RAPID COMMUNICATION

Normal thermal conduction in lattice models with asymmetric harmonic interparticle interactions*

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We study the thermal conduction behaviors of one-dimensional lattice models with asymmetric harmonic interparticle interactions. Normal thermal conductivity that is independent of system size is observed when the lattice chains are long enough. Because only the harmonic interactions are involved, the result confirms, without ambiguity, that asymmetry plays a key role in normal thermal conduction in one-dimensional momentum conserving lattices. Both equilibrium and nonequilibrium simulations are performed to support the conclusion.

Keywords: anharmonicity, normal thermal conduction, Green–Kubo formula

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1. Introduction

The thermal transport properties of low-dimensional systems have evoked intensive studies for decades,[1–13]. These studies are aimed at verifying the validity of Fourier's law of thermal conduction

$$J = -\kappa \nabla T. \tag{1}$$

Here, J is the thermal current, ∇T is the temperature gradient along the chain, and κ is the thermal conductivity. For one-dimensional (1D) momentum conserving fluids and lattices, it is generally believed that the thermal conductivity should diverge as $\kappa \sim L^{\alpha}$ with the increase of the system size L,[14–22] though some counterexamples with size-independent thermal conductivities have also been found, such as the rotator model,[23,24] a 1D lattice in effective magnetic fields,[25] and the variant ding-a-ling model.[26]

Recently, we found that, via nonequilibrium molecular dynamical simulations, momentum conserving chains with asymmetric interparticle interactions[27] can also result in normal thermal conduction. This result is further confirmed by investigating the time-dependent behavior of current autocorrelation function at equilibrium.[28] The current autocorrelation function is defined as

$$C(t) = \langle J(t)J(0)\rangle,$$

where $J(t)$ represents the total current fluctuations at time t and $\langle\cdot\rangle$ denotes the equilibrium thermodynamic average. Following the linear response theory,[30,31] the thermal conductivity may be calculated by the Green–Kubo formula

$$\kappa = \lim_{\tau\to\infty}\lim_{N\to\infty}\frac{1}{k_{\mathrm{B}}T^2N}\int_0^{\tau} C(t)\,\mathrm{d}t, \tag{2}$$

where τ is the evolution time, L is the linear dimension of the system along which the current flows, k_{B} is the Boltzmann constant, and T is the temperature. Differing from the direct nonequilibrium calculation based on equation (1), the thermal conductivity here is calculated with current fluctuations at equilibrium. After studying different types of interaction potentials, it is found[28] that with a proper degree of asymmetry, the current autocorrelation decays rapidly, which leads to the convergence of the Green–Kubo formula.

It is well known that the asymmetric interaction can induce thermal expansion, while the symmetric one can not, and real materials usually show the thermal expansion effect.[29] Thus, our finding has particular importance for real materials. It implies that low-dimensional materials may also have size-independent thermal conductivity in the thermal limit as the bulk materials, and Fourier's law of thermal conduction is generally valid for low-dimensional materials. However, as mentioned above, at present it is generally accepted that the thermal current autocorrelation decays in power-law, and the thermal conductivity diverges with the system size in 1D momentum conserving systems. Meanwhile, the models we studied[27,28] have a potential with a combination of anharmonicity and asymmetry. Therefore, whether the convergent thermal conductivity results from the anharmonicity or the asymmetric feature needs to be clarified.

2. Model and results

We study a 1D momentum conserving lattice with simple asymmetric interparticle interactions: thermal expansion or thermal shrinkage is governed by different harmonic potentials. In more detail, we study the lattice described by the

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Hamiltonian

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + V(x_i - x_{i-1}), \tag{3}$$

where p_i and x_i represent the momentum and the deviation from its equilibrium position of the i-th particle, respectively. The potential is as follows:

$$V(x) = \begin{cases} \frac{1}{2}(1+r)x^2 & \text{if } x < 0 \\ \frac{1}{2}(1-r)x^2 & \text{otherwise}, \end{cases} \tag{4}$$

where r controls the degree of asymmetry. The potentials with different r are plotted in Fig. 1. These potentials and the higher order derivatives are continuous at $x = 0$, except the second derivative.

