Heat conduction and reversed thermal diode: The interface effect

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The important role of interface collisions on the thermal-diode effect, of the two-segment lattices is studied. In the high-average temperature region, it is found that the thermal-diode effect may be significantly weaken and even annihilated. In the low-temperature region, where the thermal diode is inhibited in the collisionless case, an interesting reversed thermal diode is achieved. These behaviors are interpreted in terms of phonon-band mixing induced by interface collisions. The regime where a reversed thermal diode can be observed by resorting to the dependence of the heat current on the average temperature, and a critical temperature exists. The results proposed in this paper reveal that thermal-diode effect can be qualitatively influenced if the interface collisions could not be neglected.

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I. INTRODUCTION

Heat conduction is a rather old yet unsolved problem. In the past decades, much effort has been focused on the first-principles derivation of Fourier's law from statistical mechanics and the validity of this law in low-dimensional systems [1–8]. Compared to these fundamental explorations, the possibility in controlling heat conduction, such as the design of a thermal diode, attracted increasing attention due to its important potential-energy-saving applications in recent years [9–16]. An encouraging progress is that a nanoscale solid-state thermal rectifier has recently been demonstrated experimentally [13]. Furthermore, the models of thermal transistor and even thermal logic gates, which provide the possibility to design a "phononic computer," have been proposed [14,15]. All of these amazing progresses are based on the model of thermal diode. A typical thermal diode [10] consists of two segments of Frenkel-Kontorova (FK) lattices with different parameters. It allows heat flow in one direction but inhibits the flow in the opposite direction. However, there are several problems to be solved about this model and a more in-depth understanding of the asymmetric heat conduction is needed.

The explanation of the asymmetric heat conduction lies on the temperature dependence of the phonon bands. For appropriate parameters, the phonon bands of the two segments may change from overlapping to separation when the positions of the two heat baths are reversed. As a result, the thermal-diode system may change from a good thermal conductor to a good thermal insulator. It is trivial to get an asymmetric thermal conduction in an asymmetric structure. The main attraction is the significant rectification efficiency (about 100 times), which is crucial in achieving a high stability of the thermal-diode effect. Depending on the previous works [10–12], a weak interface link k_{int} is an important and necessary condition of a high rectification efficiency. However, one problem naturally arises for very low k_{int}; i.e., the particles at the interface may swarm up the substrate barrier and collide with each other because the repulsive force between them can be neglected when they are close to each other.

Much progress have been achieved on the heat conduction in the presence of the hard-core collisions, such as the one-dimensional hard-particle gas model and gas channels [1,7]. It is significant to explore the influence of the interface collisions on the thermal-diode effect. Our simulations show that the collisions between neighboring particles can be frequently observed. Interfacial collisions may change the heat transfer behaviors of the thermal-diode system drastically. In this paper, we find that the thermal-diode effect disappears at high temperature while a reversed thermal-diode effect can be observed at low temperature if we take into account the hard-core collisions in our simulations experiment.

The rest of the paper is organized as follows. In Sec. II, we describe the thermal-diode model. In Sec. III, we demonstrate and discuss the annihilation of the thermal-diode effect at high system temperature. Section IV is devoted to the reversed thermal-diode effect. In Sec. V, we show the dependence of thermal rectification effect on the system temperature and size. Finally, we conclude the paper by conclusions and discussions in Sec. VI.

II. THERMAL-DIODE MODEL

Let us consider two segments of FK lattices connected by a harmonic link k_{int}. The Hamiltonian of the whole system is given by [10,11]

$$H = H_L + H_R + \frac{1}{2}k_{int}(x_{N/2+1} - x_{N/2} - a)^2, \tag{1}$$

where

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$$H_{L/R} = \sum_i \left[\frac{p_i^2}{2m} + \frac{1}{2}k_{L/R}(x_{i+1} - x_i - a)^2 - \frac{V_{L/R}}{(2\pi)^2}\cos 2\pi x_i \right] \tag{2}$$

denotes the Hamiltonian of the left/right segment. m, a, V, and N represent the mass, the lattice constant, the strength of the external potential, and the system size, respectively. We set the parameters as $m=1$, $a=1$, $V_L=5.0$, $V_R=1.0$, $k_L=1.0$, and $k_R=0.2$. Fixed boundary conditions are adopted. The two ends of the chain ($i=1$, $i=N$) are connected with two Nose-Hoover heat baths at temperature $T_L=T_0(1+\Delta)$ and $T_R=T_0(1-\Delta)$, where T_0 denotes the average temperature of the system and Δ is the dimensionless temperature difference.

