Heat Conduction in One-Dimensional Systems with Hard-Point Interparticle Interactions

A. V. Savin,[1,2] G. P. Tsironis,[2] and A. V. Zolotaryuk[2,3]

[1]*State Institute for Physics and Technology, Prechistenka str. 13/7, 119034 Moscow, Russia*

[2]*Physics Department, University of Crete and Foundation for Research and Technology–Hellas, P.O. Box 2208, 71003 Heraklion, Crete, Greece*

[3]*Bogolyubov Institute for Theoretical Physics, 03143 Kiev, Ukraine*

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Results of extensive and accurate numerical studies on heat transfer in a system of particles with unequal masses, interacting through hard-point potentials with two types of symmetry, are reported. The particles are confined in a one-dimensional box with fixed ends coupled to heat reservoirs at different temperatures. The study aims to throw light upon recent controversial results on thermal conductivity in one-dimensional systems. When the particles interact through elastic hard-point collisions (a standard asymmetric case), the system is shown to have always infinite (anomalous) thermal conductivity as follows from the Prosen-Campbell theorem.

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The problem of finding a one-dimensional (1D) Hamiltonian system that obeys Fourier's law of heat conduction has attracted considerable interest [1], resulting recently in important contributions on this very old problem [2–12]. The study reported in this Letter has been inspired by the following recent controversial results. On one side, Prosen and Campbell [8] have proved a theorem according to which any 1D system with momentum conserving dynamics and nonzero pressure has infinite (anomalous) thermal conductivity. On the other side, the recent numerical study of Garrido *et al.* [12] on a 1D gas of elastically colliding particles of unequal masses is against this theorem, showing that the thermal conductivity in this system is normal, whereas Dhar's result [10] on the same system reveals a slow divergence of the conductivity. Therefore we have undertaken here an extensive and accurate numerical study of the same system, i.e., the 1D gas with different interparticle hard-point interactions.

Let us consider a system of N point particles (numbered by $n = 1, \ldots, N$) with unequal masses moving in a one-dimensional box $0 \le x \le L = Na$, where a is the average distance between the particles (or the "lattice spacing"). From here onwards we take $a = 1$. The only interaction considered is between the nearest-neighbor particles through a *hard-point* potential $V(r)$, with r being the displacement from the "equilibrium" distance $a = 1$. The mass, position on the line, and velocity of the nth particle are denoted by m_n, x_n, and v_n, respectively.

We consider three interparticle hard-point potentials, each plotted in Fig. 1. The first of these shown in the left panel (a) is of a standard type with *one* reflecting wall,

$$V(r) = \infty \text{ if } r \le -1 \text{ and } V(r) = 0 \text{ if } r > -1 . \quad (1)$$

This potential describes the elastic repulsion under collisions, when the adjacent particles meet each other at *zero* distance, i.e., $r = -1$. The second one has *two* symmetrically located reflecting walls, as illustrated by the middle panel (b),

$$V(r) = \infty \text{ if } |r| \ge 1 \text{ and } V(r) = 0 \text{ if } |r| < 1 . \quad (2)$$

It also describes an elastic reflection of the adjacent particles when they meet each other at zero distance ($r = -1$), but besides this type of collisions the adjacent particles are assumed to collide elastically also "inside," when the distance between them becomes $2a$ ($r = 1$), as they would be "roped" at this distance. As illustrated by the right panel (c), the third potential is also symmetric, but it has metastable equilibria, so that each pair of the adjacent particles on the line can be found with two different energies, 0 or 1,

$$V(r) = \infty \text{ if } |r| \ge 1, \quad V(r) = 1 \text{ if } d \le |r| < 1 , \quad \text{and } V(r) = 0 \text{ if } |r| < d , \quad (3)$$

where the parameter d determines the relative "population" of the particles in the metastable and the ground states.

