Fourier Law in the Alternate-Mass Hard-Core Potential Chain

Baowen Li,[1] Giulio Casati,[2,3,1] Jiao Wang,[4] and Tomaž Prosen[5]

[1]*Department of Physics, National University of Singapore, Singapore 117542, Republic of Singapore*
[2]*Center for Nonlinear and Complex Systems, Universita' degli studi dell'Insubria, Como, Italy*
[3]*Istituto Nazionale di Fisica della Materia, Unita' di Como, and Istituto Nazionale di Fisica Nucleare, Sezione di Milano, Milano, Italy*
[4]*Temasek Laboratories, National University of Singapore, Singapore 119260, Republic of Singapore*
[5]*Physics Department, Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia*

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We study energy transport in a one-dimensional model of elastically colliding particles with alternate masses m and M. In order to prevent total momentum conservation, we confine particles with mass M inside a cell of finite size. We provide convincing numerical evidence for the validity of Fourier law of heat conduction in spite of the lack of exponential dynamical instability. Comparison with previous results on similar models shows the relevance of the role played by total momentum conservation.

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After several decades of intensive investigations [1–9], the precise conditions that a dynamical system of interacting particles in 1D must satisfy in order to obey the Fourier law of heat conduction are still not known.

For noninteracting particles in external potential, it has been shown [3] that exponential local instability leads to Fourier law. Actually, even linear mixing without exponential instability, such as that found in generic polygonal billiards [10], has been shown to be sufficient for a diffusive heat transport [4]. In addition, several interacting nonintegrable many-particle systems which clearly obey the Fourier law have been proposed and investigated [1]. However, it should be noted that in the above models, the total momentum is not conserved. In several recent papers [5,6,8] it has been suggested that total momentum conservation does not allow Fourier law. Moreover, using renormalization group [8], it is argued that a generic momentum conserving particle chain should, in a macroscopic limit, be equivalent to 1D hydrodynamics with thermal noise where the coefficient of thermal conductivity should diverge with the system size L as $\kappa(L) \propto L^{1/3}$. However, most existing numerical data do not support this universal constant. Instead, it has been proposed that $\kappa(L) \propto L^{2-2/\alpha}$ [9], where α is the exponent of the diffusion ($\langle \Delta x^2 \rangle = 2Dt^{\alpha}$), $0 < \alpha \leq 2$.

We remark that there exists a model [11] [a particle chain with interparticle potential $V(x) = 1 - \cos(x)$] in which, in spite of momentum conservation, the heat conduction seems to obey the Fourier law. The reason for such behavior is not clear and the precise role of the total momentum conservation needs to be clarified.

In previous papers two models have been considered; both are mixing and without exponential instability: (i) the triangular billiard channel [4], which exhibits Fourier law, and (ii) the alternate mass hard-point gas model [7], in which the coefficient of thermal conductivity diverges with the system size. The difference between the two models is that in case (ii) the total momentum is conserved, while in case (i) it is not.

On the other hand, model (i) has been criticized since, in spite of the fact that one can perfectly well define an internal local temperature, there is no mechanism to provide local thermal equilibrium due to lack of interparticle interaction, and this may look somehow unsatisfactory. In this Letter, we consider a model which is identical to the alternate mass hard-point gas [7]; namely, it consists of a one-dimensional chain of elastically colliding particles with alternate masses m and M. Here, however, in order to prevent total momentum conservation, we confine the motion of particles of mass M (bars) inside unit cells of size l. Schematically, the model is shown in Fig. 1 in which particles with mass m move horizontally and collide with bars of mass M which, besides suffering collisions with the particles, are elastically reflected back at the edges of their cells. In between collisions, particles and bars move freely. Our numerical results clearly indicate that our model, contrary to the translationally invariant model [7], obeys the Fourier law. The only difference between the two models is total momentum conservation.

The total length of the system is $L = Nl$, where N is the number of fundamental cells. In all the calculations presented in this Letter, we fix $l = 1$ so that $L = N$. We

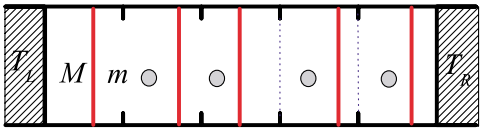

FIG. 1 (color online). The geometry of the model. The elementary cell (indicated by two dotted lines) has unit length $l = 1$. The bars have mass $M = 1$, and the particles have mass $m = (\sqrt{5} - 1)/2$. The two heat baths at temperatures T_L and T_R are indicated.

also take $M = 1$, $m = (\sqrt{5} - 1)/2$ and we verify that the numerical value of the mass ratio is not relevant.

