Simple One-Dimensional Model of Heat Conduction which Obeys Fourier's Law

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(Received 13 February 2001)

We present the computer simulation results of a chain of hard-point particles with alternating masses interacting on its extremes with two thermal baths at different temperatures. We found that the system obeys Fourier's law at the thermodynamic limit. This result is against the actual belief that one-dimensional systems with momentum conservative dynamics and nonzero pressure have infinite thermal conductivity. It seems that thermal resistivity occurs in our system due to a cooperative behavior in which light particles tend to absorb much more energy than the heavier ones.

Fourier developed his theory of heat conduction at the beginning of the nineteenth century. It states (in actual notation) that the temperature profile of an isolated system will evolve following the conservation equation

$$c_v(T) \frac{\partial}{\partial t} T(\underline{r}, t) = \underline{\nabla} \cdot [\kappa \underline{\nabla} T], \tag{1}$$

where $T(\underline{r}, t)$ is the temperature measured by a probe at position $\underline{r}$ at time t, $c_v(T)$ is the specific heat per unit volume, and κ is the thermal conductivity. Fourier's law may be applied, in particular, to a system in contact with two heat reservoirs at different temperatures placed at $x = 0$ and $x = L$. In this case, the stationary state has the property of

$$J = -\kappa(T) \frac{dT}{dx} = \text{const}, \tag{2}$$

where J is the stationary heat flux through the system. Notice that one should assume that there is not mass transport and/or other mechanisms different than heat conduction. This law has been extensively tested in experiments in fluids and crystals. However, we do not understand yet many of its fundamental aspects (see, for instance, the review in [1]). In particular, its derivation from a microscopic Hamiltonian dynamics and the existence of a local equilibrium that gives meaning to the local temperatures are open problems.

Actually, heat transport in one-dimensional systems is an interesting problem in the context of both nonlinear dynamics and statistical physics. Long ago, Peierls proposed a successful perturbative theory, based on a phonon scattering mechanism, in order to explain the thermal conductivity in solids [2]. In particular, Peierls theory predicts that we do not expect a finite thermal conductivity in one-dimensional monoatomic lattices with interactions between nearest neighbors. Accordingly, the temperature profile of a chain of N harmonic oscillators is flat and its thermal conductivity goes like $\kappa(N) \simeq N$ for large enough N. More generally, any integrable Hamiltonian system is expected to have such divergent conductivity because its

associated normal modes behave like a gas of noninteracting particles carrying energy from the hot source to the cold one with no loss. On the other hand, there are nonintegrable systems, to which the Peierls theory does not apply directly, whose behavior is known to agree with its prediction. For example, the thermal conductivity of the Fermi-Pasta-Ulam-β model goes like $\kappa(N) \simeq N^\alpha$, with $\alpha = 0.43$. The value of α can be predicted by using a mode coupling approximation to the corresponding interacting gas of phonons [3]. An exception to these results is systems with translation invariant Hamiltonian that have zero pressure. For instance, a one-dimensional chain of rotators shows normal heat conduction [4].

In general, as an extension of the prediction from the Peierls argument, it is presently believed that one should not expect in general a finite thermal conductivity in one-dimensional systems with momentum conserving interactions and nonzero pressure [5]. The goal of this Letter is to show a counterexample to the above belief. We introduce a system that, although its particle interaction conserves momentum and the pressure is nonzero, the energy behavior has a diffusive character and Fourier's law holds. Therefore, we think that in one-dimensional systems with nonzero pressure, the conservation of momentum does not seem to be a key factor to find anomalous heat transport.

