Asymmetric Properties of Heat Conduction in a One-Dimensional Frenkel-Kontorova Model

Bambi Hu\textsuperscript{1,2}, Lei Yang\textsuperscript{1}, and Yong Zhang\textsuperscript{1,*}

\textsuperscript{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
\textsuperscript{2}Department of Physics, University of Houston, Houston, Texas 77204-5005

In this Letter, we show numerically that the rectifying effect of heat flux in a one-dimensional two-segment Frenkel-Kontorova chain demonstrated in recent literature is merely available under the limit of the weak coupling between the two constituent segments. Surprisingly, the rectifying effect will be reversed when the properties of the interface and the system size change. The two types of asymmetric heat conduction are dominated by different mechanisms, which are all induced by the nonlinearity. We further discuss the possibility of the experimental realization of thermal diode or rectifier devices.

PACS numbers: 44.10.+i, 05.60.-k, 05.70.Ln

Understanding of the phonon transport behavior under nonequilibrium stationary states is much less than the electron in charge conduction. It is a key distinction between them that the former is related to nonequilibrium statistic mechanics, while the latter is basically the transport behavior under thermal equilibrium states. Even for the phonon thermal conduction in the simplest solid model, such as the Fermi-Pasta-Ulam $\beta$ model, in low dimensional cases, it is still an open question to get full microscopic dynamics description of macroscopic thermal transport behavior, i.e. the Fourier law\textsuperscript{[1, 2, 3, 4]}. On the other hand, the band theory predicts the unidirectional transport of the electrons in heterogeneity semiconductor junctions, which have very useful applications in modern electronics. This property is basically attributed to the facts that the electrons obey Fermi statistics and only the valence electrons take part in the transport process. In contrast, the phonons obey Bose-Einstein statistics and all take part in thermal transport. In this respect, a phonon, viewed as a collective exciton in crystal lattices, is not expected to exhibit intrinsic asymmetric transport properties, unless the heat conduction of material dramatically changes when the heat baths are exchanged.

Recently, however, the asymmetric heat conduction in one-dimensional inhomogeneous chains with nonlinear on-site potentials has been reported via computer simulations\textsuperscript{[5, 6, 7, 8]}. They proposed some mechanisms which allow the heat flux in one direction while the systems act almost like an insulator when the heat baths are exchanged. These mechanisms are based on a common idea that phonon bands of the different segments of the chain change from overlap to separation when the heat baths are exchanged. The phonon band shift controlled by temperature is attributed to the different contribution of nonlinearity to the effective phonon spectra at different temperatures. The effective phonon spectrum can be obtained quantitatively by self-consistent phonon method\textsuperscript{[9]} and qualitatively by linearization treatment of Hamiltonians\textsuperscript{[10]}. On the other hand, the numerical results in previous work\textsuperscript{[5, 6, 7]} show that the rectifying effect decreases as the system size and the coupling of the interface increase. Nevertheless, the picture of overlap/separation of phonon bands, which treats each of the different segments of the chain independently, is totally independent of the system size and the coupling of the interface. Thus, this picture fails to explain numerical results on the decreasing of the rectifying effect. Surprisingly, as shown by our numerical results in this paper, the rectifying effect will be reversed when these parameters further increase. So, more in-depth understanding is needed to assess possible applications of this counterintuitive phenomenon discovered by computer simulations.

In this Letter, we implement extensive numerical studies about a one-dimensional two-segment Frenkel-Kontorova (FK) chain that is exactly the same as the model studied by Ref.\textsuperscript{[6]}. We find that the rectifying effect demonstrated in Ref.\textsuperscript{[6]} will be reversed when the properties of the interface and the system size change. A simple physical picture was proposed to understand the reversal of the rectifying effect, and a new but very intuitive mechanism for the new type of asymmetric heat transport was addressed. We further argue that the experimental realization is a hard task, because the asymmetric heat conduction dramatically depends on the properties of the interface and the system size.

