Asymmetric Heat Conduction in Nonlinear Lattices

Bambi Hu,[1,2] Lei Yang,[1,3] and Yong Zhang[1,*]

[1]*Department of Physics, Centre for Nonlinear Studies, and The Beijing-Hong Kong-Singapore Joint Centre for Nonlinear and Complex Systems (Hong Kong), Hong Kong Baptist University, Kowloon Tong, Hong Kong, China*
[2]*Department of Physics, University of Houston, Houston, Texas 77204-5005, USA*
[3]*Institute of Modern Physics, Chinese Academy of Science, and Department of Physics, Lanzhou University, Lanzhou 730000, China*
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In this Letter, we conduct an extensive study of the two-segment Frenkel-Kontorova model. We show that the rectification effect of the heat flux reported in recent literature is possible only in the weak interfacial coupling limit. The rectification effect will be reversed when the properties of the interface and the system size change. These two types of asymmetric heat conduction are governed by different mechanisms though both are induced by nonlinearity. An intuitive physical picture is proposed to interpret the reversal of the rectification effect. Since asymmetric heat conduction depends critically on the properties of the interface and the system size, it is probably not an easy task to fabricate a thermal rectifier or thermal diode in practice.

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The problem of phonon transport is much less well understood than that of electron transport. The key distinction lies in the fact that the former is a thermal nonequilibrium problem, while the latter is a thermal equilibrium problem. Even in a simple model such as the Fermi-Pasta-Ulam model, it is difficult to get a complete microscopic explanation of its macroscopic thermal transport behavior as described by the Fourier law [1–4]. On the other hand, the band theory predicts a unidirectional transport of electrons in a heterogeneous semiconductor junction. This property is basically due to the fact that electrons obey Fermi-Dirac statistics and only the valence electrons will take part in the transport process. In contrast, phonons obey Bose-Einstein statistics and all of them will take part in the transport process. In this respect, phonons, viewed as a collective excitation of a crystal lattice, are not expected to exhibit intrinsic asymmetric transport unless the thermal conductivity of the material changes dramatically when the positions of the heat baths are reversed.

Recently, asymmetric heat conduction in one-dimensional inhomogeneous chains with nonlinear on-site potentials has been reported [5–9]. The system acts like a good thermal conductor in one direction but a good thermal insulator in the opposite direction when the positions of the heat baths are reversed. An explanation of this phenomenon is that the phonon bands of different segments of the chain will change from overlap to separation when the heat baths are reversed. The reason why temperature can control the phonon band shift is due to the presence of nonlinearity in the effective phonon spectrum at different temperatures. The effective phonon spectrum can be obtained qualitatively by a linearization of the Hamiltonian [6] and quantitatively by the self-consistent phonon theory [10]. On the other hand, the numerical results reported in previous works [6,8] show that the rectification effect will decrease as the system size and the interfacial coupling increase. Nevertheless, the overlap or separation of the phonon bands, obtained by treating each segment of the chain independently, is independent of the system size and the interfacial coupling constant. Moreover, we have checked explicitly that the single-particle frequency spectrum used in Ref. [6] under nonequilibrium states is very much independent of the system size (Fig. 1). Thus this picture fails to explain the decrease of the rectification effect. Surprisingly, our results show that the rectification effect will be reversed when these parameters increase further. Therefore, a more in-depth understanding of asymmetric heat conduction is needed before one can ascertain the rectification effect and apply it to the design of thermal devices.

In this Letter, we have conducted an extensive study of the two-segment Frenkel-Kontorova (FK) model [6]. We

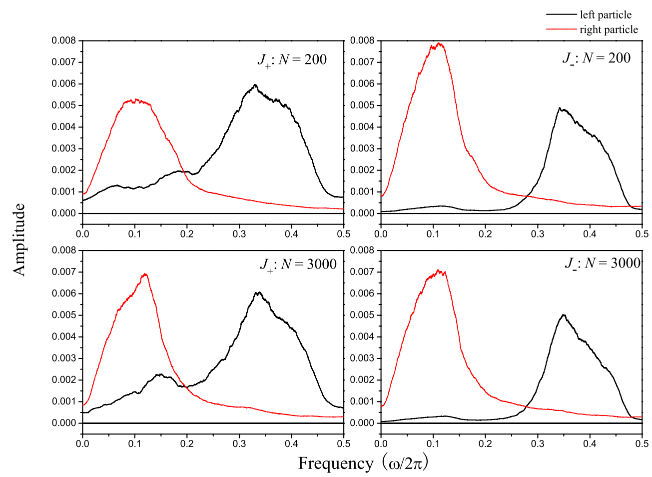

FIG. 1 (color online). Single-particle frequency spectrum of the two coupled particles ($k_{\rm int} = 0.2$) on the left (solid line) and the right (dotted line) of the interface for $N = 200$ and $N = 3000$.

find that the rectification effect will be reversed when the properties of the interface and the system size change. A simple physical picture is proposed to understand the reversal of the rectification effect, and a new mechanism for this new type of asymmetric heat transport is proposed. Moreover, we argue that, since asymmetric heat conduction depends critically on the properties of the interface and the system size, the actual fabrication of a thermal rectifier or thermal diode is probably not an easy task.