A direct way to test whether the system obeys the Fourier law is to put two heat baths with small temperature difference into contact with the two ends of the system and check the dependence of the thermal current on the system size. Here statistical thermal baths are used; that is, when the first (last) bar collides with the left (right) side of the first (last) cell, it is injected back with a new speed generated from the distribution

$$P_{L,R}(v) = \frac{M|v|}{T_{L,R}} \exp\left(-\frac{Mv^2}{2T_{L,R}}\right). \tag{1}$$

This assures, for small temperature gradients, that the edge particles have canonical (Maxwellian) velocity distribution. In our simulations we fixed $T_L = 1.1$ and $T_R = 0.9$.

For any given initial condition, after a long enough transient time, the system reaches a stationary state. Then one may compute the local temperature, defined as

$$T(x) = \langle M v_i^2 \rangle \quad \text{for} \quad x = x_i^{\text{bar}} = (i - 0.5), \quad i = 1, \ldots N, \qquad T(x) = \langle m u_j^2 \rangle \quad \text{for} \quad x = x_j^{\text{part}} = j, \quad j = 1, \ldots N - 1. \tag{2}$$

Here x_i^{bar} and x_j^{part} can be regarded roughly as the time-averaged positions of the ith bar and the jth particle.

In Fig. 2 we plot the temperature profile versus the scaled length x/N for different values of N. Notice the good linear scaling behavior. In both Figs. 2 and 3, the average time measured by the total collisions number is larger than 5×10^{10} for $N = 512$, which is the largest system size we have considered.

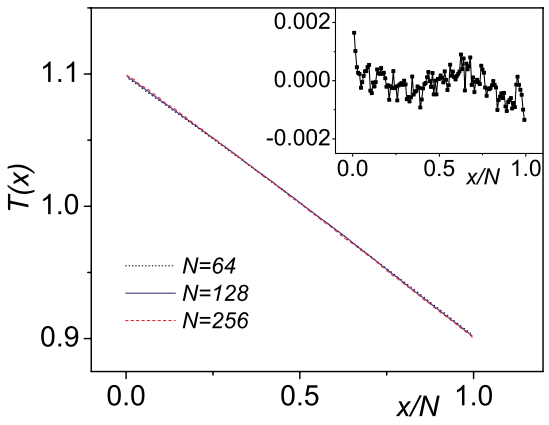

FIG. 2 (color online). Internal local temperature as a function of the rescaled position x/N. The total number N of cells is $N = 64$ (dotted line), $N = 128$ (solid line), and $N = 256$ (dashed line). Notice the good scaling behavior of the temperature field. The inset shows kurtosis of the local velocity distribution.

We should emphasize that in previous models [3,4,7] the local thermal equilibrium cannot be established, whereas in the model considered here, the local thermal equilibrium is well established independently of the thermal baths used. We have checked that the velocity distribution function for each bar and particle is a Gaussian function whose width gives the local temperature, whereas the kurtosis, defined by $K(x_i^{\text{bar}}) = (\langle v_i^4 \rangle / 3\langle v_i^2 \rangle^2) - 1$, for bars, and $K(x_j^{\text{part}}) = (\langle u_j^4 \rangle / 3\langle u_j^2 \rangle^2) - 1$, for particles, are close to zero. The kurtosis versus the bar/particle site is plotted in the inset in Fig. 2.

In Fig. 3 we show the stationary time-averaged heat flux $\langle j \rangle$ as a function of the system size N. The best fit of numerical data gives $\langle j \rangle = 0.24 N^{-\gamma}$ with $\gamma = 0.99 \pm 0.01$. The coefficient of thermal conductivity appears therefore to be independent of N, which means that the Fourier law is obeyed. Its numerical value reads as $\kappa = -(\langle j \rangle / \nabla T) = 1.20 \pm 0.05$.

To investigate how the energy diffuses along the system, we set $T_L = T_R = 1$. Then, after the equilibrium state is reached, the middle particle [i.e., the 100th one for $N = 200$ in Fig. 4(a)] is given a speed $u = 2/\sqrt{m}$, so that its energy is 4 times bigger than the equilibrium average. The evolution of the energy profile along the chain is then recorded afterwards. To suppress statistical fluctuations, 10^6 realizations are taken into account for the average. The width of the energy profile can be measured by its second moment

$$\sigma^2(t) = \frac{\int [E(x,t) - E_0](x - x_0)^2 dx}{\int [E(x,t) - E_0] dx}, \tag{3}$$

where $E(x,t) = \sum_j (m u_j^2/2) \delta(x - x_j^{\text{part}}) + \sum_i (M v_i^2/2) \times \delta(x - x_i^{\text{bar}})$. In our calculations for Fig. 4, $E_0 = 0.5$ and $x_0 = 100$. The energy profile spreads as $\sigma^2(t) = 2Dt$ with $D = 1.20 \pm 0.01$ [Fig. 4(b)], which agrees with the thermal conductivity $\kappa = 1.20 \pm 0.05$ very well.

