal diffusion [12], a property that is strictly connected to the requirement of full hyperbolicity along transport direction (see, for instance, [13] to see how relaxing this requirement may induce anomalous diffusion). Our simulations show that in this dynamical system the heat conductivity is normal and that for small temperature gradients the Fourier conduction law is valid. For larger temperature gradients the temperature profile is not linear anymore in the transport direction. It is a rational function depending on the temperatures of the heat reservoirs. This function scales with the length of the system. We expect that for dynamical systems sharing the same properties, as the system consider here, normal heat transport can be established. It would be interesting to obtain the heat conductivity coefficient for the system from a Liouvillian description, as considered in [3]. From the point of view of quantum mechanics, the ideas needed to understand from firm grounds transport processes are still in early stages of development [14]. It would be interesting to treat models, as the one presented here, in a quantum context to see whether it is possible or not to establish conditions under which transport takes place in a normal way. The fact that in the classical limit the system is chaotic, and the persistence of some traces of chaotic dynamics in the quantum case, for instance, in the structure of wave functions, may play in this respect an important role.

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