Let us introduce our model. In a line of length L, there are N point particles of different masses interacting exclusively via elastic collisions. In order to minimize the finite size effects, the particles have only two different masses and they alternate along the line, i.e., $m_{2l-1} = 1$ and $m_{2l} = (1 + \sqrt{5})/2$ with $l = 1, \ldots, N/2$. We have chosen the masses of the even particles to be the most irrational number in order to minimize possible periodicities, resonances, or nonergodic behaviors. At the extremes of the line there are thermal reservoirs at fixed temperatures $T_1 = 1$ and $T_2 = 2$ at $x = 0$ and $x = L$, respectively. We simulate the reservoirs by using the following process: each time particle 1 (L) hits the boundary at $x = 0$ ($x = L$) with velocity v, the particle is reflected with the velocity modulus

$$v' = \left[\frac{-2}{m_{1(L)}\beta_{1(2)}} \ln\left(1 - e^{-\frac{\beta_{1(2)}}{2}m_{1(L)}v^2} \right) \right]^{1/2}, \quad (3)$$

where $\beta_{1(2)} = 1/T_{1(2)}$. This reversible and deterministic map is due to van Beijeren [6]. In order to check the influence of the type of reservoir into the system properties we have also used more conventional stochastic boundary conditions, but only different finite size effects and no other relevant behavior have been observed. For $T_1 \neq T_2$ there is a flow of energy from the high temperature reservoir to the low one, and the system then evolves to a nonequilibrium stationary state. A version of this model in which the masses are randomly placed was already studied by us [7]. In this work, the system thermodynamic limit behavior was not considered, but the local equilibrium property was demonstrated. Our goal in this Letter is to check if the system has a finite thermal conductivity in the thermodynamic limit $N, L \rightarrow \infty$ with $N/L = 1$. With this aim we performed a detailed numerical analysis along the following lines.

(1) The existence of a nontrivial thermal profile.—We define the local temperature by measuring the mean kinetic energy of each particle and its mean position at the stationary state. We computed the profiles for $N = 50$, 100, 500, 1000, 2000, with fixed $N/L = 1$, $T_1 = 1$, and $T_2 = 2$. Figure 1 shows the local temperature as a function of x/N (by seeking clearer figures, we have performed local averaging of the temperatures and positions to draw only 100 points; no difference is found by drawing all the points). We see in Fig. 1 that the temperatures follow linear profiles in the interval $x/N \in [0.4, 0.6]$ with slopes depending on the system size. This slope apparently tends to converge to unity but we find that the convergence is so slow that we cannot
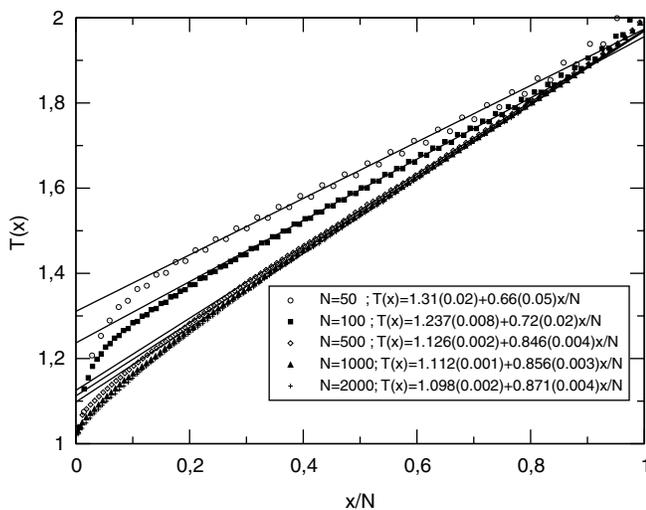
(numerically) exclude the possibility that the limiting temperature profile is nonlinear (which is not against Fourier's law). In any case, a nonflat profile is clearly expected in the thermodynamic limit.

(2) The averaged heat current.—If Fourier law holds and the heat conductivity is finite, the mean heat current, $J = N^{-1} \sum_{i=1}^{N} m_i v_i^3 / 2$, should go to zero as $1/N$ whenever $T_{1,2}$ and N/L are kept fixed. The data do not give us a conclusive answer. In fact, we fitted the experimental points (J corresponding up to seven different N's) to behaviors like $J = aN^{-0.71}$, $J = aN^{-1}(1 + bN^{-1})$, $J = aN^{-1}(1 + b\ln N)$, and $J = aN^{-1}(1 + b/\ln N)$ all of them with regression parameters of order 0.999. This reflects that the corrections to the leading order are dominant and that we are far from the asymptotic regime for the observable heat current [8]. Therefore, the direct use of the Fourier law $\kappa = JN/(T_2 - T_1)$ does not clarify (from the numerical point of view) the existence of a finite heat conductivity in the thermodynamic limit.

