Reversal of thermal rectification in one-dimensional nonlinear composite system*

Zhan Si-Qi(詹斯琦), Huang Wei-Qing(黄维清)†, and Huang Gui-Fang(黄桂芳)

Department of Applied Physics, Key Laboratory for Micro-Nano Physics and Technology of Hunan Province, Hunan University, Changsha 410082, *China*

(Received 7 March 2014; revised manuscript received 29 April 2014; published online 24 September 2014)

Using nonequilibrium molecular dynamics simulations, a comprehensive study of the asymmetric heat conduction in the composite system consisting of the Frenkel–Kontorova (FK) model and Fermi–Pasta–Ulam (FPU) model is conducted. The calculated results show that in a larger system, the rectifying direction can be reversed only by adjusting the thermal bias. Moreover, the rectification reversal depends critically on the system size and the properties of the interface. The mechanisms of the two types of asymmetric heat conduction induced by nonlinearity are discussed. Considering the novel asymmetric heat conduction in the system, it may possess possible applications to manage the thermal rectification *in situ* directionally without re-building the structure.

Keywords: thermal rectification, reversal, nonlinearity, composite system

PACS: 44.10.+i, 05.70.Ln, 63.20.Ry **DOI:** 10.1088/1674-1056/23/11/114401

1. Introduction

Recently, many investigations have been conducted to elucidate a comprehensive theory about the heat conduction in low-dimensional system.[1–8] Great efforts have been made to expound the macroscopic phenomenon of heat conduction in the sight of a microscopic dynamics mechanism by using analysis methods or nonequilibrium molecular dynamics simulations. Although many problems remain unsolved, some intriguing findings have established the foundation for the phononics,[9] such as the thermal rectification effect,[10] negative differential thermal resistance (NDTR),[11,12] and Kapitza resistance.[13] It has been demonstrated that the phonons in the form of heat can be controlled and manipulated analogous to the electrons in a heterogeneous semiconductor junction.

Particularly, the thermal rectification effect is widely utilized to build a thermal diode. Various nonlinear models have been proposed to construct a thermal diode theoretically.[10,14–24] Moreover, benefiting from the boost of nanotechnology, solid thermal diodes have been fabricated in experiments successfully by using specific materials, which paves the way for the practical applications of thermal diode and transistor.[25–28] These researches revealed that a one-dimensional thermal diode model must satisfy two essential conditions: the nonlinear (unharmonic) interaction and asymmetric structure of the system. As for the classic nonlinear system, it can be divided into two categories: one is the system with on-site potential, such as the Frenkel–Kontorova (FK) model typically; the other is the system without on-site potential, such as the Fermi–Pasta–Ulam (FPU-α/β) model and Toda model. The asymmetric structure can be realized by setting different system parameters in a unitary model, or by coupling different models which possess inherent asymmetry. For examples, the unitary thermal diode model consists of two FK segments with different system parameters,[14] and the FPU thermal diode model builds the asymmetric structure by introducing a mass gradient.[29] Coupling the FK and FPU models also forms the composite asymmetric system, in which the high-efficiency rectification can be obtained by changing the system parameters.[15] An explanation of the asymmetric heat conduction in the models given above is that the phonon bands of different segments of the chain will change from overlap to separation.

In this work, a comprehensive study of the one-dimensional composite system consisting of the FK model and the FPU model is conducted by using nonequilibrium molecular dynamics (NEMD) simulations. The calculated results show that the thermal rectifying direction in a larger system is found to be reversed when the thermal bias is greater than a certain value. The thermal rectification reversal has to rebuild the system structure in previous studies.[30,31] In the system we studied here, for the first time, the rectifying direction can be reversed only by adjusting the thermal bias. The proposed system whose thermal rectification can be managed *in situ* directionally without re-building the structure may have great potential applications in phononics.

2. Model and calculation method

The system consists of FK lattices and FPU lattices, as is illustrated in Fig. 1. The two segments are connected by a

*Project supported by the Natural Science Foundation of Hunan Province, China (Grant No. 12JJ3009), the Changsha Science and Technology Plan Projects, China, and the Science and Technology Plan Projects of Hunan Province, China (Grant No. 2013SK3148).