We consider a FK chain consisted of two segments of $N/2$ particles. The two segments are connected by a harmonic spring with spring constant k_{int}. The Hamiltonian of the whole system is

$$H = H_A + H_B + \tfrac{1}{2}k_{\text{int}}(x_{N/2+1} - x_{N/2} - a)^2, \qquad (1)$$

where H_A and H_B are the Hamiltonian of the left (A) segment and the right (B) segment, respectively:

$$H_{A,B} = \sum_i \frac{p_i^2}{2m} + \frac{1}{2}k_{A,B}(x_{i+1} - x_i - a)^2 - \frac{V_{A,B}}{(2\pi)^2} \times \cos 2\pi x_i. \qquad (2)$$

m is the mass of the particles, a the lattice constant, and V the strength of the external potential. We set $m = a = 1$, $V_A = 5$, $V_B = 1$, $k_A = 1$, and $k_B = 0.2$. The main adjustable parameters are k_{int} and N.

In our simulations we use fixed boundary conditions and the chain is connected to two heat baths at temperatures T_+ and T_-, respectively. We take $T_+ = 0.105$ and $T_- = 0.035$. We use Nosé-Hoover heat baths and integrate the equations of motion by using the fourth-order Runge-Kutta algorithm [11]. The local temperature is defined as $T_i = m\langle \dot{x}_i^2 \rangle$. The local heat flux is defined as $j_i = k\langle \dot{x}_i(x_i - x_{i-1})\rangle$, and the total heat flux is $J = Nj$. The simulations are performed long enough to allow the system to reach a steady state in which the local heat flux is constant along the chain. We denote the absolute value of total heat flux from left to right as J_+ and the heat flux from right to left as J_- when the positions of the two heat baths are reversed.

Figure 2 shows the dependence of $J_\pm$ on k_{int} for different system sizes $N = 100$, 1000, and 2000. As k_{int} increases there exists a crossover from $J_+ > J_-$ to $J_+ < J_-$; i.e., the rectification effect is reversed. When $J_+ > J_-$, our results are in agreement with those reported in Ref. [6] and the explanation based on the effective phonon theory. When the heat flux flows from A to B, there is a big overlap between the phonon bands of A and B; however, there is almost a complete separation when the positions of the two heat baths are reversed. Only phonons with frequencies within the overlapping range contribute to the heat flux. So $J_+ > J_-$, and J_- is nearly zero. Moreover, the overlapping bandwidth of A and B is almost unchanged when the two segments are very weakly coupled. $J_\pm$ are only determined by the transmission of phonons crossing the interface, i.e., k_{int}. One expects that $J_\pm$ will increase in the same way as

