Heat conductivity in linear mixing systems

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We present analytical and numerical results on the heat conduction in a linear mixing system. In particular we consider a quasi-one-dimensional channel with triangular scatterers with internal angles which are irrational multiples of π, and we show that the system obeys the Fourier law of heat conduction. Therefore, deterministic diffusion and normal heat transport which are usually associated with full hyperbolicity, actually take place in systems without exponential instability.

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Given a particular classical, many-body Hamiltonian system, neither phenomenological nor fundamental transport theory can predict whether or not this specific Hamiltonian system yields an energy transport governed by the Fourier heat law [1]. Heat flow is universally presumed to obey a simple diffusion equation which can be regarded as the continuum limit of a discrete random walk. In consequence, transport theory requires that the underlying deterministic dynamics yield a truly random process. Therefore, it is not mere idle curiosity to wonder what class, if any, of many-body systems satisfy the necessary stringent requirements. Moreover, it now becomes increasingly meaningful to seek example of many-body systems which, using dynamics alone, can be shown to obey the Fourier heat law. A large number of papers have recently approached this problem, mainly via numerical simulations [2–12]. Leaving aside, for the purpose of the present paper, systems which conserve the total momentum, the general picture which emerges is that the positive Lyapunov exponent is a sufficient condition to ensure Fourier heat law. In particular, the paper [10] was precisely aimed at answering this question. Indeed in Ref. [10] the thermal conductivity was studied for a Lorentz channel—a quasi-one-dimensional billiard with circular scatterers—and it was shown to obey the Fourier law. The conclusion at which the above numerical computations point out appears quite natural. Indeed modern ergodic theory tells us that for K systems, a sequence of measurements with finite precision mimics a truly random sequence, and therefore these systems appear precisely those deterministically random systems tacitly required by transport theory. On the other hand we do not have rigorous results and in spite of several efforts, the connection between Lyapunov exponents, correlations decay and diffusive properties is still not completely clear. In a recent paper [13], a model has been presented which has a zero Lyapunov exponent and yet it exhibits an unbounded Gaussian diffusive behavior. Since diffusive behavior is at the root of normal heat transport, the above results constitutes a strong suggestion that normal heat conduction can take place even without the strong requirement of exponential instability. If this would be the case, then it may turn out to be an important step in the general attempt to derive macroscopic statistical laws from the underlying deterministic dynamics. Indeed, systems with zero Lyapunov exponent have zero algorithmic complexity and, at least in principle, are analytically solvable.

In this paper we consider a two-dimensional billiard model that consists of two parallel lines of length L at distance d and a series of triangular scatterers (Fig. 1). In this geometry, no particle can move between the two reservoirs without suffering elastic collisions with the triangles. Therefore this model is analogous to that studied in Ref. [10] with triangles instead of discs, and the essential difference is that in the triangular model discussed here the dynamical instability is linear and therefore the Lyapunov exponent is zero. Strong numerical evidence has been recently given [14] that the motion inside a triangular billiard, with all angles irrational with π is mixing, without any time scale. Moreover, an area preserving map, which was derived as an approximation of the boundary map for the irrational triangle, when considered on the cylinder shows a nice Gaussian diffusive behavior even though the Lyapunov exponent of the map is zero [13]. It is therefore reasonable to expect that the motion inside the irrational polygonal area of Fig. 1 is diffusive thus leading to normal conductivity.

In the following we present careful numerical investigations of the energy transport in the system of Fig. 1 both by direct numerical simulation of energy flow for the system in contact with thermal baths as well as via the Green-Kubo approach. Our results provide convincing evidence that, if

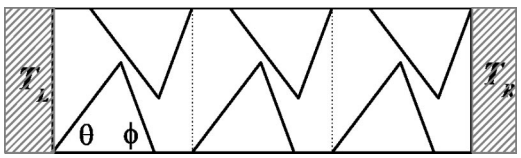

FIG. 1. The geometry of the model. Particles move in the region outside the triangular scatterers. The x coordinate goes along the channel and y is perpendicular to it. The two heat reservoirs at temperatures T_L and T_R are indicated. The length of each cell is $l=3$, the base of the triangles is $a=2.19$, and the distance between the two parallel lines is $d=1.8$. The geometry is then uniquely specified by assigning the internal angles θ and ϕ.

the angles θ and ϕ are irrational multiples of π, the system obeys Fourier law and the coefficients of thermal conductivity computed via the two approaches, coincide.

