PHYSICAL REVIEW E **67**, 015203(R) (2003)

Anomalous heat conduction in a one-dimensional ideal gas

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(Received 2 April 2002; published 24 January 2003)

We provide firm convincing evidence that the energy transport in a one-dimensional gas of elastically colliding free particles of unequal masses is anomalous, i.e., the Fourier law does not hold. Our conclusions are confirmed by a theoretical and numerical analysis based on a Green-Kubo-type approach specialized to momentum-conserving lattices.

DOI: 10.1103/PhysRevE.67.015203 PACS number(s): 05.45.−a, 44.10.+i, 05.70.Ln

Understanding the dynamical origin for the validity of the Fourier law of heat conduction in deterministic one-dimensional particle chains is one of the oldest and most frustrating problems in nonequilibrium statistical physics [1–3]. Due to some very basic unresolved issues the problem has been a source of many recent publications [4–9]. In the absence of analytical results, these papers are mainly oriented towards a numerical analysis of the problem. However, due to the delicate nature of the questions under discussion, numerical results sometimes lead to different conclusions. This is the case, for example, of the one-dimensional (1D) hard-point particles with alternating masses for which opposite conclusions have been reached [5,7,8]. This disagreement is not extremely surprising since this system lies in the foggy region which separates clear, regular integrable systems from the totally chaotic, deterministic, motion. Indeed this system has a zero Lyapounov exponent and therefore it lacks the exponential local instability which characterizes chaotic systems. On the other hand, it has been shown [10] that such systems can exhibit Gaussian diffusive behavior and, more recently [11], an example has been shown of a system with a zero Lyapounov exponent which, however, obeys the Fourier law. From the point of view of a general theoretical understanding, the fact that the alternating mass problem lies in this critical region renders it particularly important to establish, beyond any reasonable doubt, its conducting properties. This is what we set out to do in the present paper. In particular, we confirm the breakdown of the Fourier law and formulate a proper Green-Kubo formalism of momentum-conserving models on a lattice in terms of velocity-current correlation.

We consider a one-dimensional gas of interacting particles with the Hamiltonian

$$H=\sum_{n=0}^{N-1} h_n, \quad h_n=\frac{p_n^2}{2m_n}+V(q_{n+1}-q_n) \tag{1}$$

in the canonical coordinates q_n, p_n. The energy current from site n to site $n+1$ is defined as $j_n=\{h_{n+1},h_n\}$, with the Poisson bracket $\{f,g\}=\Sigma_n \partial_{p_n} f \partial_{q_n} g - \partial_{q_n} f \partial_{p_n} g$, and satisfies the continuity equation $(d/dt)h_n=\{H,h_n\}=j_n-j_{n-1}$. In particular, we focus our attention on the ideal gas model of elastically colliding particles, $V(q>0)=0, V(q<0)=\infty$, with alternating masses, $m_{2n-1}=m_1=\sqrt{r}$, $m_{2n}=m_2=1/\sqrt{r}$, where the ratio $r=m_1/m_2$ serves as a model parameter. We have mainly considered the value $r=(\sqrt{5}-1)/2$; however, all the reported numerical results have been checked also for several other values of r $(0<r<1)$ where we found no qualitative distinction.

We place our system of N particles between two stochastic Maxwellian heat reservoirs at temperatures $T_{\rm L}$ and $T_{\rm R}$ (see [2] for a description of the reservoir model). We chose the temperatures of the reservoirs, $T_{\rm L}=1$ and $T_{\rm R}=2$, and measure the long-time averaged heat current $\langle J\rangle = \lim_{t\to\infty}(1/t)\int_0^t dt' J(t')$ versus the system size N, where $J=(1/N)\Sigma_{n=1}^{N-1} j_n$. We note that our definition of the lattice current simply accounts for the energy transferred during collisions and, since particles cannot be exchanged with the baths, obviously gives the correct heat transfer between the baths. However, its equivalence to the "free particle" current $j_n=m_n v_n^3/2$ used by some authors, e.g. [8], which is connected to the real space current density $j(x)=\Sigma_n j_n \delta(x-q_n)$ in the absence of collisions, is not obvious (see the discussion in [9]).