The 1D gas with any of these hard-point potentials can be considered as a limiting case of the chain with an appropriate sequence of the interparticle soft interaction. Thus, as shown in Fig. 1(a), a convergent sequence for the potential (1) is obtained from the Lennard-Jones (LJ) family, i.e., using the (2,1)-LJ potential:

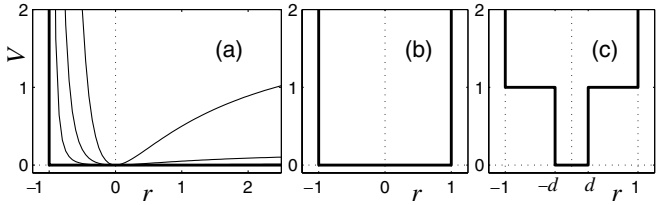

FIG. 1. Three types of the interparticle hard-point potential. (a) Asymmetric potential (1) with one reflecting wall (thick lines) and the sequence of Lennard-Jones potentials (thin curves) converging to the hard-point one. (b) Symmetric potential (2) with two reflecting walls. (c) Symmetric potential (3) with metastable states ($d = 0.25$).

$$V(r) = \lim_{\varepsilon \to 0} V(\varepsilon; r), \quad V(\varepsilon; r) = \varepsilon[(1 + r)^{-1} - 1]^2, \tag{4}$$

with the binding energy between the chain particles ε. Similarly, the potential (2) can also be constructed as a "lattice" limit of appropriate symmetric functions, modeling interparticle interaction of the β-Fermi-Pasta-Ulam type [3], which are infinite at $r = \pm 1$.

The numerical scheme for solving the equations of motion describing the dynamics of the 1D hard-point gas interacting with a thermal bath has been developed in a series of papers [4,10,12,13]. The key point is that after a collision between adjacent particles, their new velocities are obtained from momentum and energy conservation [see, e.g., Eqs. (1) in Ref. [10]]. Between collisions, the particles travel with constant velocity. The coupling of the gas to the heat reservoirs placed at the box walls $x = 0$ and $x = N + 1$ is given using the Maxwell boundary conditions. Thus, when a particle of mass m collides with a wall at temperature T, it is reflected back with a velocity chosen from the distribution $f(v) = (m|v|/T) \exp(-mv^2/2T)$. The temperatures at the left and the right walls are denoted by T_L and T_R ($T_L > T_R$), respectively. This method can easily be modified for simulations of the dynamics with the hard-point potentials (2) and (3). Note that in the case of the potential (3), we need to consider the energy $E_n = m_n m_{n+1}(v_{n+1} - v_n)^2/2(m_n + m_{n+1})$. Whenever $E_n \leq 1$, the collisions occur at the distances $1 - d$ and $1 + d$, but when $E_n > 1$, the particles collide at distances 0 and 2.

Initially, one can distribute the particles uniformly on the line, forming a regular chain with the lattice spacing $a = 1$, and choose Boltzmann's distribution on the initial velocities. Then, solving the equations of motion, we find a time t_1 of the first collision between some pair of the adjacent particles, next a time t_2 of the second collision, in general between another pair of the adjacent particles, and so on. As a result, we obtain a sequence $\{t_i, n_i\}_{i=1}^{\infty}$, where t_i is the time of the ith collision in the system, and n_i and $n_i + 1$ are the particles participating in this collision. Since we need to implement numerical simulations as long as possible, in order to find the time asymptotic of the flow-flow correlation function entering the Green-Kubo formula, we modify the numerical scheme used previously [10,12] as follows. First, we incorporate the energy change of the n_ith particle during the ith collision as $\Delta E_{n_i} = m_{n_i}(v_{n_i}'^2 - v_{n_i}^2)/2$, where v_{n_i} and v_{n_i}' are velocities of the n_ith particle before and after the ith collision, respectively. Next, we introduce a time step Δt, which is significantly less than the simulation time, but satisfies the inequality $\Delta t \gg t_0$, where $t_0 = \lim_{i \to \infty}(t_i/i)$ is the mean time between successive collisions. Then, for each $k = 0, 1, \ldots$, we define the local energy flow as a piecewise constant (in time) function

$$j_n(t) = \frac{a}{\Delta t} \sum_{i \in I_{kn}} \Delta E_{n_i}, \quad k\Delta t \leq t < (k + 1)\Delta t, \tag{5}$$