†Corresponding author. E-mail: wqhuang@hnu.edu.cn

© 2014 Chinese Physical Society and IOP Publishing Ltd

harmonic spring of elastic constant $k_{\rm int}$. The Hamiltonian of the whole system is

$$H = H_{\rm FK}^{\rm L} + H_{\rm FPU}^{\rm R} + \frac{1}{2}k_{\rm int}(x_{N+1} - x_N - a)^2, \tag{1}$$

where N is the number of particles of each segment. The total number of particles in the system is $2N$. Each segment of the system is described by

$$H_{\rm FK}^{\rm L} = \sum_{i=1}^{N}\left[\frac{p_i^2}{2m_i} + \frac{1}{2}k_{\rm FK}(x_i - x_{i-1} - a)^2 - \frac{V}{(2\pi)^2}\cos(2\pi x_i)\right], \tag{2}$$

$$H_{\rm FPU}^{\rm R} = \sum_{i=N+1}^{2N}\left[\frac{p_i^2}{2m_i} + \frac{1}{2}k_{\rm FPU}(x_{i+1} - x_i - a)^2 + \frac{\beta}{4}(x_{i+1} - x_i - a)^4\right], \tag{3}$$

where p_i and x_i in $H_{\rm FK}^{\rm L}$ and $H_{\rm FPU}^{\rm R}$ denote the momentum and the displacement of the i-th particle, respectively. The mass of the i-th particle is $M_i = 1$. We set $k_{\rm FK} = k_{\rm FPU} = 1$ and $a = 1$, which represent the harmonic interaction strength between particles and the lattice constant, respectively. The strength of on-site potential in the FK model is taken by $V = 5$, and the strength of unharmonic interaction in the FPU model is $\beta = 1$.

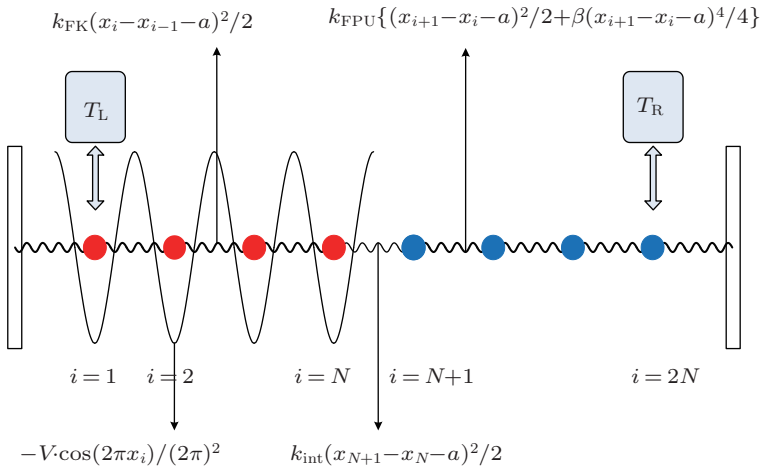


Fig. 1. (color online) Schematic picture of the system. The left and right segments are the Frenkel–Kontorova model with on-site potential and the Fermi–Pasta–Ulam model, respectively. The two segments are connected by a weak harmonic spring of elastic constant $k_{\rm int}$. The particles at the left and right ends are coupled with the heat baths of temperatures $T_{\rm L}$ and $T_{\rm R}$, respectively.

In our simulations, we use the fixed boundary conditions ($x_0 = 0, x_{2N+1} = (2N+1)a$), and the first and last particles are coupled with the NOSE-HOOVER heat baths, keeping temperatures at $T_{\rm L}$ and $T_{\rm R}$. For simplicity, we define the average temperature of the system $T_0 = (T_{\rm L} + T_{\rm R})/2$, and the thermal bias $\Delta T = T_{\rm L} - T_{\rm R} = 2T_0\Delta$. When $\Delta > 0$, the left-end particle is connected with the higher-temperature heat bath and vice versa as $\Delta < 0$. The improved Runge–Kutta algorithm is used to integrate the equations of motion of each particle, in which the local temperature and heat flux at site i defined as $T_i = m\langle\dot{x}_i^2\rangle$, $J_i = k\langle\dot{x}_i(x_i - x_{i-1} - a)\rangle$ for the FK model and $J_i = k\langle\dot{x}\{(x_i - x_{i-1} - a) + \beta(x_i - x_{i-1} - a)^3\}\rangle$ for the FPU model respectively are investigated ($\langle\ \rangle$ denoting time average). The simulations are performed long enough so that the system can reach a nonequilibrium steady state where J is a constant independent of the site of a lattice. We denote the absolute value of the heat flux from left to right as J_+, the heat flux from right to left as J_- when the heat baths are reversed. The thermal rectifier efficiency of the system is denoted by $r = J_+/J_-$.