(3) The current-current self-correlation function.—The heat conductivity is connected to the current-current self-correlation function evaluated at equilibrium via its time integral (Green-Kubo formula). The integral has
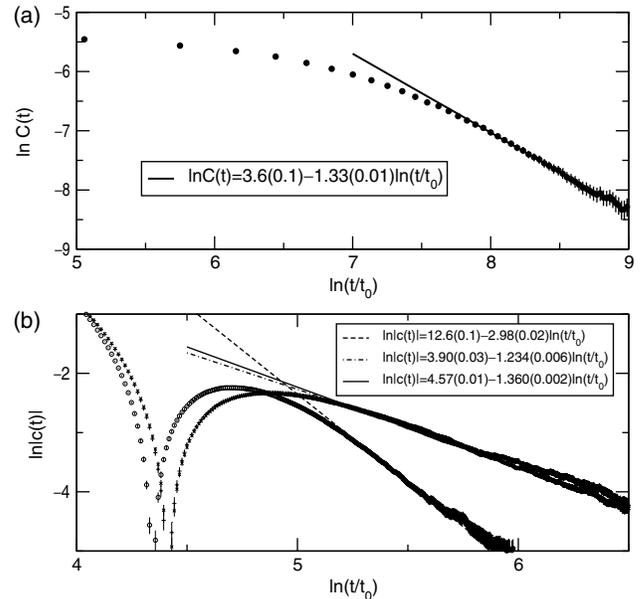

FIG. 1. Temperature profile at the stationary state for N particles. Lines are the best fits of the data in the interval $x/N \in [0.4, 0.6]$. The corresponding equations are shown in the box. Errors in the coefficients are in brackets.

FIG. 2. (a) Logarithm of the total heat current self-correlation function versus logarithm of t. The data correspond to a system with $N = 500$. The solid line is the best fit for the asymptotic region. The number of independent averaged histories is of order 10^7. (b) The logarithm of the absolute value of the local heat current self-correlation function versus logarithm of t (see text). ($+$) and ($\times$) symbols correspond to a system with $N = 500$ and $N = 1000$, respectively. ($\circ$) are the results for a system of $N = 500$ particles with equal masses. Lines are the best fits to the asymptotic regions. Their equations are shown in the box. Slope 2.98(0.02) corresponds to the equal masses case. Slopes 1.234(0.006) and 1.360(0.002) correspond to $N = 500$ and $N = 1000$ with different masses, respectively. In all cases, the number of independent averaged histories is of order 10^9.

some meaning whenever the correlation function decays as $t^{-1-\Delta}$ with $\Delta > 0$. We measured the current-current correlation function with periodic boundary conditions and total momentum equal to zero. We find that the simulation has strong finite size effects. Nevertheless, we can see a clear tail of order $t^{-1.3}$ [see (a) in Fig. 2]. In order to confirm such a result we computed the local current-current correlation function since it has much better averaging properties. We show in Fig. 2(b) the behavior of the logarithm of $c(t) = \langle j_i(0)j_i(t) \rangle$ with $j_i(t) = m_i * v_i(t)^3/2$, where the average is evaluated at the equilibrium state with $T_1 = T_2 = 1.5$ and we average over all the particles and different initial states. In order to check that we are doing right we first computed $c(t)$ when the system has equal masses. In this case we know from Jepsen that the exact solution [9] behaves like $c(t) \simeq t^{-3}$ for t large enough. In Fig. 2(b) we see how this behavior is obtained numerically and we also see that for the different masses case $c(t)$ decays as $t^{-1-\Delta}$ where Δ is again close to 0.3. This implies that we can define a finite thermal conductivity via Green-Kubo. We think that the decay of correlations is so slow that it explains the strong finite size effects observed in the temperature profile and in the mean heat current. In fact, we can argue that $JN/(T_2 - T_1) = \kappa - AN^{-\Delta}$ which explains why we do not see a clear behavior of J with N with system sizes of order 10^3 (the corrections are of order unity for those sizes).