The local temperature of the lattice system is defined as the average value of the kinetic energy $T_i=m\langle\dot{x}_i^2\rangle$, where $\langle\cdot\rangle$ stands for temporal average. Taking into account the nonlocality of the particles, we adopt the following definition of the local heat flux proposed in Ref. [1],

$$j_i = \frac{1}{2}(x_{i+1} - x_i)(\dot{x}_{i+1} + \dot{x}_i)F(x_{i+1} - x_i) + \dot{x}_i h_i, \tag{3}$$

where

$$h_i = \frac{p_i^2}{2m} - \frac{V_{L/R}}{(2\pi)^2}\cos 2\pi x_i + \frac{1}{2}[U(x_{i+1} - x_i) + U(x_i - x_{i-1})] \tag{4}$$

denotes the local energy density at the ith particle,

$$U(x_{i+1} - x_i) = \frac{1}{2}k_{L/R}(x_{i+1} - x_i - a)^2 \tag{5}$$

represents the interaction potential, and

$$F(x_{i+1} - x_i) = - U'(x_{i+1} - x_i). \tag{6}$$

is the force acting on the $(i+1)$th particle by the ith particle.

III. ANNIHILATION OF THE THERMAL RECTIFICATION EFFECT

We denote the two interface particles [the $(N/2)$th and the $(N/2+1)$th particle]) by A and B, respectively. In order to obtain a high rectification efficiency, the interaction between A and B must be very weak ($k_{int}=0.05$ in Ref. [10].). As we have mentioned above, for such low k_{int}, the repulsive force between A and B is so weak that they may collide with each other. If such collisions have not be taken into account in simulation experiment, the particles will pass through each other, as shown in Fig. 1(a). It is not a reasonable physical picture.

In this paper, we take into account the collisions between particles in the typical two-segment thermal-diode model. In order to simplify the model, the particle size is neglected and the collisions between particles are considered to be elastic, as shown in Fig. 1(b). The collisions between the right-segment particles ($i>N/2+1$) can also be observed, but not so frequently as the situation of the collisions between A and B because the right interaction ($k_R=0.2$) is strong than k_{int}.

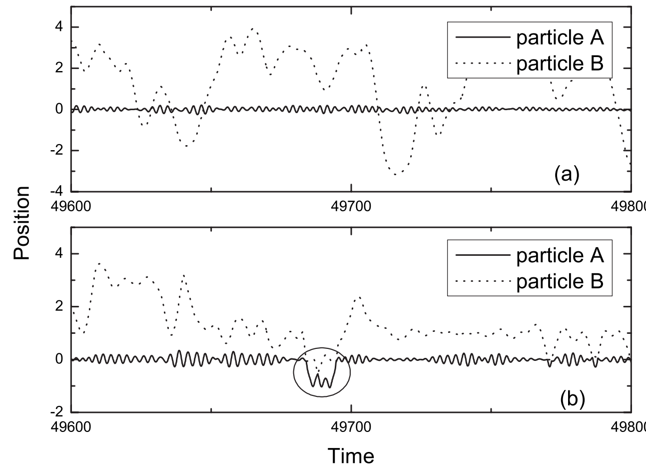

FIG. 1. The evolution of the positions of interface particles A and B for (a) the collisionless case, and (b) in the presence of elastic collisions. The equilibrium positions of particles A and B are set as 0 and 1, respectively. Here, $N=100$, $k_{int}=0.05$, $T_0=0.07$, and $\Delta=-0.5$.

As for the left-segment particles ($i<N/2$), we can hardly observe the collisions between them due to the strong left interaction ($k_L=1.0$).

The collisions drastically change the qualitative behavior of heat conduction. Figure 2 gives the heat current J versus Δ for different system temperature T_0. In Fig. 2(a), the $J-\Delta$ relation given by solid squares shows a typical thermal-diode effect in the collisionless case: the current in the region of $\Delta<0$ (J_-) is much smaller than the current in the region of $\Delta>0$ (J_+) [see the enlarged plot (c)]. We are concerned with the influence of hard-core interactions on the heat flux, which is shown by the empty-square line in Fig. 2(a). We find that there is no great difference between the value of $|J_-|$