In order to ensure that our results are not affected by finite size effects we have taken particular care in using an efficient numerical scheme which allows us to reach high N values. Our algorithm, developed in Ref. [3], searches in a partially ordered tree (*heap*) of precomputed candidates pairs for the next collision and, due to this, it requires only $\log_2 N$ computer operations per collision. As a consequence, we were able to simulate very long chains and we have obtained reliably converged results for lattices with sizes N up to 30 000. Convergence has been controlled by checking the constancy of the finite-time-averaged heat current $(1/t)\int_0^t dt' J(t')$, and to this end simulations for the largest system sizes had to be carried on up to 10^{12} pair collisions. It is also clear that convergence problems suggest to keep far away form the r values too close to one or to zero. The analysis made in [2] indicated that the range $0.15<r<0.6$ was the most effective in attenuating solitary pulses and the value $r=0.2$ was chosen. In the present paper we take the somehow "standard" choice $r=(\sqrt{5}-1)/2$.

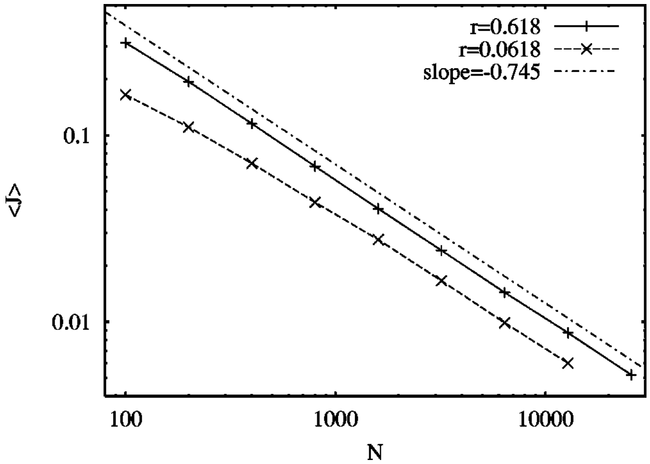

FIG. 1. Time-averaged energy current of a system of N particles between heat baths at temperatures $T_{\mathrm{L}}=1$ and $T_{\mathrm{R}}=2$ vs the size N, at two different mass ratios $r=m_1/m_2=(\sqrt{5}-1)/2$ and $r=(\sqrt{5}-1)/20$. The suggested scaling $\langle J\rangle \propto N^{-\alpha}$ with $\alpha=0.745$ is shown for comparison.

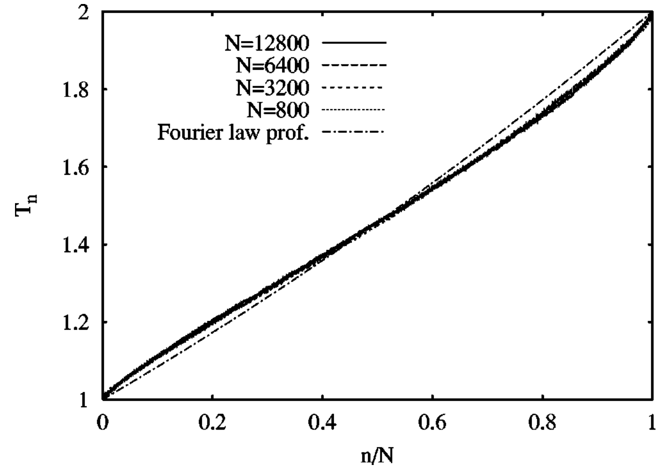

FIG. 2. Temperature profile for $T_{\mathrm{L}}=1$, $T_{\mathrm{R}}=2$, and different sizes N from 800 to 12 800 (dotted-dashed-solid curves), as compared to the Fourier law prediction (chain curve).