We consider a one-dimensional chain consisting of two segments of $N/2$ particles. The two segments are connected by a linear spring of constant $k_{\text{int}}$. The Hamiltonian of the whole system is

\begin{equation}
H = H_A + H_B + \frac{1}{2}k_{\text{int}}(x_{N/2+1} - x_{N/2} - a)^2,
\end{equation}

where $H_A$ and $H_B$ are the Hamiltonian of the left segment (A segment) and the right one (B segment), respec-

*Author to whom correspondence should be addressed. Electronic address: yzhang@phys.hkbu.edu.hk
We set the mass of the particles and the lattice constant \( m = a = 1 \), and fix \( V_A = 5, V_B = 1, k_A = 1 \) and \( k_B = 0.2 \). The main adjustable parameters in this paper are \( k_{\text{int}} \) and \( N \).

In our numerical simulations we use fixed boundary conditions and the chain is coupled, at the two ends, with heat baths at temperatures \( T_+ \) and \( T_- \) respectively. We take \( T_+ = 0.105 \) and \( T_- = 0.035 \) through our paper. We use Nosé-Hoover heat baths and integrate the differential equations of motion by using the fourth-order Runge-Kutta algorithm as described in [10]. We compute the temperature profile inside the system, i.e., the local temperature at site \( i \) defined as \( T_i = m \langle \dot{x}_i^2 \rangle \), where \( \langle \rangle \) stands for temporal average, the local heat flux \( j_i = k \langle x_i(x_i - x_{i-1}) \rangle / 2 \) and \( J = N j \) the total heat flux. The simulations are performed long enough to allow the system to reach a steady state where the local heat flux is constant along the chain. We denote the absolute value of total heat flux from left to right as \( J_+ \) when the bath at higher temperature \( T_+ \) is at the left end of the chain and as \( J_- \) when the baths are exchanged.

Figure 1 shows \( k_{\text{int}} \) dependence of \( J_+ \) and \( J_- \) in different system size \( N = 100, 1000, 2000 \). As \( k_{\text{int}} \) increases there exist a crossover from the situation with \( J_+ > J_- \) to that with \( J_+ < J_- \), that is, the rectifying effect is reversed. In the situation \( J_+ > J_- \), our numerical results are in agreement with those reported in Ref.[2] at the same parameters and the prediction by the effective-phonon analysis (as shown by the Fig.4 in the Ref.[2]). When the heat flux flows from A to B there is a big overlap between the phonon bands of A and B, while there is almost a separation between them when the baths are exchanged. Only phonons with the frequencies within the overlap range have contributions to heat flux. So \( J_+ > J_- \) and \( J_- \) is near zero. Moreover, the overlapping bandwidth between A and B is almost unchanged when the two segments are very weakly coupled. So in this case the \( J_\pm \) are only determined by the transmission of the phonons crossing the interface, i.e., \( k_{\text{int}} \). One can expect that \( J_\pm \) increase in the same way as \( k_{\text{int}} \) increases. This is confirmed by the numerical result that \( J_\pm \sim k_{\text{int}}^2 \) with small \( k_{\text{int}} \) and \( N \) (as shown by the Fig.2(a) in Ref.[3]). In fact, this relationship is universal when one consider the transmission of phonons crossing the interface between two kind of material that are weakly joined by a harmonic spring [11, 12]. In the situation \( J_+ < J_- \), the results are strikingly different. \( J_\pm \) have sharp increases compared to the former case, and almost independent of the \( k_{\text{int}} \) as shown in Fig.1(b) and Fig.1(c). These results are disagreement with the above prediction based on the effective-phonon analysis, and strongly suggest that phonon bands of A and B mix up. It is obvious that the band mixing is due to the interaction among phonons induced by the nonlinearity in the chain. In fact, the effective-phonon analysis in Ref.[6] treated each of the two segments of the chain independently, and it could be based on the condition \( k_{\text{int}} \to 0 \). Consequently, the prediction, i.e. \( J_+ > J_- \), is well agreement with the numerical results for very small \( k_{\text{int}} \) (a typical value in simulations is 0.05). As \( k_{\text{int}} \) increases the two-segment chain behaves as a whole. The phonons of the chain in this situation become different from the ones of A and B due to the band mixing. Therefore, the individual effective-phonon analysis to each of A and B fails to explain the new type of asymmetric heat conduction.