If the system obeys the Fourier law, its thermal conductivity can also be obtained via the Green-Kubo formula

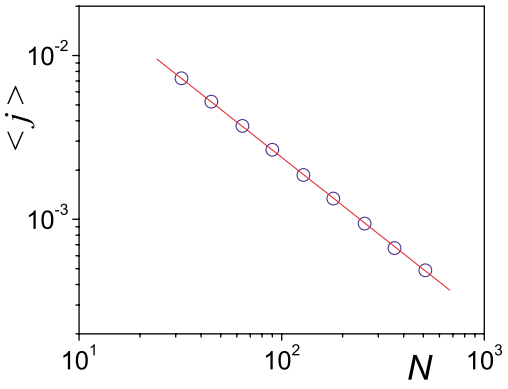

FIG. 3 (color online). Scaling behavior of the stationary time-averaged heat flux $\langle j \rangle$ as a function of the system size N. The least squares fit gives a slope -0.99 ± 0.01.

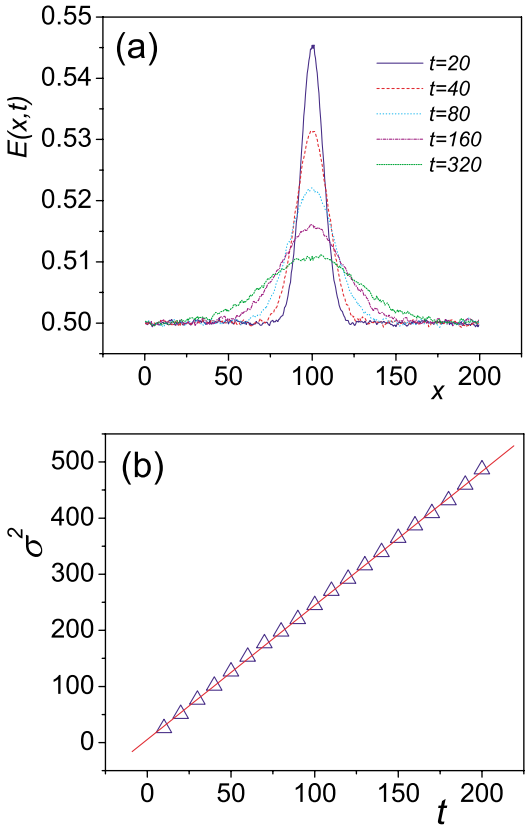

FIG. 4 (color online). Diffusive property of our model. Initially, the system is at equilibrium with temperature $T = 1$; then an impulse is given to the particle in the middle of the chain. (a) Energy distribution along the channel at different times. (b) The second moment of the energy distribution versus time.

$$\kappa = \lim_{t\to\infty} \lim_{N\to\infty} \frac{1}{NT^2} \int_0^t \langle J(\tau)J(0)\rangle d\tau, \tag{4}$$

where the heat current can be written as [12]

$$J = \sum_{i=1}^{N} \frac{1}{2}(Mv_i^3 + mu_i^3). \tag{5}$$

In applying Green-Kubo theory, a periodic boundary condition is imposed on the system.

In Fig. 5 we plot the quantity

$$\kappa(t) = \frac{1}{NT^2} \int_0^t \langle J(\tau)J(0)\rangle d\tau, \tag{6}$$

as a function of time t for $N = 24$. Since $\langle J(\tau)J(0)\rangle$ decays in time very fast (see Fig. 6), one has that $\kappa(t)$ tends to κ very fast as well. The numerical result gives $\kappa = 1.22$, in excellent agreement with the heat conductivity obtained via simulations with thermal baths ($\kappa = 1.20$).