In our computations we model the heat baths by stochastic kernels of Gaussian type, namely, the probability distribution of velocities for particles coming out from the baths is

$$P(v_x)=\frac{|v_x|}{T}\exp\left(-\frac{v_x^2}{2T}\right),$$

$$P(v_y)=\frac{1}{\sqrt{2\pi T}}\exp\left(-\frac{v_y^2}{2T}\right), \tag{1}$$

for v_x and v_y, respectively.

The total length of the channel is $L=Nl$ where N and l are the number and the length of the fundamental cells. For the irrational angles we take $\theta=(\sqrt{2}-1)\pi/2$ and $\phi=1$. By increasing L, the number of particles per cell must be kept constant. However, since the particles do not interact we will consider the motion of a single particle over long times and then rescale the flux.

We turn now to the definition of the two relevant quantities: the internal temperature and the heat flux. The temperature field at the stationary state is calculated following the idea used in Ref. [10], namely, we divide the configuration space in slices $\{C_i\}$. The time spent by the particle within the slice in the jth visit is denoted by t_j and the total number of crossings of a slice C_i during the simulation is M. The temperature is defined by

$$T_{C_i}=\frac{\sum_j^M t_j E_j(C_i)}{\sum_j^M t_j}, \tag{2}$$

where $E_j(C_i)$ is the kinetic energy at the jth crossing of the slice C_i. Since the energy changes only at collisions with the heat baths, we define the heat flux as

$$j(t_c)=\frac{1}{t_c}\sum_{k=1}^{N_c}(\Delta E)_k, \tag{3}$$

where $(\Delta E)_k=E_{in}-E_{out}$ is the change of energy at the kth collision with the heat bath and N_c is the total number of such collisions which occur during time t_c.

For sufficiently long integration times ($>10^{10}$ time unit) both the internal temperature field and the heat flux reach a stationary value. We have checked that the temperature profile obeys the law given in Ref. [10]. For small temperature differences ΔT, it is a linear function, as illustrated in Fig. 2,

$$\nabla T=\frac{T_R-T_L}{L}. \tag{4}$$

In the calculation of the temperature profile shown in Fig. 2 and heat flux shown in Fig. 3, the total simulation times are larger than 1.2×10^{11} units for system size $N<100$, and larger than 2.4×10^{11} units for $N>100$. The time unit is defined as the time a particle, with velocity $v=1$, takes to cross a unit length of the channel.

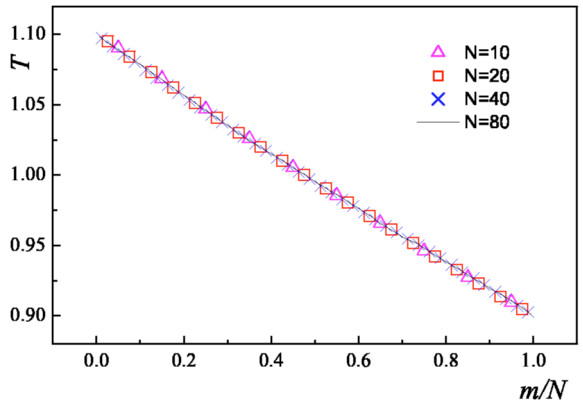

FIG. 2. Internal local temperature as a function of the rescaled cell number m/N for the irrational case with $\theta=(\sqrt{2}-1)\pi/2$ and $\phi=1$. The total number N of cells is $N=10$ ($\triangle$), $N=20$ ($\square$), $N=40$ ($\times$), and $N=80$ (solid line). Here $T_L=1.1$, $T_R=0.9$, $l=3$. Notice the quite good scaling behavior of the temperature field.

In order to study the dependence of the heat flux on the system size, we need to consider larger and larger systems, keeping the particles density constant. The corresponding heat flux (for a density of one particle per unit length) is $J=Lj$, where j is the flux computed with a single particle simulation. In Fig. 3, we plot the heat flux J as a function of the system size N. For the irrational case, the best fit gives $J=AN^{-\gamma}$, with $\gamma=0.99\pm0.01$ and $A=0.015$. The coefficient of thermal conductivity is therefore independent on N, which means that the Fourier law is obeyed and its numerical value is $\kappa=-(J/\nabla T)=0.225$.