3. Results and discussion

We first study the asymmetric heat conduction of the composite system ($N = 50$) coupling by a weak harmonic spring ($k_{\rm int} = 0.05$). Figure 2 shows the normalized temperature T/T_0 versus lattice site i for three different dimensionless temperatures with fixed $|\Delta| = 0.5$. It is obvious that, in all cases, there exists a temperature jump caused by interface thermal resistance (ITR, $R \equiv \Delta T/J$) at the interface. When $T_0 = 0.1$, owing to the asymmetric ITR in the system, the temperature gradient distributions are asymmetric as the heat baths are reversed. However, the asymmetry of heat conduction relies on the average temperature T_0. In the case of $T_0 = 0.01$, the two parts of the system are both in the low-temperature limit where the phonons cannot propagate through the system, especially the interface. On the contrary, in the case of $T_0 = 0.5$, the two parts are both in the high-temperature limit where the phonons vibrate strongly and can propagate through the system from each direction. As a result, the asymmetric heat conduction vanishes in both high- and low-temperature limits. To extend a better study on asymmetric heat conduction of the system, the average temperature is fixed at $T_0 = 0.1$ in the following

discussion (unless otherwise stated).

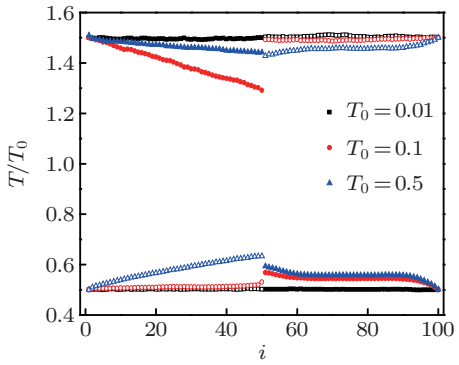


Fig. 2. (color online) T/T_0 versus lattice site i at fixed $|\Delta| = 0.5$ for $T_0 = 0.01$, 0.1, and 0.5. In all cases, $N = 50$ and $k_{\rm int} = 0.05$. The solid symbols are for the cases of $\Delta > 0$ and the empty symbols are for the cases of $\Delta < 0$ (the same below).

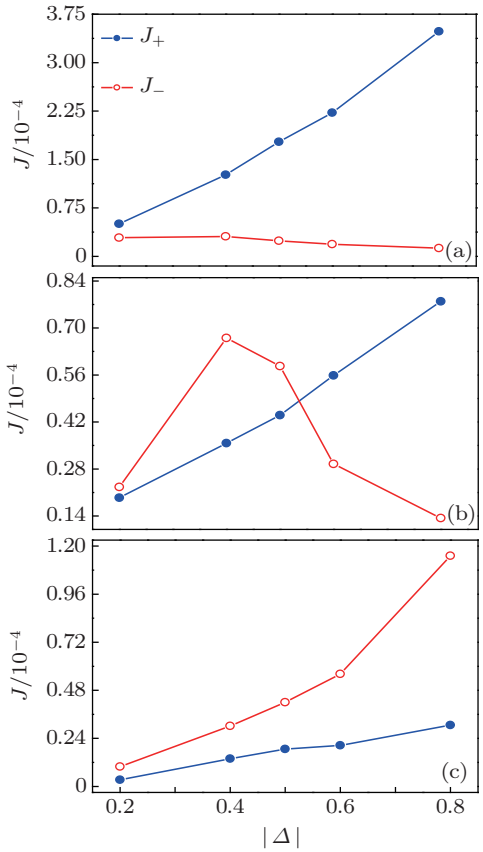


Fig. 3. (color online) The heat flux J versus $|\Delta|$ for (a) $N = 50$, (b) $N = 500$, (c) $N = 2000$. In all cases, $T_0 = 0.1$ and $k_{\rm int} = 0.05$.