Validity of Fourier law implies the scaling $J\propto\nabla T\propto N^{-1}$. Our numerical results shown in Fig. 1 clearly demonstrate instead a different power-law behavior, namely $J\propto N^{-\alpha}$ with $\alpha\approx 0.745\pm 0.005$ over a very large range in N. We have also found that the scaling exponent α does not change appreciably with the mass ratio r. For example, for ten times smaller value of r the asymptotic scaling only sets in later (i.e., for larger values of N, see Fig. 1). The possibility of a slow convergence to the asymptotic value might be at the origin of the slightly different numerical values for α found in previous numerical experiments ($\alpha\approx 0.65$ by Hatano [5], $\alpha\approx 0.83$ by Dhar [7]). Since the model under consideration is energy scaling we do not expect any dependence of the exponent α on the reservoirs temperatures.

The above results therefore solve the existing controversy and clearly show that the alternating mass, 1D hard point gas does not obey Fourier heat law. We turn now to the analysis of other quantities which, besides providing additional confirmation of the above conclusions, illuminate interesting aspects of the heat conduction problem. A quantity of main interest is the internal local temperature profile $T_n=\langle p_n^2/m_n\rangle$ in the nonequilibrium steady state for the system placed in between the heat reservoirs. First we notice that the temperature profile in the discrete index variable n is different than the temperature profile in position variable q_n [7] since the inverse density $dq/dn=\langle q_{n+1}-q_n\rangle$ is nonuniform in nonequilibrium, in fact it is simply proportional to the temperature due to the constancy of pressure [7]. Now, in the case of Fourier law, the thermal conductivity κ scales with temperature like $\kappa\propto\sqrt{T}$. Therefore, from $\sqrt{T}(dT/dn)dn/dq=\mathrm{const}$ one obtains the temperature profile $T_n^{\mathrm{kin}}=[T_{\mathrm{L}}^{1/2}+(T_{\mathrm{R}}^{1/2}-T_{\mathrm{L}}^{1/2})n/N]^2$. Extensive numerical simulations showed (see Fig. 2) that the temperature profile in our model converges, for sufficiently large N, to a well-defined scaling function $T_n^{\mathrm{scal}}=f(n/N)$ which is slightly, but *significantly*, different from the kinetic temperature profile T_n^{kin}. This is another piece of evidence for the anomalous heat transport and for the nonvalidity of the Fourier law in our system. It should be remarked that the convergence to the temperature profile predicted by kinetic theory observed in [7], which has indeed been considered as surprising by the author himself, actually does not take place.

A standard theoretical analysis of transport laws is based on the Kubo formulas [12,13]. However, applicability of the Kubo formula in momentum-conserving cases, i.e., for translationally invariant systems like model (1), is not very clear. This is particularly critical in view of a recent claim [6] that the Kubo formula diverges for a momentum-conserving lattice with nonvanishing pressure. For this latter type of models we have an additional difficulty in applying the Kubo formalism, namely, as we show below, the result depends not only on the temperature gradient, but also on other thermodynamic properties of the initial nonequilibrium state—i.e., the *isobaric* case (constant pressure profile) or the *isochoric* case (constant density profile). There is no *a priori* argument which favors either of these two options: the choice depends on the specific physical situation of interest. For instance, the steady-state heat current simulation considered above (Figs. 1 and 2) is clearly described by the isobaric state. Since we want to consider both situations we need to revise the derivation of the Kubo formula by following the time evolution of a general nonequilibrium initial state in an isolated system with periodic boundary conditions $q_N\equiv q_0+N, p_N\equiv p_0$. To this end, we prepare the initial state in a local-equilibrium state described by the inverse temperature profile β_n and by an additional thermodynamic potential γ_n,

$$\rho_{\mathrm{neq}}=Z_{\mathrm{neq}}^{-1}\exp\left(-\sum_n \beta_n h_n-\sum_n \gamma_n(q_{n+1}-q_n)\right). \quad (2)$$