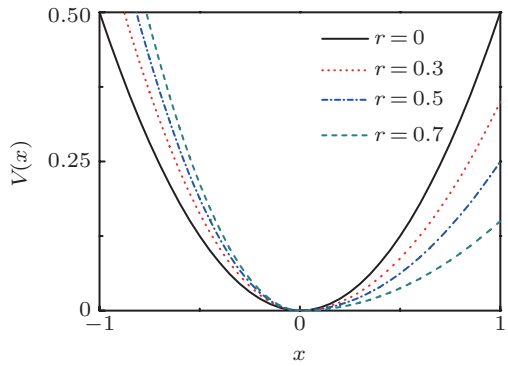


Fig. 1. (color online) The asymmetric harmonic interaction potentials.

To perform the nonequilibrium simulations, Nose-Hoover thermal baths[32,33] with temperatures T_L and T_R are coupled to the left and right particles, respectively. The fixed boundary conditions are applied in the simulation. The equations of the motion of the particles in the thermal baths is given by

$$\begin{aligned} \dot{x}_{1,N} &= \frac{p_{1,N}}{\mu}, \\ \dot{p}_{1,N} &= -\frac{\partial H}{\partial x_{1,N}} - \zeta_{L,R} p_{1,N}, \end{aligned} \tag{5}$$

$$\dot{\zeta}_{L,R} = \frac{p_{1,N}^2}{T_{L,R}} - 1 \tag{6}$$

and the motions of the other $N-2$ particles are described by

$$\dot{x}_i = \frac{p_i}{\mu}, \quad \dot{p}_i = -\frac{\partial H}{\partial x_i}. \tag{7}$$

We integrate the equations of motion using the leap-frog integrating algorithm. The local temperature and local thermal current at the i-th site are calculated by $T_i \equiv \langle p_i^2 \rangle$ and $J_i \equiv \langle \dot{x}_i \partial H / \partial x_i \rangle$, respectively.[8] The simulations are performed with a sufficiently long time, usually $t > 10^7$, to ensure that the system has reached a stationary state. In such a state, the local current is independent of the particle site. To avoid the finite-size effect, the system size N is extended until the temperature profiles fit with each other by rescaling the x variable with factor $1/N$, in which $\mathrm{d}T/\mathrm{d}x \approx N/(T_L - T_R)$, and the thermal conductivity can thus be calculated following $\kappa = \langle J \rangle N/(T_L - T_R)$.

Figure 2(a) shows the temperature profiles with $r = 0.5$ for several system sizes. One can see that for $N > 10^4$, the temperature profiles are well-rescaled together. Figure 2(b) shows the thermal conductivity as a function of system size. It can be seen that κ converges gradually to be a size-independent constant. The convergence threshold of the system size is quite long in this model, and this feature also appears in our previous work[27,28], where a different asymmetric interaction potential is applied. We guess that this may be one of the reasons why previous researchers have not observed convergent thermal conductivity, though they have also investigated lattice models with certain asymmetric potentials.

The convergence threshold is related to the degree of asymmetry. In Fig. 2, we also show the results with $r = 0.3$ and 0.7, respectively. It is clear that the threshold of convergent thermal conductivity increases with the decrease in the asymmetry degree. However, a further increase of r may result in simulation difficult. We have to apply a very small integral step to guarantee the integral precision.

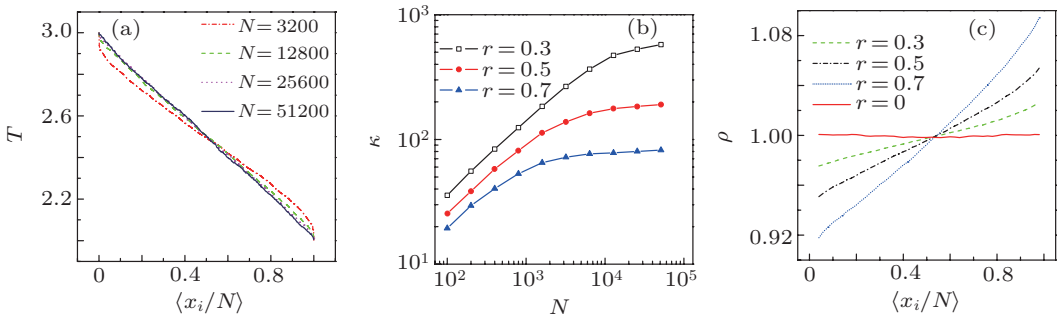


Fig. 2. (color online) (a) The temperature profiles for our model with fixed $r = 0.5$. (b) The thermal conductivity κ vs the number of particles N in our lattice model for various values of interaction asymmetry parameter r. (c) The mass density functions for our model with $r = 0.0$, 0.3, 0.5, and 0.7, respectively. The system size is $N = 2000$. In our simulations, the temperatures of the thermal baths are $T_L = 3$ and $T_R = 2$.