There is the difference between curves of the \( J_+ \) and \( J_- \) in Fig.1(a). \( J_+ \) reaches saturation as \( k_{\text{int}} \) increases. \( J_- \) reaches its maximum value at the middle \( k_{\text{int}} \) value with \( (k_A + k_B) / 2 = 0.6 \), but decreases as \( k_{\text{int}} \) further increases. Specially, \( J_+ \) is larger than \( J_- \) again when \( k_{\text{int}} \) increases larger than the value \( k_{\text{int}} \sim k_A + k_B = 1.2 \) as shown in Fig.1(a). These phenomena can be understood as follow. The role of \( k_{\text{int}} \) changes to an impurity in the two-segment chain when \( k_{\text{int}} \gg (k_A + k_B) / 2 \). The impurity just scatters the high-frequency phonons, and does not affect the low-frequency ones. We speculate that, for the mixing phonon spectrum, the high-frequency phonons have main contributions to \( J_+ \) and the low-frequency ones to \( J_- \). As a result, \( J_- \) drops due to the impurity scattering, while \( J_+ \) is almost unchanged as \( k_{\text{int}} \) increases. The effect of the impurity on the heat conduction reduces with \( N \) increasing. So the reduction of...
FIG. 2: Total heat current $J_{\pm}$ versus the system size $N$ in the log-log plot for (a) $k_{\text{int}} = 0.05$; (b) $k_{\text{int}} = 0.2$; (c) $k_{\text{int}} = 0.6$.

$J_-$ decrease as $N$ increase as shown by Fig.1. It is clear seen that both $J_+$ and $J_-$ almost saturate as $k_{\text{int}}$ increases as shown in Fig.1(c). This means that the heat conduction behavior of the chain is almost independent of $k_{\text{int}}$ when the two segments are well coupled. Note also that the crossover occurs at $k_{\text{int}} \approx 0.5$, 0.24, 0.15 for $N = 100$, 1000, 2000. This result strongly implies that the crossover will also appears as $N$ increases under certain fixed $k_{\text{int}}$. It is confirmed by Fig.2.

Figure 2 depicts the $N$ dependence of $J_+$ and $J_-$ at different $k_{\text{int}}$. For a typical weak coupling value, $k_{\text{int}} = 0.05$, the crossover does not occur, i.e. $J_+ > J_-$, up to $N = 3000$. It is clear, however, seen that the increasing of $J_-$ is more faster than $J_+$ as shown in Fig.2(a). This implies that the crossover will occur at a larger $N$. In Fig.2(b), the crossover appears at $N \approx 1500$ for $k_{\text{int}} = 0.2$. In Fig.2(c), the two-segment chain exhibits $J_+ < J_-$ for the whole regime of $N$ used for simulations. This result can also be understood by the role of $k_{\text{int}}$ in the limit case $N \rightarrow \infty$. Strictly speaking, there is not a geometric boundary within a one-dimensional system in thermodynamic limit, unless the coupling of the two segments is exact zero. For any finite $k_{\text{int}}$, the interface of two segments behaves like an impurity in the limit $N \rightarrow \infty$, and the effect of the impurity on heat conduction of the whole system reduces with $N$ increasing, as stated above. This suggest that the two-segment chain will exhibit the behavior of $J_+ < J_-$ in the thermodynamical limit.

Up to now, it is clear seen that there are two types of asymmetric heat conduction in the two-segment FK model (1), and the transition between them will occur by varying the $k_{\text{int}}$ and $N$. When the two segments are very weakly coupled, $J_+$ is larger than $J_-$; while $J_-$ is larger than $J_+$ when the two segments are well coupled or the chain is long enough. Phonon band shift and phonon mixing play important roles in the former case and the latter case, respectively. It is interesting that these two contrary behaviors are all attributed to the nonlinearity.