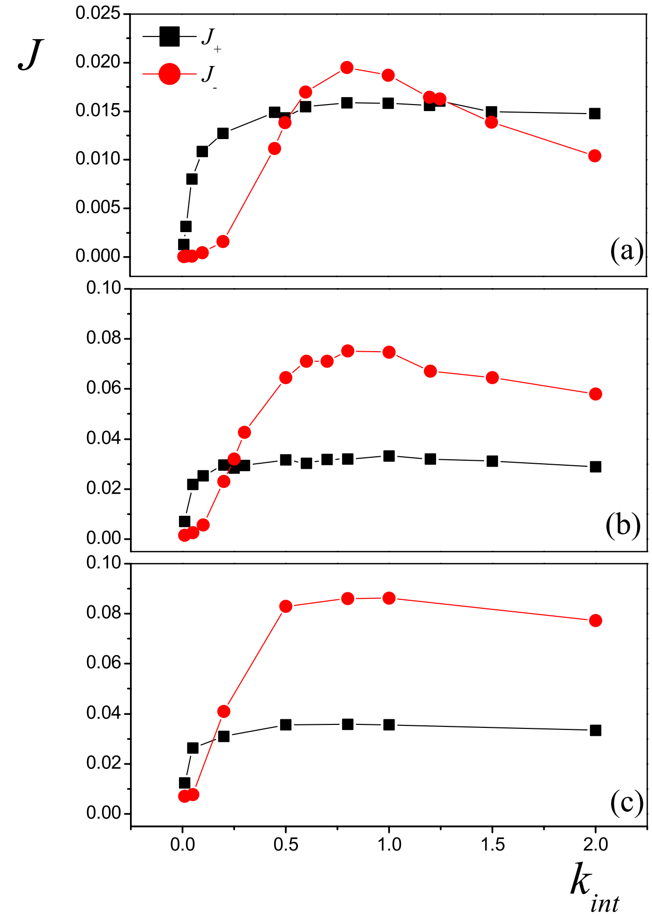

FIG. 2 (color online). Dependence of the total heat flux $J_\pm$ on the interfacial harmonic coupling strength k_{int} for (a) $N = 100$, (b) $N = 1000$, and (c) $N = 2000$.

k_{int} increases. This is confirmed by the numerical result that $J_\pm \sim k_{\text{int}}^2$ for small k_{int} and N. In fact, this relationship is universal when one considers the transmission of phonons crossing the interface between two kinds of material that are weakly joined by a harmonic spring [12,13]. However, when $J_+ < J_-$, the results are strikingly different. $J_\pm$ increase sharply and they are almost independent of k_{int}, as shown in Figs. 2(b) and 2(c). These results are in disagreement with the prediction based on the effective phonon theory. They strongly suggest that the phonon bands of A and B are no longer separable; instead they become mixed and form a whole. The mixing of phonon bands is due to interactions between phonons of A and B induced by the nonlinearity in the chain. In fact, the validity of the effective phonon theory that treats each of the two segments of the chain independently is predicated on the assumption $k_{\text{int}} \to 0$. As a consequence, the numerical results show $J_+ > J_-$ only for very small k_{int} (typically $k_{\text{int}} = 0.05$). As k_{int} increases the two segments of the chain behave as a whole. The phonon spectrum of the whole chain is different from those of A and B separately. Therefore, the effective phonon theory applied to A and B

separately fails to explain this new type of asymmetric heat conduction.

Figure 2(a) shows that J_+ and J_- behave quite differently. J_+ reaches saturation as $k_{\rm int}$ increases, whereas J_- reaches its maximum at $k_{\rm int} \approx (k_A + k_B)/2 = 0.6$ and decreases as $k_{\rm int}$ further increases. Specifically, $J_+ > J_-$ again when $k_{\rm int} > (k_A + k_B) = 1.2$. These results can be understood intuitively as follow. The role of $k_{\rm int}$ is like an impurity in the two-segment chain when $k_{\rm int} \gg (k_A + k_B)/2$. The impurity scatters only high-frequency phonons and does not affect low-frequency ones. We speculate that, in the mixed phonon spectrum, both low-frequency and high-frequency phonons contribute to J_-, whereas mainly low-frequency phonons contribute to J_+. As a result, J_- decreases due to impurity scattering, whereas J_+ is almost unchanged as $k_{\rm int}$ increases. The effect of the impurity on heat conduction is reduced when N increases. From Fig. 2(c), it is clearly seen that both J_+ and J_- almost saturate as $k_{\rm int}$ increases. This means that the heat conduction behavior of the chain is almost independent of $k_{\rm int}$ when the chain is long enough. Note also that the crossover occurs at $k_{\rm int} \approx 0.5$, 0.24, and 0.15 for $N = 100$, 1000, and 2000. This result strongly suggests that the crossover will occur as N increases.

Figure 3 shows the dependence of $J_\pm$ on N for different $k_{\rm int}$. For a typical weak coupling, $k_{\rm int} = 0.05$, the crossover does not occur until $N = 3000$. It is clear, however, that J_- increases much faster than J_+, as shown in Fig. 3(a). This implies that the crossover will occur at a much larger N. In Fig. 3(b), the crossover appears at $N \approx 1500$ for $k_{\rm int} = 0.2$. In Fig. 3(c), $J_+ < J_-$ for all N. This result can also be understood from the role of $k_{\rm int}$ in the limit $N \to \infty$. Strictly speaking, there is no geometric boundary in a one-dimensional system unless the coupling of the two segments is exactly zero in the thermodynamic limit. For any finite $k_{\rm int}$, the interface of the two segments behaves like an impurity as $N \to \infty$, and the effect of the impurity on the heat conduction of the whole system is reduced when N increases. This suggests that, in the two-segment chain, $J_+ < J_-$ in the thermodynamical limit.