where the integer sets I_{kn}'s are defined by $I_{kn} = \{i | k\Delta t \leq t_i < (k + 1)\Delta t, n_i = n\}$. The set I_{kn} takes into account those collisions that occur between particles n and $n + 1$ during the time interval $k\Delta t \leq t < (k + 1)\Delta t$. Equilibration times were typically occurring in the system of the order 10^6. After these times have passed, we define the time-averaged local thermal flow

$$J_n = \langle j_n(t) \rangle_t \equiv \lim_{t \to \infty} \frac{1}{t} \int_0^t j_n(\tau)\, d\tau \tag{6}$$

and the temperature distribution $T_n = m_n \langle v_n^2(t) \rangle_t$, where $v_n(t)$ is the velocity of particle n calculated at a time t. To find these averaged quantities, we have used times up to 10^7. Note that previously [10,12] the time averaging was implemented through the formula

$$J_n = m_n \langle v_n^3(t) \rangle_t / 2. \tag{7}$$

In order to avoid nonlinear temperature profiles obtained by Dhar [10], in our calculations we have used only small temperature gradients. Specifically, we have chosen $T_L = 1.05$ and $T_R = 0.95$. At least for these values, both the definitions (5), (6) and (7) lead to the same results.

In order to compare our results with those found by Garrido *et al.* [12], we take the same masses, i.e., $m_1 = 1$ and $m_2 = (\sqrt{5} + 1)/2$, and simulate the time evolution of the gas with $N = 40$, 80, 160, 320, and 640. As shown in Fig. 2, the local heat flow J_n is constant along the system [if defined according to Eqs. (5) and (6)] and the linear temperature gradient is formed. As demonstrated by Fig. 2(a), averaging times 10^7 are not sufficient to attain a *constant* flow along the system, when the definition (7) is used. For this purpose, times 10^8 or even 10^9 are required.

Upon calculating the averaged local flow J_n and the temperature gradient T_n, one can find the thermal conductivity κ directly as the limit

$$\kappa = \lim_{N \to \infty} \kappa(N), \quad \kappa(N) = \sum_{n=1}^{N} J_n/(T_1 - T_N), \tag{8}$$

at the mean temperature $T = (T_L + T_R)/2$. For the mass ratio $m_2/m_1 = (\sqrt{5} + 1)/2$, the system size dependence $\kappa(N)$ plotted in Fig. 3 gives the asymptotic $\kappa \sim N^{\alpha}$ with $\alpha = 0.24$, being close to that found by Dhar [10], but for another mass ratio, namely $m_2/m_1 = 1.22$ ($\alpha < 0.2$). Thus, our result together with Dhar's findings clearly shows that the diatomic 1D gas with the interparticle hard-point interaction (1), which is confined in a finite box, has *infinite* (anomalous) thermal conductivity, as stated by Prosen and Campbell [8]. However, recently [12], based on the long-time behavior of the flow-flow correlation function, the opposite conclusion has been asserted. Therefore we have also undertaken a systematic numerical study of time behavior of the correlation function, using both our techniques and those used previously [12]. Moreover, we have in parallel implemented calculations for the "lattice" approximation given by the (2,1)-LJ sequence (4), in order to demonstrate a *uniform*