In order to further verify the role of nonlinearity in the asymmetric heat conduction in model (1), we add a quartic nonlinear coupling to the interface in model (1), as described by

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

Figure 3 plots the $J_{\pm}$ versus $\beta_{\text{int}}$ for $N = 100$ and $N = 1000$ at a typical weak coupling parameter $k_{\text{int}} = 0.05$. By increasing the $\beta_{\text{int}}$, one can also see the similar crossover as shown in Fig.1 and Fig.2. The crossover occurs at $\beta_{\text{int}} \approx 0.06$ and $\beta_{\text{int}} \approx 0.02$ for $N = 100$ and 1000, respectively. These results confirm that the phonon mixing due to the nonlinearity leads to the crossover from the case $J_+ > J_-$ to the one $J_+ < J_-$, even if the nonlinearity is very small.

A problem immediately arises from the above analysis: why is $J_-$ larger than $J_+$ when the phonon bands of A and B mix up? In the thermodynamical limit, it can be expected that the heat conduction of this two-segment chain is independent of the properties of interface and the system size and determined by the heat transport properties of A and B. In Fig.4, we plot the temperature dependence of the heat conductivity $\kappa$ for A and B, respectively. As the temperature change from 0.02 to 0.12, $\kappa_A$ decreases, and $\kappa_B$ increase. Thus, both A and B have the higher heat conductivity when A is contacted with $T_- = 0.035$ and B with $T_+ = 0.105$. When the baths are exchanged, both A and B have the lower heat
conductivity. It is very intuitive that $J_{-}$ is larger than $J_{+}$.

In summary, we find the reversal of the rectifying effect in the one-dimensional two-segment FK model via computer simulations. We distinguish two different (even contrary) effects of the nonlinearity on the heat conduction behaviors. For the weak coupling of the two segments, the phonon band shift due to the nonlinearity leads to $J_{+} > J_{-}$. In an other case, the nonlinearity causes the mixing of phonon bands and leads to $J_{+} < J_{-}$. These two types of asymmetric heat conduction can transit to each other by varying the properties of the interface and the system size.

The asymmetric heat conduction discovered by computer simulations opens new possibilities to design a thermal rectifier or thermal diode in theory\footnote{[5, 6]}. However, as shown by our numerical results, the function of such a thermal device will dramatically depend on the properties of the interface. To exactly control the interface properties is very difficult in the lab\footnote{[10]}, and this difficulty really leads to the poor reproducibility of the experimental measurement of the thermal boundary resistance. As a result, the function of the thermal devices based on the principles stated here will be unpredictable due to the unknown interface conditions, such as the weak nonlinear atom-atom interaction. Thus, this is a hard task to make a thermal rectifier or thermal diode in the lab.

YZ is indebted to Prof. Hong Zhao for very helpful discussions. We would also like to thank Dr. D. He and members of the Centre for Nonlinear Studies for useful discussions. This work was supported in part by grants from the Hong Kong Research Grants Council (RGC) and the Hong Kong Baptist University Faculty Research Grant (FRG).

[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 421, 327 (2003).
[4] Focus Issue on 50th anniversary of Fermi-Pasta-Ulam model, edited by D. K. Campbell, P. Rosenau, and G. Zaslavsky.
[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. Hu and L. Yang, Chaos 15, 015119 (2005).
[8] Baowen Li, Jinghua Lan, and Lei Wang, Phys. Rev. Lett. 95, 104302 (2005).
[9] T. Dauxois, M. Peyrard, and A.R. Bishop, Phys. Rev. E 47, 684 (1993).
[10] W.H. Press, S.A. Teukolsky, W.T. Vetterling, and B.P. Flannery, Numerical Recipes (Cambridge University Press, Cambridge, 1992).
[11] Kelly R. Patton and Michael R. Geller, Phys. Rev. B 64, 155320 (2001).
[12] Bambi Hu, D. He, Lei Yang, and Yong Zhang, preprint CNS-05-05, (2005).
[13] E.T. Swartz and R.O. Pohl, Rev. Mod. Phys. 61, 605 (1989).