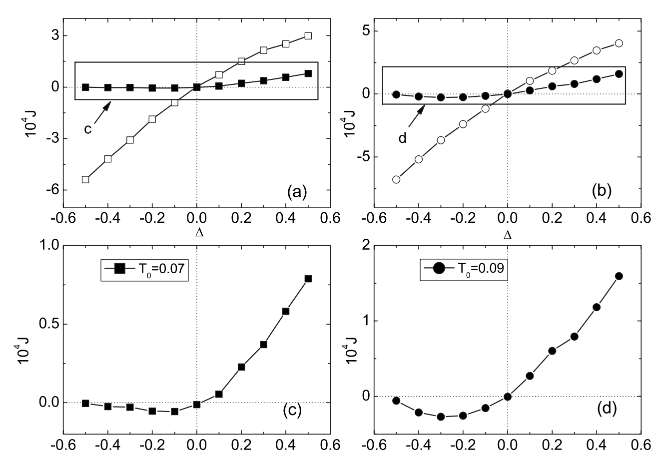

FIG. 2. The heat flow J versus Δ for different values of T_0: Squares in (a) denote the results for $T_0=0.07$, and circles in (b) for $T_0=0.09$. Solid symbols give the result following Ref. [10], while the empty ones denote the results by taking into account the collisions. For the sake of clarity, the solid squares and circles in Figs. 1(a) and 1(b) are enlarged in (c) and (d), respectively. Here the parameters are $N=100$ and $k_{int}=0.05$. The lines are drawn to guide eyes.

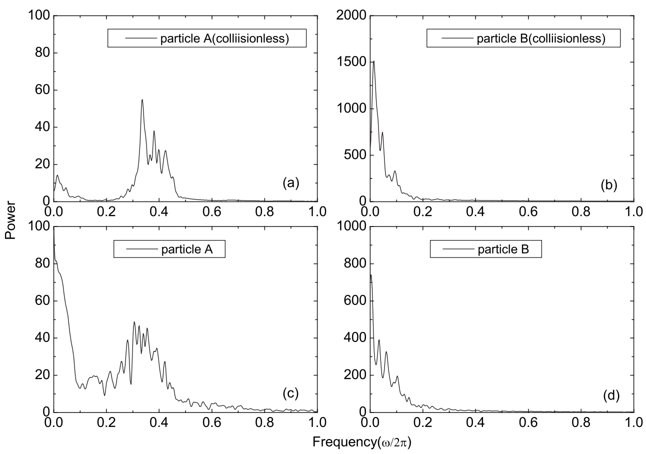

FIG. 3. (a) and (b) show the single-particle spectrum of interface particles A and B for the collisionless case in Fig. 1(a). While (c) and (d) give the phonon bands of particles A and B for the case in Fig. 1(b).

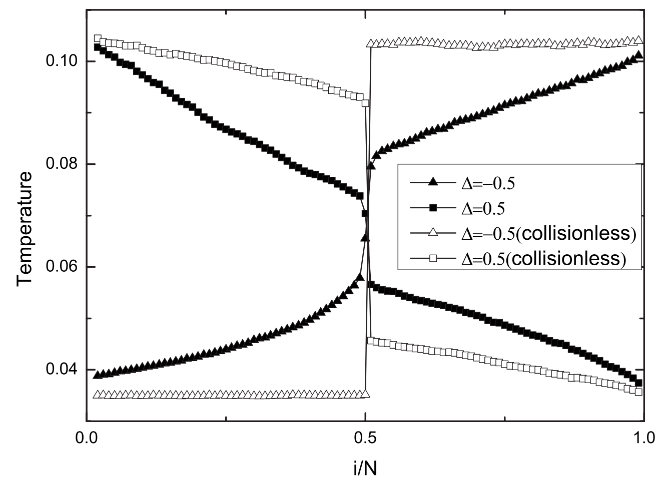

FIG. 4. Temperature profile for $T_0=0.07$. Solid symbols show the results in the presence of collisions, while empty symbols give the results for collisionless case. Here, $N=100$ and $k_{int}=0.05$.

and J_+ in the presence of elastic collisions. Instead, they are in the same order of magnitude ($|J_-/J_+|\sim 2$). So the rectification effect of heat current obviously disappears if we take into account the collisions.

The result for the case of $T_0=0.09$ is similar to $T_0=0.07$, as shown in Figs. 2(b) and 2(d) by circles. We have checked that the annihilation of the rectification effect can also be observed if we use Langevin heat baths. This emphasizes the significant role of hard-core collisions, and it may even lead to the disappearance of the thermal-diode effect.