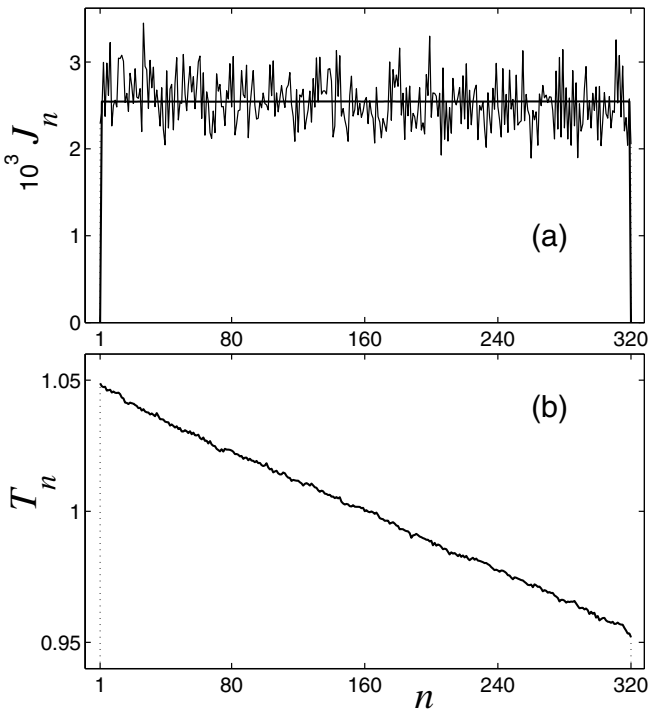

FIG. 2. (a) Time-averaged local heat flow J_n calculated using the definition given by Eqs. (5) and (6) and shown by thick line, and the definition according to Eq. (7) and illustrated by thin randomlike curve. (b) Local temperature profile T_n ($T_L = 1.05$, $T_R = 0.95$, and $N = 320$).

convergence of the thermodynamic pressure and to show a *similarity* of the correlation function behavior.

To find the flow-flow correlation function $C(t)$ numerically, we calculated the time mean $\langle J(\tau)J(\tau - t)\rangle_\tau/N$, with $J(t) = \sum_n j_n(t)$ being the total heat flow through the gas/chain system consisting of $N = 500$ particles, averaged over 10^4 realizations of initial thermalization. Since in this case $t_0 \simeq 0.004$, the step Δt was fitted to be 0.1. In the gas case, the local heat flow $j_n(t)$ is calculated according to Eqs. (5) and (6), whereas in the lattice case, this flow is calculated analytically [5,7,8,14] using the specific form (4). The time behavior of $C(t)$ obtained for both the gas and the LJ chain and plotted in Fig. 4 appears to be of the type $C(t) \sim t^{-\sigma}$ as $t \to \infty$, with more complicated behavior of σ compared to that found recently by Garrido *et al.* [12]. Note that in order to attain the same "level" of averaging (as shown, e.g., by curve 3), using the standard formula (7), one would require the number of realizations 10–100 times as large. More precisely, we have found that at $T = 1$ and $\varepsilon \leq 2$ the correlation function $C(t)$ reveals the *similar* behavior as that of the 1D gas with the hard-point interaction (1), as illustrated by Fig. 4. Thus, for comparatively short times, $t < e^9 t_0$, we have $\sigma > 1$ ($\sigma = 1.22$ if $\varepsilon = 2$, $\sigma = 1.25$ if $\varepsilon = 0.2$, and $\sigma = 1.28$ as $\varepsilon \to 0$). Note that the value $\sigma = 1.28$ is in good agreement with the estimate $\sigma = 1.33$ obtained by Garrido *et al.* [12]. However, for longer times shown in Fig. 4 by the shaded (gray) area, the decrease becomes essentially slower with $\sigma < 1$ ($\sigma = 0.89$ if $\varepsilon = 2$, $\sigma = 0.86$ if $\varepsilon = 0.2$, and $\sigma = 0.83$ as $\varepsilon \to 0$). In this case, the integral in the Green-Kubo formula diverges and therefore the thermal conductivity becomes infinite. This effect of different rates of the correlation function decrease is observed at $m_2/m_1 < 1.9$, but practically vanishes if $m_2/m_1 \geq 2$. However, the inequality $\sigma < 1$ is *always* valid as $t \to \infty$.

On the other hand, since the key point in the derivation of the Prosen-Campbell theorem is the existence of a