(4) The energy diffusion.—We also wanted to check if the dynamical version [see Eq. (1)] of Fourier's law holds. With this aim, we prepared the system with zero energy (all particles at rest) and positions $x(i) = i - 1/2$, $i = 1, \dots, N$. Then, we give to the light particle $i = N/2 + 1$ a velocity chosen from a Maxwellian distribution with temperature $T = 1.5$. We monitored how the energy flows through the system until any boundary particle moves. Finally, we average over many initial conditions. If the system follows the Fourier's law we should see a diffusive type of behavior (if the thermal conductivity is constant). Figure 3 shows the energy distribution for $N = 100$ and different times measured in units $t_0 = 0.032$. Let us remark here that to apply Eq. (1) the temperature should have a smooth variation in the microscopic scale to guarantee that local equilibrium holds. In Fig. 3 we see that, for times larger than $t = 200t_0$, the average variation in the local temperature is of order 0.001. Therefore, we may assume that we are in a regime where Eq. (1) holds. Initially, the energy of the light particle is transferred to the neighbors very fast and then the particle stays very cold, much colder than its neighbors. In fact, in this initial regime, the energy maxima are moving outwards at constant velocity. This behavior ends at around $t = 100t_0$. The system then begins to slow down and, at $t \simeq 300t_0$, the structure of the energy distribution changes, and one can then differentiate the behavior corresponding to light particles and heavy ones at least around the maxima of the distribution. We mea-
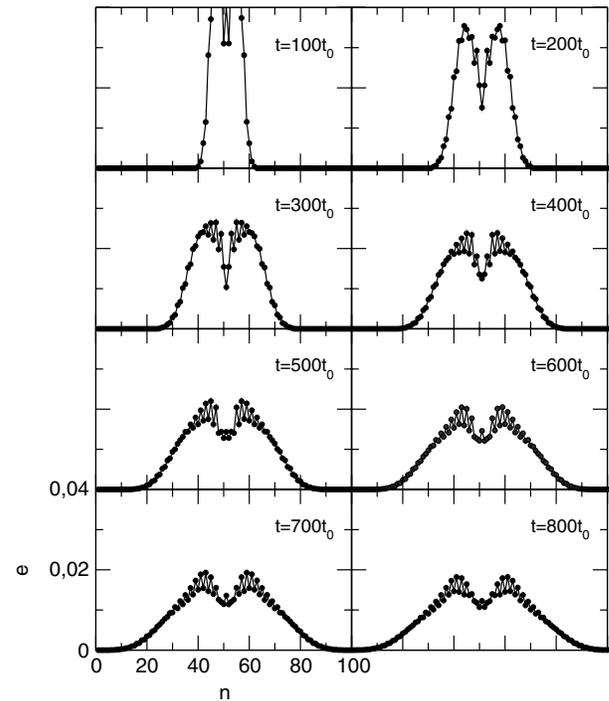

FIG. 3. Evolution of the energy distribution for an initial condition in which all particles, $N = 100$, are at rest except particle 51 which has an averaged energy corresponding to temperature 1.5. The figure shows averages over 10^7 independent realizations and $t_0 = 0.032$.

sured the mean square displacement of the energy distribution at each time: $s(t) = \sum_n (n - 51)^2 e(n, t)$. We found that we can fit $\ln s(t) = -6.39(0.04) + 2.05(0.01) \ln t$ for $t/t_0 \in (30, 100)$, thus, a ballistic behavior that changes smoothly until for $t > 400t_0$ where we find a diffusive behavior $\ln s(t) = -1.00(0.01) + 1.005(0.002) \ln t$. This last result confirms that our system follows even the dynamical aspects of Fourier's law.