The point under discussion here is very delicate and numerical experiments must be very accurate and reliable in order to reach clear conclusions. We have therefore checked the validity of our result by an independent approach, via a Green-Kubo type formalism, by studying the diffusive properties of our model isolated from thermal baths.

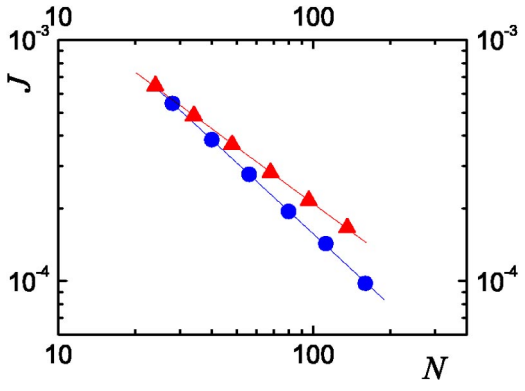

FIG. 3. Scaling behavior of the stationary heat flux J as a function of the system size for the irrational case of Fig. 1 (●) and for the rational case (▲) (see later in the text). N is the number of fundamental cells. The best-squares fit gives a slope -0.99 ± 0.01 for the irrational case and -0.78 ± 0.01 for the rational one.

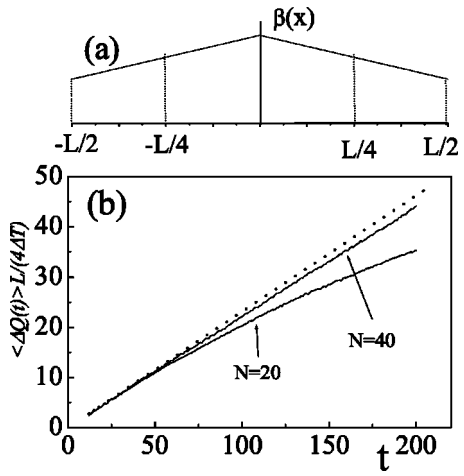

FIG. 4. (a) Initial temperature distribution $\beta(x)=1/T(x)$ with $\beta(0)=1.1, \beta(\pm L/2)=0.9$. (b) The rescaled heat flow $\langle \Delta Q(t)\rangle/2T^2\nabla\beta$ versus time t for different values of chain length N for the irrational case. The dotted line has slope 0.225.

In our numerical calculations, we follow Ref. [3], namely, we consider the system with periodic boundary conditions and with an initial temperature distribution $\beta(x)$ given in Fig. 4(a). Then we calculate how the heat flows from the half hotter part ($L/4<|x|<L/2$) of the system to the half colder part ($-L/4<x<+L/4$). At time $t=0$ we take a Maxwellian distribution of velocities, namely, $P(v_{x,y})=\exp\{-v_{x,y}^2/[2T(x)]\}/\sqrt{2\pi T(x)}$. If we denote by $Q(t)$ the energy contained in the cold half part of the chain then, if the system obeys the Fourier law, the quantity $\langle \Delta Q(t)\rangle = \langle Q(t)-Q(0)\rangle$ must increase linearly with time t, $\langle \Delta Q(t)\rangle = (2\kappa T^2\nabla\beta)t$. Clearly the linear increase takes places only for times smaller than the sound transit time across channel. The numerical results are shown in Fig. 4(b) where the dotted line, which fits the initial linear increase of the curve for $N=40$, has slope $\kappa=0.225$ thus indicating a very good agreement with simulations with thermal baths.

Another important characteristic which is relevant for transport properties is the decay of the velocity autocorrelation function. In Fig. 5 we show the decay of the absolute value of the normalized velocity autocorrelation $C(t)=\langle v_x(0)v_x(t)\rangle/\langle v_x^2(0)\rangle$ for the irrational case. This function decays as $|C(t)|\sim t^{-\alpha}$ with $\alpha\approx 3/2$.

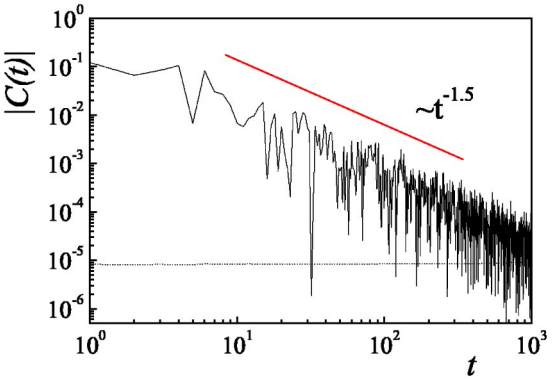

FIG. 5. The absolute value of the velocity autocorrelation function $|C(t)|$ averaged over 6×10^5 orbits initially with unit velocity amplitude but random directions. The solid line has slope $-3/2$. The dotted line shows the statistical errors.