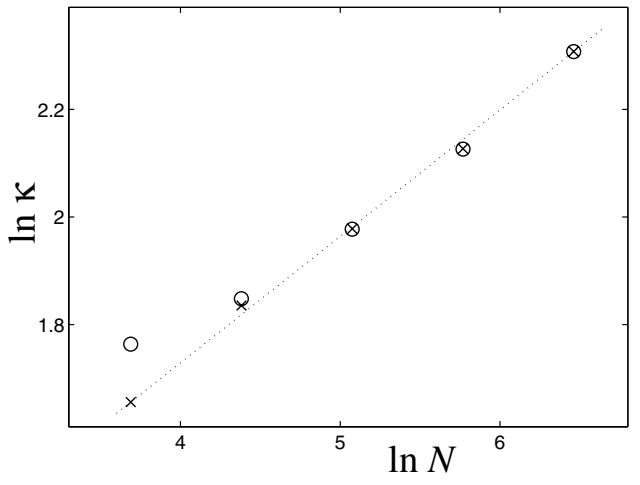

FIG. 3. Logarithm of thermal conductivity $\kappa(N)$ against the logarithm of length $L = N$ calculated for asymmetric hard-point potential (1) when using Eq. (8). Empty balls represent the results obtained from the use of the definition of local heat flow by Eqs. (5) and (6), whereas crosses show the values calculated according to Eq. (7). In the thermodynamic limit ($N \to \infty$) both the definitions give the same values and the discrepancy revealed at smaller N does not depend on the simulation time.

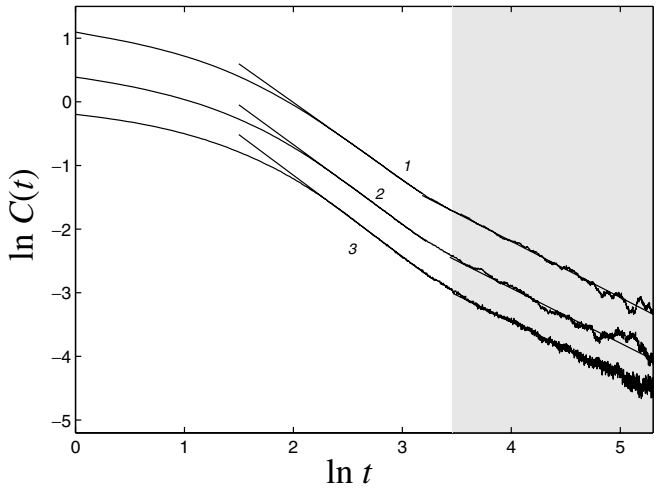

FIG. 4. Logarithm of correlation function $C(t)$ against logarithm of time t for the diatomic $[m_2/m_1 = (\sqrt{5} + 1)/2]$ gas/chain with the (2,1)-Lennard-Jones potential (4) for $\varepsilon = 2$ (curve 1, $\sigma = 1.22$ and 0.89) and $\varepsilon = 0.2$ (curve 2, $\sigma = 1.25$ and 0.86), and for the limiting case ($\varepsilon \to 0$) with hard-point potential (1) (curve 3, $\sigma = 1.28$ and 0.83). The first values for exponent σ are obtained from calculations during times used in Ref. [12], $t < e^9 t_0$ (for $N = 500$, $t_0 = 0.003944$), whereas the second numbers are obtained from calculations for much longer times shown by gray area.

nonzero lower bound for the thermodynamic pressure $P = \lim_{N\to\infty}[N^{-1}\sum_n \langle V'(x_{n+1} - x_n - 1)\rangle_t]$, where the prime denotes the derivative of a function over its argument, we have also calculated P for the "soft" sequence (4) as a function of ε. As seen from Table I, at the constant temperature $T = 1$, the pressure P tends to 1 if $\varepsilon \to 0$. Moreover, one can prove analytically the existence of a *uniform* (in ε) lower bound implying *infinite* conductivity also in the limit $\varepsilon \to 0$, as mentioned in Ref. [8] as well. Thus, the estimate $\sigma = 1.3$ obtained by Garrido *et al.* [12] is an artifact. It is an early time estimate based only on numerical calculations for the times prior to those in the shaded region of Fig. 4. In this region, we have found that $\sigma = 0.83 < 1$. Hence, in the vicinity of the left edge of the gray area, there exists a *point of inflection* if $m_2/m_1 = (\sqrt{5} + 1)/2$. In general, the existence of this point depends on the mass ratio m_2/m_1, but still the absence of this point does not eliminate the divergence of κ in the Green-Kubo formula.

Thus, we conclude that the 1D diatomic gas confined in a finite box (and therefore having the total momentum equal to zero on average) always has infinite conductivity, independently on the mass ratio, and this result does not contradict the Prosen-Campbell theorem, the proof of which is based on a canonical ensemble *without any constraints* being therefore in contradiction with a remark of Ref. [1]. One may argue which correlation function has to enter the Green-Kubo formula when working in a canonical ensemble (e.g., subtracting the longest wavelength mode that arises in momentum conserving systems), but these arguments have no relevance to our study here and will be considered elsewhere.