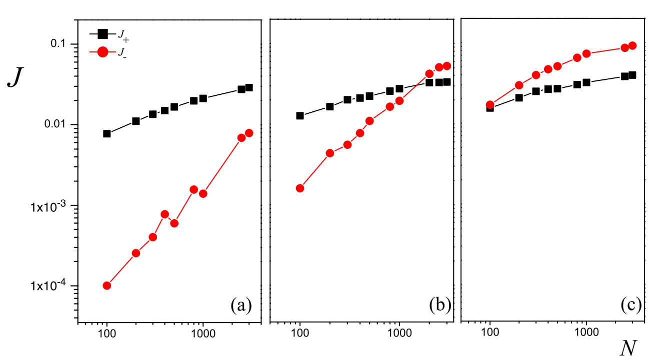

FIG. 3 (color online). Dependence of the total heat flux $J_\pm$ on the system size N in the log-log plot for (a) $k_{\rm int} = 0.05$, (b) $k_{\rm int} = 0.2$, and (c) $k_{\rm int} = 0.6$.

It is thus clear that there are two types of asymmetric heat conduction in the two-segment FK model, and a crossover will occur as $k_{\rm int}$ and N change. When the two segments are very weakly coupled, $J_+ > J_-$. When the two segments are well coupled or the chain is long enough, $J_+ < J_-$. The phonon band shift plays an important role in the former case, whereas phonon band mixing plays an important role in the latter case. It is remarkable that these two opposite behaviors can both be attributable to the presence of nonlinearity.

In order to further verify the role of nonlinearity in asymmetric heat conduction, we add a quartic coupling to the interfacial Hamiltonian in Eq. (1):

$$H = H_A + H_B + \tfrac{1}{2}k_{\rm int}(x_{N/2+1} - x_{N/2} - a)^2 + \tfrac{1}{4}\beta_{\rm int}(x_{N/2+1} - x_{N/2} - a)^4. \quad (3)$$

Figure 4 shows the dependence of $J_\pm$ on $\beta_{\rm int}$ for $N = 100$ and 1000 at a typical weak coupling $k_{\rm int} = 0.05$. By increasing $\beta_{\rm int}$, one can also see a similar crossover, as shown in Figs. 2 and 3. The crossover occurs at $\beta_{\rm int} \simeq 0.06$ and $\beta_{\rm int} \simeq 0.02$ for $N = 100$ and 1000, respectively. These results confirm that phonon band mixing will lead to a crossover from $J_+ > J_-$ to $J_+ < J_-$ even if the nonlinearity is very small.

A problem immediately arises from the above analysis: Why is $J_+ < J_-$ when the phonon bands of A and B mix?

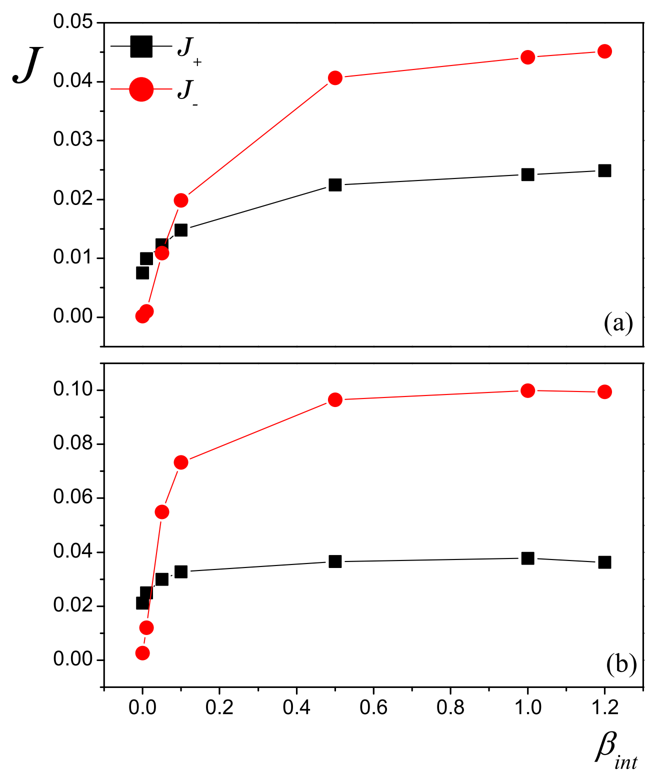

FIG. 4 (color online). Dependence of the total heat flux $J_\pm$ on the interfacial anharmonic coupling strength $\beta_{\rm int}$ for (a) $N = 100$ and (b) $N = 1000$.