The thermal bias is another critical factor for the asymmetry of heat conduction. Figure 3 shows the dependence of heat flux on thermal bias for different system sizes with fixed $k_{\rm int} = 0.05$. In Fig. 3(a) ($N = 50$), one can see that as the thermal bias increases, J_+ almost exhibits linear growth, while J_- exhibits negative growth, which is caused by the NDTR. The asymmetric heat conduction is captured by the phenomenon of $J_+ > J_-$, and the rectifier efficiency increases with the thermal bias. Moreover, the appearance of NDTR as $\Delta < 0$ further improves the asymmetric heat conduction of the system. However, as shown in Fig. 3(b), the asymmetric heat conduction is reversed in a larger system ($N = 500$). There exists a rectification reversal from $J_+ < J_-$ to $J_+ > J_-$ at $|\Delta| \approx 0.53$. To the best of our knowledge, the rectification reversal in other systems appears only when the system structure is rebuilt.[30,31] While the rectifying direction in our study, for the first time, can be reversed in site only by adjusting the thermal bias without re-building the structure. It can be seen intuitively that the NDTR leads to the rectification reversal. Moreover, the appearance region of the NDTR shifts towards greater thermal bias with the increase of N. As a result, for $N = 2000$, the rectification reversal varying simultaneously with the NDTR disappears eventually and the asymmetric heat conduction is captured by $J_+ < J_-$ (Fig. 3(c)).

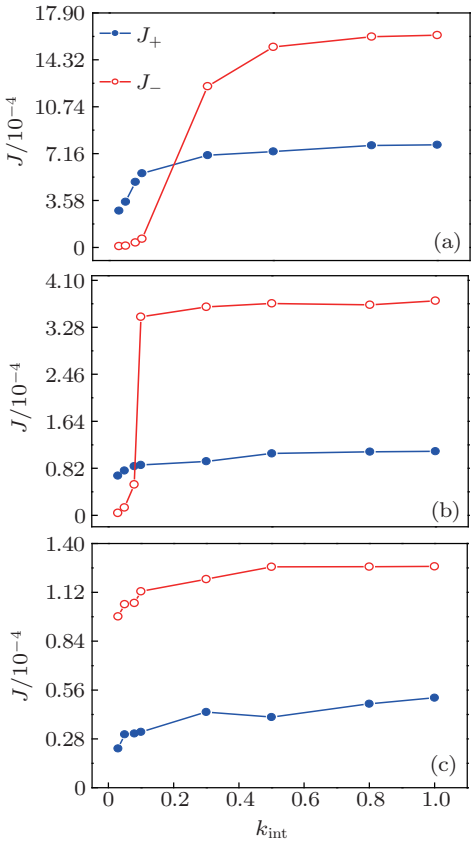


Fig. 4. (color online) Dependence of the heat flux J on $k_{\rm int}$ for (a) $N = 50$, (b) $N = 500$, (c) $N = 2000$. In all cases, $T_0 = 0.1$ and $|\Delta| = 0.8$.

To understand the rectification reversal existing in the larger system, we investigate the dependence of $J_\pm$ on $k_{\rm int}$ for different system sizes with fixed $|\Delta| = 0.8$, as shown in Fig. 4. It is clearly seen that, as $k_{\rm int}$ increases, the two segments are strongly coupled and behave as a whole in all cases. The $J_\pm$ would approach to saturation gradually and the asymmetric heat conduction is captured by the phenomenon of $J_+ < J_-$. Consequently, there exists a crossover of $J_\pm$ in Figs. 4(a) and 4(b), while the crossover disappears in a long chain (for example, $N = 2000$) with $J_+ < J_-$ (seen in Fig. 4(c)). The crossover

can be traced from the asymmetric ITR, which is regarded as a direct manifestation of thermal rectification. Here, we can see the rectification reversal directly through the unsynchronized changes of $R_\pm$ ($R_\pm$ denote the ITR when $\Delta > 0$ and $\Delta < 0$, respectively), as shown in Fig. 5. In Fig. 5(a), when the two segments are weakly coupled, $R_- \gg R_+$, resulting in $J_+ > J_-$. As $k_{\rm int}$ increases, R_- decreases sharply and R_+ exhibits a relatively flat decrease. As a result, $R_- < R_+$ gives rise to the phenomenon of $J_+ < J_-$. Similarly, the crossover of $R_\pm$ also exists in Fig. 5(b). Because of the sharp decrease of R_- and gentle growth of R_+ with the increase of N, the asymmetric heat conduction in the larger system is captured by the phenomenon of $J_+ < J_-$. Therefore, the rectification reversal in Figs. 3(b) and 3(c) can be understood as follows. The effect of the weak interfacial spring on the system decreases with the increase of N.[30] Hence, the weakly coupled two segments in the larger system behave as a whole, analogous to the case that the two segments are well coupled.