This (small) additional term is necessary in order to equilibrate the pressure in the isobaric case. Notice that γ_n is undetermined up to an arbitrary additive constant due to a gauge invariance of the second term in Eq. (2). In order to determine the gradient of the γ potential which is necessary to keep the physical pressure ϕ constant (n independent), we compute the *generalized pressure* ϕ_l

$$\beta_l \phi_l = -\frac{\partial}{\partial a} \ln Z_l(a)\bigg|_{a=0}, \tag{3}$$

$$Z_l(a) = \int e^{-\sum_n (\beta_n V(q_{n+1}-q_n+a\delta_{ln}) - \gamma_n(q_{n+1}-q_n+a\delta_{ln}))} d\vec{q}.$$

By a simple trick, a shift of one variable $q_l \to q_l + a$ in the integral $Z_l(a)$, we find $Z_l(a) \equiv Z_{l-1}(a)$ and therefore

$$\beta_l \phi_l = \beta_{l-1}\phi_{l-1} = \text{const.} \tag{4}$$

Writing the *force* as $\phi = -\langle V'(q_{n+1}-q_n)\rangle_{\text{neq}} = \phi_n + \gamma_n/\beta_n$, multiplying by β_n, and taking the first difference $\nabla f_n := f_n - f_{n-1}$ we obtain the required "gradient"

$$\nabla \gamma_n = \phi \nabla \beta_n. \tag{5}$$

In the following we consider two specific cases: (i) The initial isochoric state with $\langle q_{n+1}-q_n\rangle_{\text{neq}} = \text{const}$. This is obtained by setting $\gamma_n \equiv 0$. (ii) The initial isobaric state with uniform pressure profile. This is obtained by specifying the γ-potential according to Eq. (5). We note again that the isobaric state (ii) is the one which is relevant for the steady nonequilibrium state of a system in contact with heat reservoirs. Carefully repeating the first few steps in the derivation of the Green-Kubo formula (following Ref. [13]) we arrive at the very general linear response formula

$$\langle A(t)-A(t_0)\rangle_{\text{neq}} = \int_{t_0}^{t} dt' \left\langle A(t') \sum_n (\nabla\beta_n j_n + \nabla\gamma_n v_n) \right\rangle_{\text{eq}}$$

where $v_n = \dot{q}_n$ are the particles' velocities. In the last step we have assumed that we are close to equilibrium ($\nabla\beta_n$ and $\nabla\gamma_n$ small) so that the right-hand side (RHS) can be evaluated in the corresponding equilibrium state $\langle\rangle_{\text{eq}}$. Let us now consider the periodic temperature profile $\beta_n = \beta + \epsilon \sin(2\pi kn/N)$, and compute the total heat that has been transported in time t from *warm* to *cold* regions of the lattice, namely $Q(t) = \int_0^t dt' J_k(t')$, where

$$J_k := N^{-1}\sum_{n=0}^{N-1} \cos(2\pi kn/N) j_n.$$

Inserting Q for A and using Eq. (5) [case (i) is obtained by formally setting $\phi = 0$] we obtain

$$\langle Q(t)\rangle_{\text{neq}} = \frac{2\pi\epsilon}{N}\int_0^t dt'(t-t')\langle J_k(t)(J_k + \phi V_k)\rangle_{\text{eq}}, \tag{6}$$

where $V_k := N^{-1}\sum_{n=0}^{N-1}\cos(2\pi kn/N) v_n$. We see that the growth of the transported heat $\langle Q(t)\rangle_{\text{neq}}$ is given by the generalized correlation function $C_k(t) = C_{JJ}(t) + \phi C_{JV}(t)$, where $C_{JJ}(t) = \langle J_k(t) J_k\rangle_{\text{eq}}$ and $C_{JV}(t) = \langle J_k(t) V_k\rangle_{\text{eq}}$. In the isochoric case (i) expression (6) reduces to the usual current autocorrelation function only. We note that an unusual form of the correlation function in Eq. (6) is due to our use of "nonstandard" lattice currents j_n.