It is important to explore the mechanism of the annihilation of thermal-diode effect based on the temperature dependence of the phonon frequency, which originates from the presence of nonlinearity. In the absence of collisions, the equation of motion for the left/right-segment particles can be linearized as [9,10]

$$m\ddot{q}_n = k_{L/R}(q_{n+1} - 2q_n + q_{n-1}) - Vq_n, \tag{7}$$

where $q_n=x_n-na$ denotes the stretching from the equilibrium position of the n-th particle. Equation (7) has plane-wave solutions, $q_{nK}(t)=e^{i(Kn-\omega t)}$, where the frequency ω and momentum K satisfy the dispersion relation

$$\omega_{L/R}^2 = V + 2k_{L/R} - 2k_{L/R}\cos K. \tag{8}$$

At low temperature, the particles is confined in the valley of the on-site potential. One can easily obtain the so-called phonon bands, $\sqrt{V}<\omega<\sqrt{V+4k}$, which is allowed by dispersion relation (8). While at high temperature, the on-site potential can be neglected and the phonon band is given by $0<\omega<\sqrt{4k}$. When $\Delta=-0.5$, the left/right segments are at the low/high-temperature side, respectively. Therefore, we have $0.36<\omega_L/2\pi<0.48$ and $0<\omega_R/2\pi<0.14$, which are separated with each other, as shown in Figs. 3(a) and 3(b). Note that there is a tiny low-frequency part in Fig. 3(a). It is induced by the interface link k_{int} and we will interpret it in the following text. If we set $\Delta=0.5$, the two heat baths are reversed and the phonon bands of the two segments will change from separation to overlapping ($0<\omega_L/2\pi<0.32$ and $0.16<\omega_R/2\pi<0.21$). Thereby, the system acts as a good thermal diode in the absence of collisions.

The dynamical behavior of the interface particles are drastically changed in the presence of the hard-core collisions, as shown in Fig. 1. The phonon bands of the interface particle will be quite different from the collisionless case. Figures 3(c) and 3(d) show the phonon bands of A and B corresponding to Fig. 1(b). It can be found that a part of low-frequency component emerges in the phonon spectrum of particle A, which overlaps with the phonon band of particle B. This phonon-band mixing consequently results in a energy flow through the interface. As a consequence, the system does not act like a thermal insulator anymore but a good thermal conductor when $\Delta<0$.

Figure 4 shows the temperature profile along the lattice for $T_0=0.07$. Compared to the collisionless case, there exits much less difference in the temperature profile between the case of $\Delta=-0.5$ and $\Delta=0.5$, which indicates the annihilation of the thermal-diode effect.

In the thermal-diode model, the match/mismatch of the phonon bands of the interface particles sensitively controls the total heat flux. The phonon band is the result of the collective dynamical behavior of all the particles along the lattice. The bands of the intrasegment particles are certainly overlapping with each other. However, in the thermal-diode model, we should consider the left- and right-segment phonon bands to be almost independent due to the weak interface link. The match/mismatch of the phonon band between the left and right segments depends on the system temperature and other parameters.

We propose that there are two dominating factors which can be responsible for the phonon-band mixing between the two segments. One is the interface harmonic interaction k_{int}. The tiny low-frequency part in Fig. 3(a), which is mentioned above, is the result of the phonon-band mixing induced by k_{int}. But it is too weak to contribute a sufficient heat flow. The higher the value of k_{int}, the better the phonon-band mixing. For sufficiently large k_{int}, the thermal-diode model should be treated as a whole system, not two parts any more.

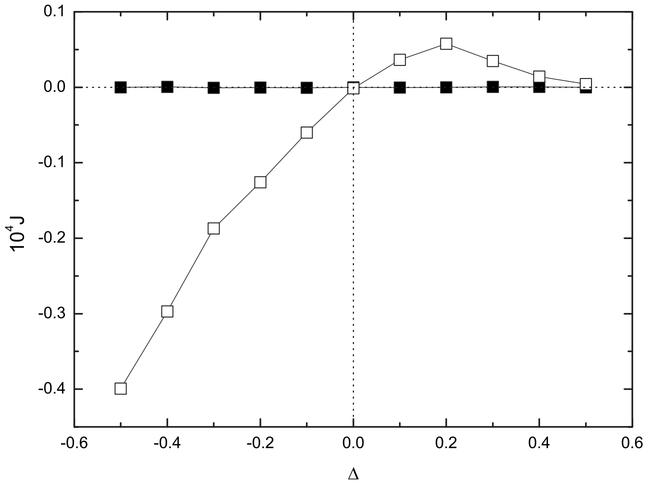

FIG. 5. The heat flow J versus Δ for T_0=0.02. Solid squares give the result in the collisionless case, while the empty ones denote the results in the presence of the collisions. N=100 and k_{int}=0.05. The lines are drawn to guide eyes.