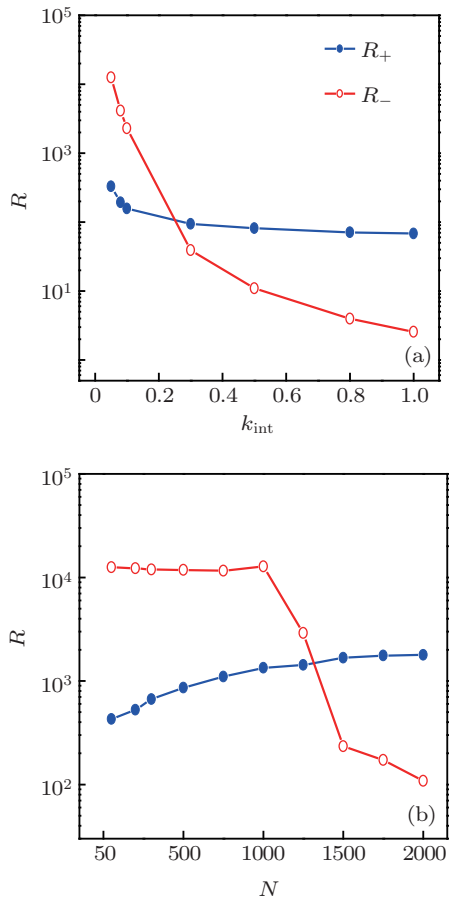


Fig. 5. (color online) Dependence of the ITR on $k_{\rm int}$ and N for (a) $N = 50$, (b) $k_{\rm int} = 0.05$. In all cases, $T_0 = 0.1$ and $|\Delta| = 0.8$.

It is thus clear that the system presents two types of asymmetric heat conduction as the system size and coupling strength of inter-models are changed: one is $J_+ > J_-$ when the two segments are weakly coupled; the other is $J_+ < J_-$ when the two segments are strongly coupled or the chain is long enough. To understand the underlying mechanisms of them, we first need to invoke the temperature-dependence of phonon frequencies of the homogeneous FK and FPU segments. As discussed in Ref. [15], in the high-temperature limit, the FK system whose on-site potential can be neglected is close to a harmonic chain with the frequency spectra

$$0 < \omega/2\pi < \frac{1}{2\pi}\left(2\sqrt{\frac{k_{\rm FK}}{M_i}}\right),$$

which gives $0 < \omega/2\pi < 0.318$ for the parameters used in our system. However, as for the FPU system, the anharmonic term is dominant and a rough theoretical estimate of frequency spectra is given by

$$0 < \omega/2\pi < \frac{C_0}{2\pi}\left(Tk_{\rm FPU}\beta\right)^{1/4},$$

with

$$C_0 = 2\sqrt{2\pi}\Gamma(3/4)\,3^{1/4}/\Gamma(1/4) \approx 2.23,$$

where Γ is the Gamma function. In the low-temperature limit, the FK particles are confined in the valley of on-site potential. By linearizing the equations of motion, the frequency spectra are obtained with

$$\frac{1}{2\pi}\sqrt{\frac{V}{M_i}} < \omega/2\pi < \frac{1}{2\pi}\left(\sqrt{\frac{V+4k_{\rm FK}}{M_i}}\right),$$

which gives $0.355 < \omega/2\pi < 0.477$. While the FPU system becomes a harmonic one with the frequency spectra

$$0 < \omega/2\pi < \frac{1}{2\pi}\left(2\sqrt{\frac{k_{\rm FPU}}{M_i}}\right),$$