In the systems with symmetric interparticle interactions of the type (2) or (3), this theorem does not apply. Here the pressure P is always zero (even if the gas is confined) and a finite thermal conductivity is expected. Using the same numerical scheme, the thermal conductivity of the diatomic gas with the symmetric interparticle hard-point interaction (2) is shown to be also anomalous, as in the asymmetric case. Here the correlation function tends to zero with the exponent $\sigma = 0.80$. Approximately, the same behavior is observed for the correlation function of the monoatomic gas ($m_1 = m_2 = 1$) , but here $\sigma = 0.85$.

On the other hand, the 1D gas with symmetric metastable hard-point potential (4) at the temperature $T = 1$ can have a finite heat conductivity. Here the correlation function $C(t)$ has a similar behavior, but the exponent σ depends on the parameter (the intermediate diameter) $d > 0$. The smaller this parameter is (the wider the metastable state is), the larger is σ. Thus, in the monoatomic chain ($m_1 = m_2 = 1$) with $d = 1/2$, this exponent is $\sigma = 0.71$; at $d = 1/4$, $\sigma = 0.87$; at $d = 1/8$, $\sigma = 0.97$; but for $d = 1/16$, we have $\sigma = 1.07 > 1$. In other words, for sufficiently wide metastable states, the gas at temperature $T = 1$ has a *finite* conductivity. When $T = 0.25$ and $T = 1.5$, the correlation function decreases slower than t^{-1}. Thus, nearby $T = 1$ there exists a narrow "temperature window" with a normal heat conduction. For lower and higher temperatures, the system has infinite thermal conductivity, though local thermal equilibrium does exist at these temperatures.

TABLE I. Pressure P in the diatomic chain with the (2,1)-Lennard-Jones potential (4) on the binding energy ε ($T = 1$).

ε	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
P	1.935	1.284	1.133	1.044	1.003	1.001

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[1] F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet, math-ph/0002052.
[2] G. Casati, J. Ford, F. Vivaldi, and W. M. Visscher, Phys. Rev. Lett. **52**, 1861 (1984).
[3] S. Lepri, R. Livi, and A. Politi, Phys. Rev. Lett. **78**, 1896 (1997); Europhys. Lett. **43**, 271 (1998); Physica (Amsterdam) **119D**, 140 (1998).
[4] R. Tehver, F. Toigo, J. Koplik, and J. R. Banavar, Phys. Rev. E **57**, R17 (1998).
[5] B. Hu, B.-W. Li, and H. Zhao, Phys. Rev. E **57**, 2992 (1998).
[6] T. Hatano, Phys. Rev. E **59**, R1 (1999).
[7] C. Giardiná, R. Livi, A. Politi, and M. Vassalli, Phys. Rev. Lett. **84**, 2144 (2000); O. V. Gendelman and A. V. Savin, Phys. Rev. Lett. **84**, 2381 (2000).
[8] T. Prosen and D. K. Campbell, Phys. Rev. Lett. **84**, 2857 (2000).
[9] B. Li, H. Zhao, and B. Hu, Phys. Rev. Lett. **86**, 63 (2001); A. Dhar, Phys. Rev. Lett. **86**, 5882 (2001); **87**, 069401 (2001); B. Li, H. Zhao, and B. Hu, Phys. Rev. Lett. **87**, 069402 (2001).
[10] A. Dhar, Phys. Rev. Lett. **86**, 3554 (2001).
[11] K. Aoki and D. Kusnezov, Phys. Rev. Lett. **86**, 4029 (2001).
[12] P. L. Garrido, P. I. Hurtado, and B. Nadrowski, Phys. Rev. Lett. **86**, 5486 (2001).
[13] J. Masoliver and J. Marro, J. Stat. Phys. **31**, 565 (1983).
[14] G. P. Tsironis, A. R. Bishop, A. V. Savin, and A. V. Zolotaryuk, Phys. Rev. E **60**, 6610 (1999).