As in Ref. [27], we calculate the mass density $\rho(x)$ along the lattice chain at nonequilibrium stationary states. The results are shown in Fig. 2(c). It can be seen that the mass gradients do set up along the chain in the asymmetry cases, while in the symmetry case of $r = 0$, there is no such gradient. The density is inversely proportional to the temperature. This is a result of positive r, where thermal expansion occurs more easily than thermal shrinkage. If one applies a negative r to the potential, where thermal expansion is more difficult than thermal shrinkage, one will find that the mass density is proportional to the temperature. This is a remarkable difference between symmetric and asymmetric lattice systems, and may provide clues to understand why the qualitative difference in thermal transport emerges. We guess that the mass gradient can induce additional scattering of the current and, together with other scattering mechanisms, results in the normal thermal conduction behavior.

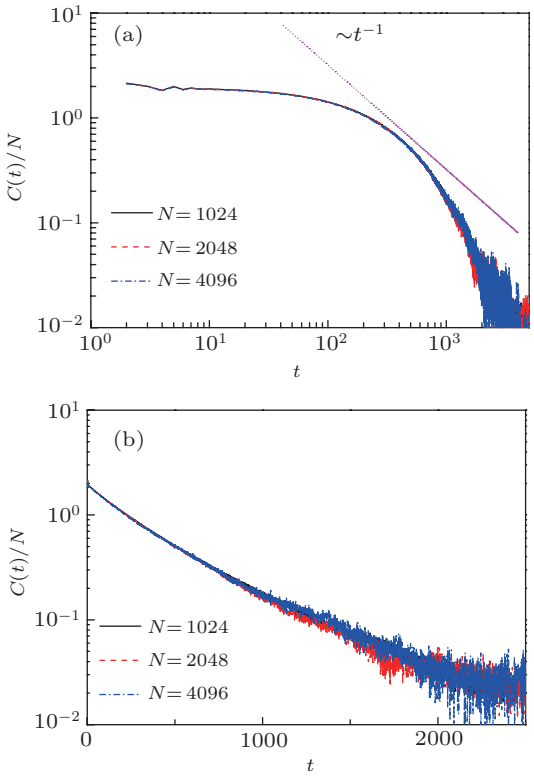


Fig. 3. (color online) The autocorrelation function of the thermal flux, $C(t)$, for the asymmetric harmonic interaction potential with $r = 0.5$ at $T = 2.5$, shown by the log–log plot (a) and the semi-log plot (b). The dashed line indicates the decay function t^{-1} for reference.

The decay behavior of the current autocorrelation can further confirm that asymmetric interparticle interactions may result in the normal thermal conduction of lattice systems. To calculate the current autocorrelation function, we first evolve the system for a sufficiently long time to relax the system to its equilibrium state. Then, the current correlation function $C(t) = \langle J(t)J(0)\rangle$ is calculated by the total current fluctuations $J(t) = \sum_{i=1}^{N} J_i(t)$. The decay behavior of $C(t)$ determines whether the thermal flux violates the Fourier law of thermal conduction. If it decays as $C(t) \sim t^{-\gamma}$ with $\gamma < 1$, the κ will diverge following the Green–Kubo formula. If it decays faster than $\gamma = 1$, particularly with an exponential decay of $C(t) \sim e^{-\delta t}$, then the Green-Kubo formula converges and the thermal conductivity is size-independent in the thermal dynamical limit. The Fourier law is thus obeyed. Figure 3 shows the current autocorrelation functions corresponding to the parameter sets applied in Fig. 2. To perform the simulation, periodic boundary conditions are applied with several simulation sizes. The temperature is set to be $T = 2.5$, which is the average temperature applied in the nonequilibrium simulations. One may see that the curves with different simulation sizes overlap with each other, indicating that the finite-size effect is avoided. It is clear, either with the log–log plot or the semi-log plot, that the decay of the autocorrelation function is quite fast, and even approaches the exponential decay manner, indicating a convergent thermal conductivity.

3. Concluding remarks

In conclusion, the 1D lattice model, even with asymmetric harmonic interparticle interactions, shows normal thermal conduction behavior. Our nonequilibrium simulations obtain a size-independent thermal conductivity when the system size is sufficiently large. Our equilibrium simulations show that the current autocorrelation decays faster than the power-law decay of $C(t) \sim t^{-1}$, implying a convergent thermal conductivity according to the Green–Kubo formula. Because this model involves only the asymmetric harmonic interactions, our results thus confirm that it is the asymmetry of the interaction potentials that result in the normal thermal conduction behavior in 1D momentum conserving lattices.