which gives $0 < \omega/2\pi < 0.318$. In case that the FK and FPU models are weakly coupled (except for the larger system), as the thermal bias increases, the two segments get into opposite temperature limits independently without a temperature gradient (seen in Fig. 2). Therefore, the frequency spectra of each model present a big overlap in a large range of frequencies as the heat flux flows from the FK model to the FPU model, implying great heat flow in the system. On the contrary, the frequency spectra of each model present complete separation once the heat baths are reversed, implying scarcely any heat flow in the system. The match/mismatch of frequency spectra well explains the phenomenon of $J_+ > J_-$. However, when the two segments are strongly coupled, the two segments become mixed and form a whole. The differences between the temperature-dependence of homogeneous FK and FPU segments are needed. As shown in Fig. 6, in the same heat bath, the heat flux in the FPU model shows absolute advantage compared with the one in the FK model. This is due to the greater total thermal resistance decided by the essential attributes of the FK model itself. The phonons in homogeneous FPU can propagate through the system with less scattering. Therefore, in the case that the two segments are well coupled or the chain is long enough, as the system reaches a nonequilibrium steady state, the temperature gradient in the FK model

can be built more easily. As shown in Fig. 7, the FK model can achieve both low- and high-temperature limits, occupying high- and low-frequency phonons simultaneously no matter when $\Delta > 0$ or $\Delta < 0$. The FPU model without an obvious temperature gradient is merely in the low- or high-temperature limit. According to the frequency spectra analyzed above, only the low-frequency phonons in the FK model can propagate to the FPU model and the high-frequency phonons will be scattered by the interface; all the low-frequency phonons in the FPU model can propagate through the interface to the FK model without any scattering. The mixing of frequency spectra decided by the different temperature-dependence of the two segments results in the phenomenon of $J_+ < J_-$. We can conclude that both the match/mismatch and the mixing of frequency spectra induce thermal rectification effects, however, with opposite directions, the competition between them contributes to the rectification reversal essentially.

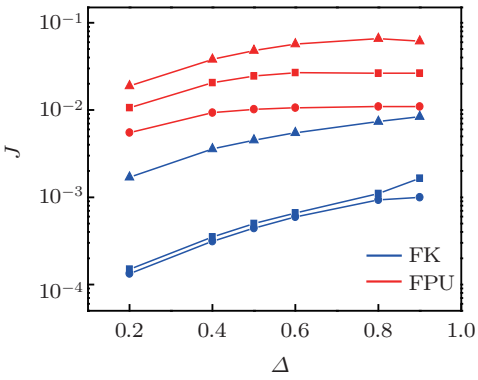


Fig. 6. (color online) Temperature dependence of the heat flux in homogeneous FK and FPU segments for $T_0 = 0.03$ (circles), $T_0 = 0.1$ (squares), and $T_0 = 0.3$ (triangles).

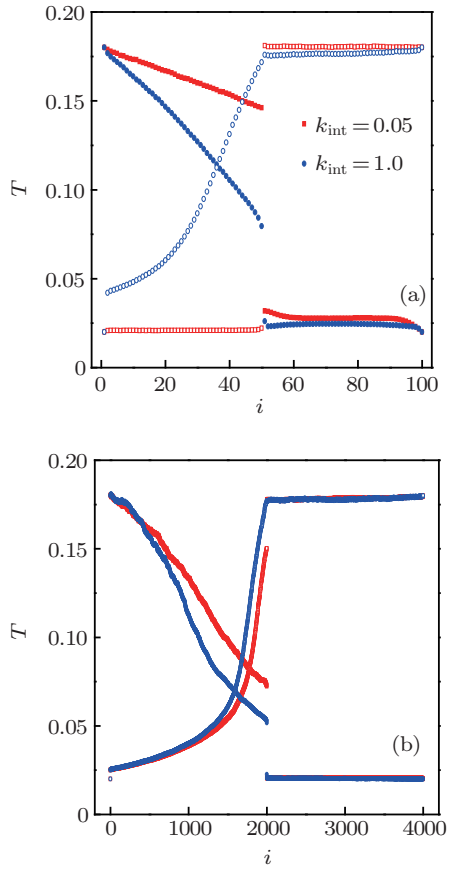


Fig. 7. (color online) The T versus lattice site i with different $k_{\rm int}$ for (a) $N = 50$, (b) $N = 2000$. In all cases, $T_0 = 0.1$ and $|\Delta| = 0.8$.

It is worth noting that the thermal rectifier efficiency of the fixed system ($N = 500$) denoted by ratio $r = |J_+/J_-|$ changes from $r \to 0.5$ to $r \to 6$ as the rectifying direction is reversed, congruous with the results observed in experiments.[25–28] It strongly suggests that our results may have practical applications in managing the thermal rectification *in situ* directionally without re-building the structure. Moreover, the system can be a good candidate to construct a thermal transistor or logic gate due to the existence of NDTR.