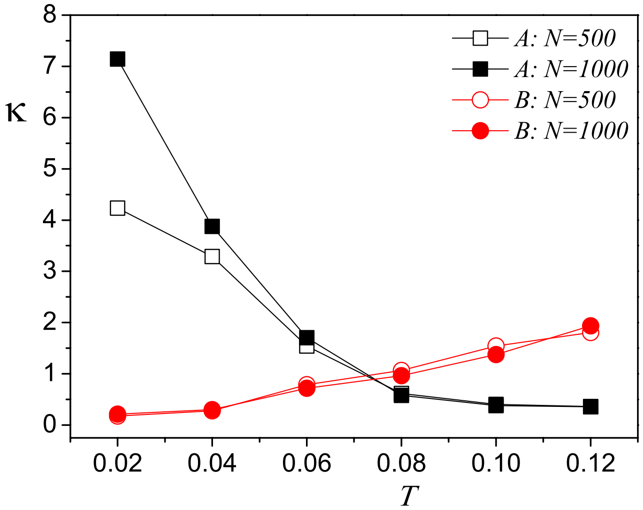

FIG. 5 (color online). Dependence of the thermal conductivity κ on the temperature T_0 for segment A and segment B, respectively. The temperature of heat baths is $T_{\pm} = T_0(1 \pm \Delta)$. $T_0 = 0.02, 0.04, 0.06, 0.08, 0.1$, and 0.12, and $\Delta = 0.1$. $\kappa = J/(2\Delta T_0)$.

In the thermodynamical limit, it can be expected that heat conduction in the two-segment chain is determined only by the heat transport properties of A and B and is independent of the properties of the interface and the system size. In Fig. 5, we plot the dependence of the thermal conductivity on the temperature for A and B, respectively. As the temperature changes from 0.02 to 0.12, κ_A decreases and κ_B increases. Thus both A and B have a higher thermal conductivity when A is in contact with a heat bath at $T_- = 0.035$ and B with a heat bath at $T_+ = 0.105$. When the heat baths are reversed, both A and B have a lower thermal conductivity; therefore, $J_+ < J_-$.

In summary, we have found a reversal of the rectification effect in the two-segment FK model. We differentiate two different (even opposite) effects of nonlinearity on the heat conduction behaviors. When the coupling of the two segments is weak, the phonon band shift leads to $J_+ > J_-$. When the coupling is strong or the chain is long enough, phonon band mixing leads to $J_+ < J_-$. A crossover between these two types of asymmetric heat conduction will occur by varying the properties of the interface and the system size.

Asymmetric heat conduction opens up the possibility for the design of thermal rectifiers and thermal diodes [5,6]. However, as shown by our numerical results, the functionability of such a thermal device depends critically on the properties of the interface. It is very difficult to control the interfacial properties precisely in practice [14]. This difficulty results in a poor reproducibility of the measurement of the thermal boundary resistance. As a result, the functionability of such thermal devices will be quite unpredictable due to insufficient information about atomic interfacial conditions. Therefore, it is probably not an easy task to fabricate a thermal rectifier or a thermal diode in practice.

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*To whom correspondence should be address.
Electronic address: yzhang@phys.hkbu.edu.hk

[1] F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet, in *Mathematical Physics 2000*, edited by A. Fokas *et al.* (Imperial College Press, London, 2000), p. 128.
[2] S. Lepri, R. Livi, and A. Politi, Phys. Rep. **377**, 1 (2003).
[3] R. Livi and S. Lepri, Nature (London) **421**, 327 (2003).
[4] Special issue on the 50th anniversary of the Fermi-Pasta-Ulam model, edited by D. K. Campbell, P. Rosenau, and G. Zaslavsky [Chaos **15**, 015101 (2005)].
[5] M. Terraneo, M. Peyrard, and G. Casati, Phys. Rev. Lett. **88**, 094302 (2002).
[6] B. Li, L. Wang, and G. Casati, Phys. Rev. Lett. **93**, 184301 (2004).
[7] B. S. Xie, H. Li, and B. Hu, Europhys. Lett. **69**, 358 (2005).
[8] B. Hu and L. Yang, Chaos **15**, 015119 (2005).
[9] B. Li, J. Lan, and L. Wang, Phys. Rev. Lett. **95**, 104302 (2005).
[10] T. Dauxois, M. Peyrard, and A. R. Bishop, Phys. Rev. E **47**, 684 (1993).
[11] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes* (Cambridge University Press, Cambridge, 1992).
[12] Kelly R. Patton and Michael R. Geller, Phys. Rev. B **64**, 155320 (2001).
[13] B. Hu, D. He, L. Yang, and Y. Zhang, Report No. CNS-05-03, 2005.
[14] E. T. Swartz and R. O. Pohl, Rev. Mod. Phys. **61**, 605 (1989).