This model has another obvious advantage. With a scale transformation $(\widetilde{x},\widetilde{t}) \to (\alpha x, t)$, the Hamiltonian changes as $\widetilde{H} \to \alpha^2 H$. Therefore, the dynamics of the system remain unchanged with scale transformation. In more detail, the systems with Hamiltonian $\widetilde{H}$ at temperature $\widetilde{T}$ and with Hamiltonian H at temperature T are identical, where $\widetilde{T} = \alpha^2 T$. Therefore, the conclusion of normal thermal conductivity can be directly extended to any temperature region.

We also observed that the mass density is set up along the lattice chain in the case of asymmetric potentials at nonequilibrium stationary states. This phenomenon may be important in understanding the microscopic mechanism of the normal thermal conductivity in nonequilibrium stationary states. In equilibrium states, there is no such stationary gradient of mass density. How a rapid decay of the current autocorrelation is caused is an open problem and deserves further studies.

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References

[1] Rieder Z, Lebowitz J L and Lieb E 1967 *J. Math. Phys.* **8** 1073
[2] Casati G, Ford J, Vivaldi F and Visscher W M 1984 *Phys. Rev. Lett.* **52** 1861
[3] Prosen T and Robnik M 1992 *J. Phys. A* **25** 3449
[4] Lepri S, Livi R and Politi A 1997 *Phys. Rev. Lett.* **78** 1896
[5] Li B, Casati G, Wang J and Prosen T 2004 *Phys. Rev. Lett.* **92** 254301
[6] Prosen T and Campbell D K 2005 *Chaos* **15** 015117
[7] Prosen T and Campbell D K 2000 *Phys. Rev. Lett.* **84** 2857
[8] Hu B, Li B and Zhao H 1998 *Phys. Rev. E* **57** 2992
[9] Hu B, Li B and Zhao H 2000 *Phys. Rev. E* **61** 3828
[10] Mai T, Dhar A and Narayan O 2007 *Phys. Rev. Lett.* **98** 184301
[11] Wang L and Wang T 2011 *Europhys. Lett.* **93** 54002
[12] Lepri S, Livi R and Politi A 2003 *Phys. Rep.* **377** 1
[13] Dhar A 2008 *Adv. Phys.* **57** 457
[14] Prosen T and Campbell D K 2000 *Phys. Rev. Lett.* **84** 2857
[15] Narayan O and Ramaswamy S 2002 *Phys. Rev. Lett.* **89** 200601
[16] Mai T and Narayan O 2006 *Phys. Rev. E* **73** 061202
[17] Lee-Dadswell G R, Nickel B G and Gray C G 2005 *Phys. Rev. E* **72** 031202
[18] Lee-Dadswell G R, Nickel B G and Gray C G 2008 *J. Stat. Phys.* **132** 1
[19] Delfini L, Lepri S, Livi R and Politi A 2006 *Phys. Rev. E* **73** 060201
[20] Delfini L, Lepri S, Livi R and Politi A 2007*J. Stat. Mech.* P02007
[21] Wang J S and Li B 2004 *Phys. Rev. Lett.* **92** 074302
[22] Wang J S and Li B 2004 *Phys. Rev. E* **70** 021204
[23] Giardiná C, Livi R, Politi A and Vassalli M 2000 *Phys. Rev. Lett.* **84** 2144
[24] Gendelman O V and Savin A V 2000 *Phys. Rev. Lett.* **84** 2381
[25] Giardiná C and Kurchan J 2005 *J. Stat. Mech.* P05009
[26] Lee-Dadswell G R, Turner E, Ettinger J and Moy M 2010 *Phys. Rev. E* **82** 061118
[27] Zhong Y, Zhang Y, Wang J and Zhao H 2012 *Phys. Rev. E* **85** 060102
[28] Chen S D, Zhang Y, Wang J and Zhao H 2012 *arXiv:*1204.5933
[29] Kittel C 1996 *Introduction to Solid State Physics* 7th edn. (New Jersey: Wiley) p. 130
[30] Green M S 1954 *J. Chem. Phys.* **22** 398
[31] Kubo R, Yokota M and Nakajima S 1957 *J. Phys. Soc. Jpn.* **12** 1203
[32] Nose S 1984 *J. Chem. Phys.* **81** 511
[33] Hoover W G 1985 *Phys. Rev. A* **31** 1695