As we noticed above, in Fig. 3 we see that the light and heavy particles seem to follow different energy distributions, at least for times longer than $t = 300t_0$. In order to get some more insight about such behavior, we computed the evolution of the total energy stored in the light (heavy) particles. The result is shown in Fig. 4 where we can detect five different time regions: (I) $t/t_0 \in (0, 16)$; only the light particle and the two heavy nearest neighbors have a nonzero velocity. (II) $t/t_0 \in (16, 23)$; the five central particles (three light and two heavy ones) are moving. The total energy stored in the light particles reaches a minimum. (III) $t/t_0 \in (23, 233)$; the heavy particles begin to release energy (on the average) until, at $t = 233t_0$, both types of particles have the same amount of energy. (IV) $t/t_0 \in (233, 600)$; light particles keep getting energy until we reach region. (V) $t > 600t_0$; where the total energy stored in the light particles reaches a constant value that exceeds to the one corresponding to the heavier ones. Let us remark that, in the asymptotic regime $t > 600t_0$,
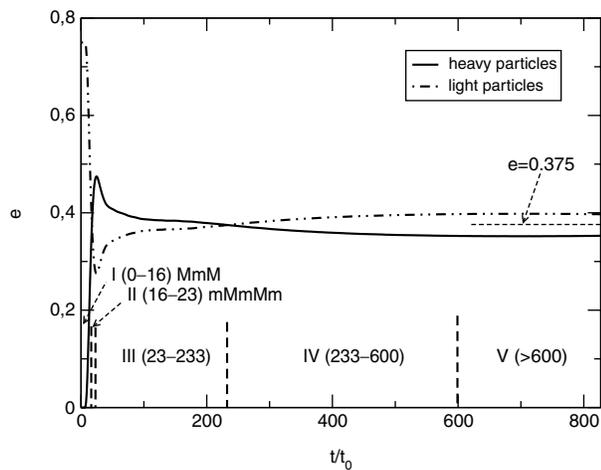
FIG. 4.   Evolution of the total energy stored in the heavy and light particles. The conditions are the same as in Fig. 3. *MmM* indicates that only the central light particle and the nearest heavy ones are moving in region I.

the energy distribution is still evolving and, therefore, this partition of energy between both degrees of freedom is an asymptotic dynamical property of the system.

In order to discard any nonergodic behavior of our system we included reflecting boundary conditions at the extremes of the chain and we did much longer simulations. We saw that the isolated system tends to the equilibrium in which equipartition of energy between all degrees of freedom holds. That is, the total energy stored in the light particles is equal to the one stored in the heavy ones. Moreover, we have checked that the system at any stationary state (equilibrium or nonequilibrium) does not present the property of nonequipartition of the energy. We think that this nonequipartition of the energy between degrees of freedom is responsible for the normal thermal conductivity. In fact, we see that, around the distribution maxima, the particles arrange in the form that hot light particles are surrounded by cold heavy ones. The energy is then trapped and released in a diffusive way. But we also see that the release is diffusive when a large enough number of those hot-cold structures develop. Therefore we think that the mechanism for the thermal resistance is somehow cooperative.

In conclusion, Peierls arguments have successfully explained the observed thermal conductivity in solids by applying a perturbative scheme around the lattice harmonic interaction. The actual belief is that strong anharmonicity is not enough to guarantee a normal thermal conduction in one-dimensional systems. Moreover, it has been proposed that the key lacking ingredient is that the dynamics of the system should not conserve linear momentum via the existence of local potentials through the line (think about particles attached to the one-dimensional substrate through some kind of nonlinear springs). In such a way, local potentials should act as local energy reservoirs that slow down the energy flow. These properties, anharmonicity and nonconservation of momentum, are in some way the ones used on the original Peierls argument. We have shown a model that does not follow such a clean picture. Although our one-dimensional model is nonlinear and it conserves linear momentum (with nonzero pressure), we find that it follows Fourier's law. We think that there are other cooperative mechanisms that can do the job of the local potentials. Maybe systems having degrees of freedom that acquire energy easily but release it in a very long time scale have, in general, normal thermal conductivity. In any case, we think that it is worth exploring such a possibility.

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