In Fig. 6 we plot the absolute value of current-current time correlation function $C(\tau) = \langle J(\tau)J(0)\rangle$ versus τ for

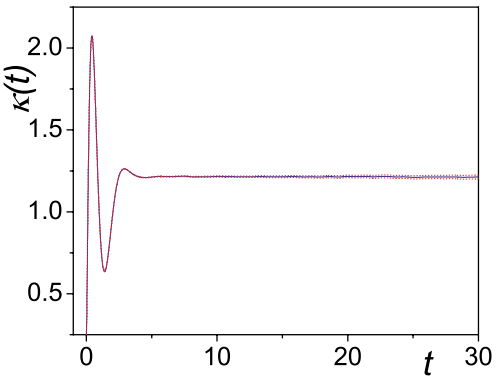

FIG. 5 (color online). The Green-Kubo integral versus t for $N = 24$ and $T = 1$. To get $\langle J(\tau)J(0)\rangle$ used in (6), a single orbit is followed up to time $t_l = 4.8 \times 10^6$; the error, $\delta\langle J(\tau)J(0)\rangle$, is estimated in the same way as in Fig. 6. Dotted lines (almost indistinguishable) indicate the error boundaries of $\kappa(t)$, obtained by replacing the integrand in (6) by $\langle J(\tau)J(0)\rangle \pm \delta\langle J(\tau)J(0)\rangle$, respectively. The errors are very small and negligible.

$N = 2$. It is interesting to remark that numerical results seem to indicate a clear exponential decay of correlation $C(\tau)$, which seems in contradiction with the linear, marginally unstable, dynamics. Indeed, as shown in [10], the existence of periodic orbits in a marginally unstable system necessarily implies an asymptotic power-law decay of correlation. The asymptotic power-law tail may be, however, very difficult or impossible to observe numerically. In fact, what we see is a transient exponential decay over several orders of magnitude which is very robust against changing system parameters, such as m/M or N.

Finally, we study the behavior of the thermal conductivity κ versus the mass ratio m/M (Fig. 7). It is

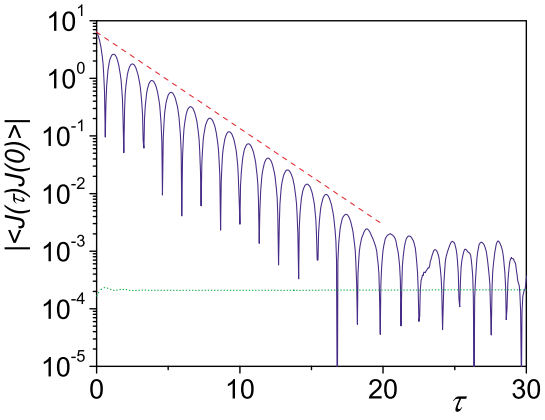

FIG. 6 (color online). Absolute heat current correlation function for $N = 2$ and $T = 1$. The time average is taken over a single orbit up to time $t_l = 5 \times 10^7$. The dotted line shows the standard deviation of $\langle J(\tau)J(0)\rangle$ estimated over $(t_l - \tau)/\delta\tau_0$ values of $J(\tau + \tau_0)J(\tau_0)$ obtained by changing τ_0 with a step $\delta\tau_0 = 0.05$ along the orbit. The dashed line indicates an exponential decay $\exp(-0.38\tau)$.

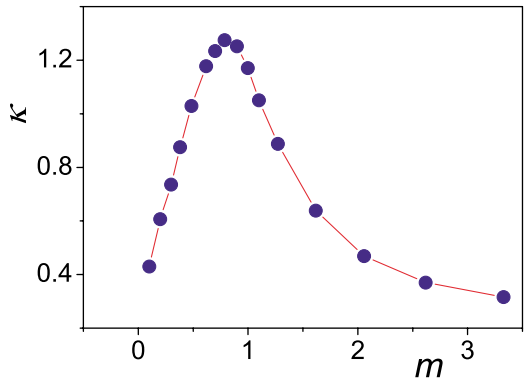

FIG. 7 (color online). The thermal conductivity κ (bullet) versus the mass m for $N = 24$ and $T = 1$. $M = 1$. The solid curve is drawn to guide the eyes.

interesting to note that even at $m = M = 1$ one finds a finite conductivity κ, which is close to the maximum of the curve in Fig. 7, in spite of the fact that in this case ($m = M$) the dynamics is *pseudo-integrable* since, for the isolated system, the set of magnitudes of the velocities of initial particles is conserved. However, the system $m = M$ is *not strictly integrable* since the topology of invariant surfaces is more complex than the one of the tori. Notice also that local thermal equilibrium is absent for $m = M$.

In the present Letter we have demonstrated diffusive energy transport and Fourier law for a marginally stable (nonchaotic) interacting many-particle system. We have thus clearly demonstrated that exponential instability (Lyapunov chaos) is not necessary for the establishment of the Fourier law. Furthermore, we have shown that breaking the total momentum conservation is crucial for the validity of Fourier law while, somehow surprisingly, a less important role seems to be played by the degree of dynamical chaos.

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[12] Notice that an alternative expression for the particle current in terms of energy transfer during collisions (such as that used in, e.g., [1]) seems to be more appropriate. The results, however, are the same.