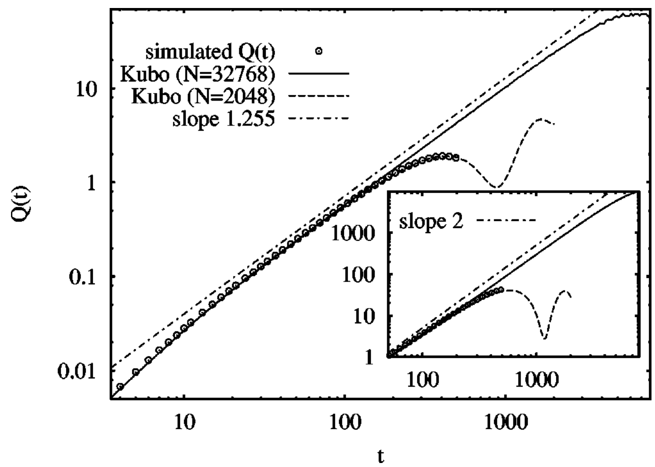

FIG. 3. Transported heat $Q(t)$ in an isolated system of size $N = 2048$ obtained by starting from a nonequilibrium *isobaric* initial state (circles) with $\epsilon = 0.2$. For comparison we show the corresponding equilibrium averaged Kubo-like expressions (6) for $N = 2048$ (dashed) and for $N = 32768$ [solid curve, multiplied by 16 to account for scaling $\langle Q(t)\rangle \propto 1/N$]. The dashed-dotted line has a slope 1.255 and gives the best fit in the range $20 < t < 2000$. The corresponding data for the *isochoric* case are shown in the inset with the slope 2.

In the case of Fourier law, we expect initial linear growth $\langle Q(t)\rangle_{\text{neq}} \approx \epsilon\kappa t$, while for the *ballistic* heat transport we expect quadratic growth $\langle Q(t)\rangle_{\text{neq}} \propto t^2$ (this has been confirmed numerically for the integrable gas of equal masses $r = 1$). However, in a generic system with momentum conservation and nonvanishing pressure $\phi \neq 0$, like our dimerized hard-point gas, we find qualitatively different behavior in cases (i) and (ii). For example, due to the result [6], $C_{JJ}(t)$ has a plateau $\propto \phi^2$ and the transport is ballistic in the isochoric case, while in the isobaric case the second term, $C_{JV}(t)$, compensates for the plateau and yields a much slower increase of the transported heat. In this latter case, independent numerical computations of $\langle Q(t)\rangle_{\text{neq}}$ and of $C_k(t)$ for N up to 32 768 shown in Fig. 3 give $\langle Q(t)\rangle_{\text{neq}} \propto t^{\nu}$ with $\nu \approx 1.255$, which is still clearly superdiffusive, and directly validate the formula (6). In Fig. 4 we show the generalized correlation function $C_k(t)$ for $k = 0$ and $k = 1$ separately. Note that the results for $k = 1$ exhibits some oscillations for longer times due to finite size effects, namely due to periodicity of the lattice, while $k = 0$ gives the *spatially homogeneous* correlation function which has the same long-time behavior with weaker finite size effects [however, the case $k = 0$ is not strictly related to the Kubo formula (6)]. We see that in the time range where $C_0(t)$ and $C_1(t)$ match, the asymptotic decay is compatible with $C_k(t) \propto t^{-\mu}$ with the exponent $\mu = 2 - \nu = 0.745$ consistent with Eq. (6), and satisfying $\mu = \alpha$.

These results can be interpreted in the following way. In the isochoric initial state the initial temperature gradients drive the heat ballistically in terms of sound waves [6]. On the other hand, in the isobaric initial state, we have density gradients which drive the lattice heat current in the opposite direction and almost exactly compensate for the effect of temperature gradients so that the net effect is a sub-ballistic,