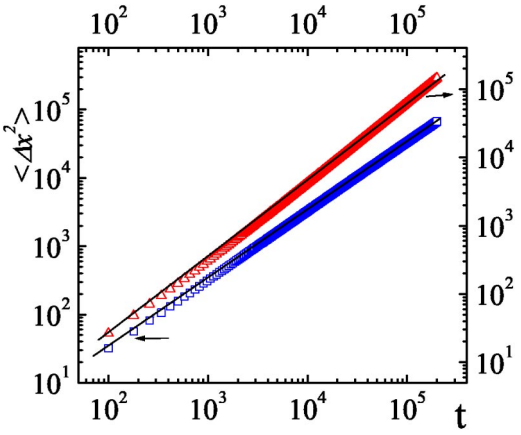

FIG. 6. Diffusive properties of our model isolated from thermal baths. In the irrational case (left scale), $\langle \Delta x^2\rangle = 0.308t^{1.007}$ (□); in the rational case (right scale), $\langle \Delta x^2\rangle = 0.082t^{1.178}$ (△). $\Delta x^2 \equiv [x(t)-x(0)]^2$. In the numerical calculation, 4×10^5 particles are used. The particles are initially at $x=0$ (in the center of the chain) and the initial velocities obey the Maxwell-Boltzmann distribution at temperature $T=1$.

In Fig. 6 we show the diffusive behavior of our model isolated from thermal baths. A clear diffusive behavior $\langle \Delta x^2\rangle = 2Dt$ for the irrational case is observed with diffusion coefficient $D=0.15$.

In fact, in our model, we can establish a connection between the thermal conductivity κ and the diffusion coefficient D. Indeed, the average time a particle takes to travel from the left to the right bath and vice versa is

$$\langle t_{LR}\rangle = \langle t_{RL}\rangle = \frac{L^2}{2D}; \tag{5}$$

then according to Eq. (3), we can write the heat current as

$$j = \frac{\int_0^\infty \frac{v^2}{2}[P(v,T_L)-P(v,T_R)]dv}{\langle t_{LR}\rangle + \langle t_{RL}\rangle}, \tag{6}$$

where $P(v,T)=(4\pi/(2\pi T)^{3/2})v^2\exp(-v^2/2T)$ is the distribution for the modulus of velocity of particles coming out from the baths [see Eq. (1)]. The thermal conductivity $\kappa = -Lj/\nabla T$ is thus

$$\kappa = \frac{3}{2}D. \tag{7}$$

We have numerically tested this formula. The thermal conductivity calculated from Figs. 2 and 3 is $\kappa=0.225$. On the other hand the diffusion coefficient calculated from Fig. 6 is $D=0.15$ which, according to the above relation, gives $\kappa = 3D/2 = 0.225$.

As expected, a completely different behavior is obtained when the angles θ and ϕ are rational multiples of π. The

case with $\theta=\pi/5$ and $\phi=\pi/3$, is shown in Fig. 6 (triangles), and leads to a clear anomalous diffusive behavior indicating the absence of the Fourier law. Correspondingly, the simulations with the heat baths (solid triangles in Fig. 3) indicate a divergent behavior of the coefficient of thermal conductivity $\kappa\sim N^{0.22}$.

In conclusion, when all angles are irrational multiples of π the model shown in Fig. 1 exhibits the Fourier law of heat conduction together with nice diffusive properties, and the numerical value of the thermal conductivity computed via a Green-Kubo approach agrees with that obtained by direct numerical simulations with thermal baths. However, when all angles are rational multiples of π, the model shows abnormal diffusion and the heat conduction does not follow the Fourier law.

One may argue that the model considered here is somehow artificial and far from realistic physical models. However, the problem discussed here is quite delicate and controversial and our main purpose is to understand which dynamical properties are necessary and sufficient to derive the Fourier law. In this respect billiards like models are very convenient, since they are more suitable for analytical and numerical analysis.

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