4. Summary

We have systematically studied the asymmetric heat conduction in a one-dimensional nonlinear composite system. The thermal rectifying direction in a larger system is found to be reversed from $J_+ < J_-$ to $J_+ > J_-$ when the thermal bias is greater than a certain value. The thermal rectification reversal ascribed to the competition between the two different types of asymmetric heat conduction depends critically on the system size and the properties of the interface. Generally, the thermal rectification reversal has to rebuild the system structure. In the system we studied here, however, the rectification effect can be reversed only by adjusting the thermal bias. Our results suggest that the systems have practical applications in managing thermal rectification *in situ* directionally without rebuilding the structure.

References

[1] Lepri S, Livi R and Politi A 1997 *Phys. Rev. Lett.* **78** 1896
[2] Hu B, Li B and Zhao H 1998 *Phys. Rev. E* **57** 2992
[3] Lepri S, Livi R and Politi A 2003 *Phys. Rep.* **377** 1
[4] Livi R and Lepri S 2003 *Nature* **421** 327
[5] Prosen T and Campbell D K 2005 *Chaos* **15** 015117
[6] Gaul C and Buettner H 2007 *Phys. Rev. E* **76** 011111
[7] Zhong Y, Zhang Y, Wang J and Zhao H 2013 *Chin. Phys. B* **22** 070505
[8] Li H B and Li Z 2010 *Chin. Phys. B* **19** 054401
[9] Li N B, Ren J, Wang L, Zhang G, Hänggi P and Li B W 2012 *Rev. Mod. Phys.* **84** 1045
[10] Terraneo M, Peyrard M and Casati G 2002 *Phys. Rev. Lett.* **88** 094302
[11] Li B W, Wang L and Casati G 2006 *Appl. Phys. Lett.* **88** 143501
[12] Wang L and Li B W 2007 *Phys. Rev. Lett.* **99** 177208
[13] Kapitza P L 1941 *J. Phys.* **4** 181
[14] Li B W, Wang L and Casati G 2004 *Phys. Rev. Lett.* **93** 184301
[15] Li B W, Lan J H and Wang L 2005 *Phys. Rev. Lett.* **95** 104302
[16] Zhang L F, Yan Y H, Wu C Q, Wang J S and Li B W 2009 *Phys. Rev. B* **80** 172301
[17] Wu L A and Segal D 2009 *Phys. Rev. Lett.* **102** 095503
[18] Zhang L, Wang J S and Li B 2010 *Phys. Rev. B* **81** 100301
[19] Yang N, Zhang G and Li B W 2009 *Appl. Phys. Lett.* **95** 033107
[20] Yang N, Zhang G and Li B W 2008 *Appl. Phys. Lett.* **93** 243111
[21] Wu G and Li B W 2007 *Phys. Rev. B* **76** 085424

[22] Xu H, Cui M L and Ma S S 2010 *Acta Phys. Sin.* **59** 7266 (in Chinese)
[23] Zhang M P, Zhong W R and Ai B Q 2011 *Acta Phys. Sin.* **60** 060511 (in Chinese)
[24] Zhang M P, Zhong W R and Ai B Q 2011 *Chin. Phys. B* **20** 100508
[25] Chang C W, Okawa D, Majumdar A and Zettl A 2006 *Science* **314** 1121
[26] Kobayashi W, Teraoka Y and Terasaki I 2009 *Appl. Phys. Lett.* **95** 171905
[27] Sawaki D, Kobayashi W and Moritomo Y 2011 *Appl. Phys. Lett.* **98** 081915
[28] Tian H, Xie D, Yang Y, Ren T L, Zhang G, Wang Y F, Zhou C J, Peng P G, Wang L G and Liu L T 2012 *Sci. Rep.* **2** 523
[29] Yang N, Li N B, Wang L and Li B W 2007 *Phys. Rev. B* **76** 020301
[30] Hu B, Yang L and Zhang Y 2006 *Phys. Rev. Lett.* **97** 124302
[31] Wang J, Li J Y and Zheng Z G 2010 *Acta Phys. Sin.* **59** 476 (in Chinese)