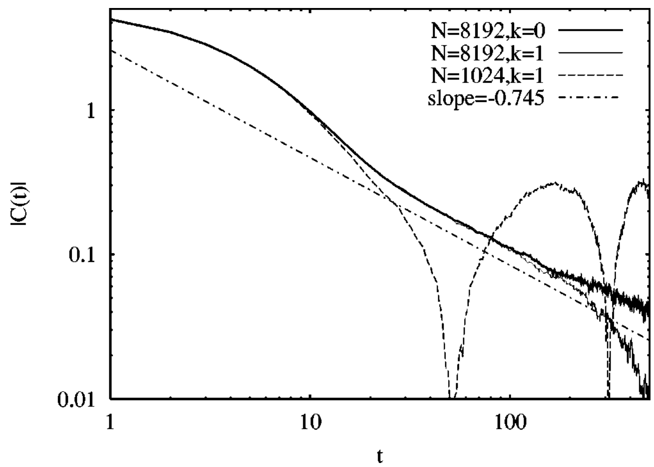

FIG. 4. The generalized time correlation function (see text) computed with canonical average at $\beta=1$ for two system sizes $N=1024$ and $N=8192$ and for the zeroth $k=0$ (dashed and solid curves, respectively) and the first $k=1$ (thin curve) spatial Fourier mode. Note the $t^{-0.745}$ decay (dashed line) in the range $20<t<200$ (for $N=8192$) whereas for longer times we see finite size effects (e.g., we have periodic oscillations for $k=1$ due to transversals of sound waves).

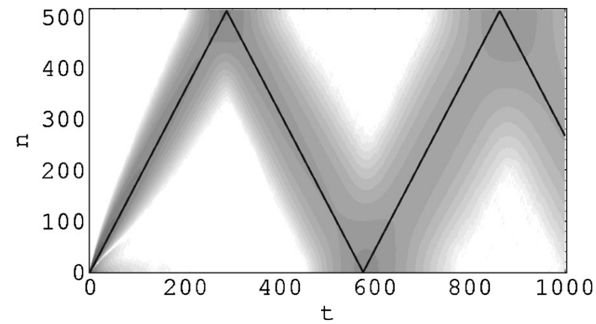

FIG. 5. The spatio-temporal current-current correlation function $c_{jj}(n,t)$ at temperature $1/\beta=1$ on a lattice of size $N=1024$ is shown with 20 different shades of grayness spaced equidistantly from 10^{-4} to 4.0 in logarithmic scale. The zigzag solid line indicates the peak ballistic sound-wave contribution moving with a uniform sound velocity $c_s=1.78$.

but still superdiffusive, energy transport. In order to illustrate the mechanism of ballistic energy transport we show in Fig. 5 the spatio-temporal current-current correlation function $c_{jj}(n,t)=\langle j_0 j_n(t)\rangle_{\rm eq}$ which exhibits clear ballistic tongues along the lines $n=\pm c_s t$ where $c_s=1.78$.

In this paper we have discussed the thermal conducting properties of a one-dimensional hard point gas with alternating masses. For the more general situation of momentum conserving systems on a lattice, we have discussed the energy redistribution in an isolated system starting from a nonequilibrium initial state and derived a Green-Kubo formula which takes into account the velocity-current correlation function. We have presented an accurate numerical analysis, made possible by a powerful integration scheme, which allows us to establish definite convincing evidence that the system under consideration does not obey the Fourier law. Moreover, by considering a typical mass ratio $r=(\sqrt{5}-1)/2$, we have found that the asymptotic scalings: (i) steady-state heat current between heat baths $\langle J\rangle\propto N^{-\alpha}$, (ii) heat transported within a nonequillibrium isobaric initial state in an isolated system $\langle Q(t)\rangle\propto t^{2-\alpha}$, and (iii) generalized current-velocity correlation in the equilibrium state $C_k(t)\propto t^{-\alpha}$, are described by just one exponent $\alpha=0.745$. After this work has been completed, two references appeared reporting quite similar results [14].

This work was partially supported by the EU, Contract No. HPRN-CT-1999- 00163 (LOCNET network) and by MURST (Prin 2000, *Caos e localizzazione in Meccanica Classica e Quantistica*). T.P. was supported by the Ministry of Science, Education and Sport of Slovenia.

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