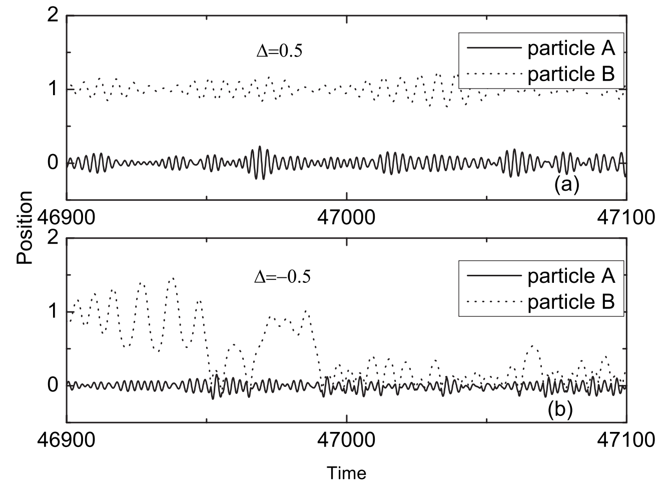

FIG. 6. The evolution the positions of interface particles A and B for the case of (a): Δ=0.5 and (b): Δ=−0.5, where the hard-core collisions are taken into account. N=100, k_{int}=0.05 and T_0=0.02.

The other dominating factor is the hard-core collisions, especially the interface collisions between A and B. Here, the interface collision play a more important role because it represents not only the interaction between interface particles A and B, but also between the two segments of the system. We may regard the hard-core collision as a simplification of high-order interactions between particles in that the high-order interaction will be significant when two particles are close with each other. So the collisions can also contribute to the phonon-band mixing inside the thermal-diode system.

In this paper, the hard-core collisions should be responsible for the phonon-band mixing between the interface particles. When $k_{int} \to 0$ (k_{int}=0.05), the mixing of phonon bands induced by the interface link between A and B can be neglected, so the hard-core collisions may induce the emergence of the low-frequency component in the phonon band of particle A. The collisions marked by a circle in Fig. 1(b) gives the evidence for this conclusion. Particle B collides with A, then particle A obtains a large kinetic energy from B and has to move far away from its original amplitude, which leads to the emergency of the low-frequency component in the phonon band of particle A.

IV. REVERSED THERMAL DIODE

The above studies focus on the cases of higher average temperatures T_0 (T_0=0.07). As we will see below, it is drastically different if T_0 is low. In Fig. 5, we plot the heat flow J versus Δ when T_0=0.02. In the absence of hard-core collisions, $J_- \approx J_+ \approx 0$ because the phonon bands of the interface particles are separated no matter $\Delta > 0$ or $\Delta < 0$. If hard-core collision effect is taken into account, a story happens, $|J_-| \gg |J_+|$, as shown by empty squares in Fig. 5. Further more, there is a region of negative differential thermal resistance when $0.2 < \Delta < 0.5$. In other words, one may recover the thermal-diode effect, which does not exist in the collisionless case! Moreover, it can be very interesting to find that this is a "reversed" thermal diode (RTD) type as compared with the diode shown in Figs. 2(c) and 2(d), i.e., when $\Delta < 0$ it acts as a thermal conductor but it inhibits the heat flow if $\Delta > 0$.

The underlying mechanism of this RTD is quite different from the one in Ref. [10]. A heuristic understanding is provided based on the presence/absence of the collisions. If $\Delta > 0$, $V_L > V_R$ and $T_L > T_R$. The left/right potential is high enough to localize the left/right particles with higher/lower kinetic energy [see Fig. 6(a)], so the phonon-band mixing cannot be achieved in the way of collisions when T_0=0.02 and $\Delta > 0$. On the other hand, k_{int} is so weak that phonon bands cannot be mixed in the way of interface harmonic interaction (Fig. 7). This leads to a nearly vanishing heat current. In the case of $\Delta < 0$, $V_L > V_R$, but $T_L > T_R$. The left particles can still be localized in the left wells, but the lower right barriers cannot localize the high energy right particles any more. B can easily overcome the barrier, then collide with other particles [see Fig. 6(b)]. The presence of the col-

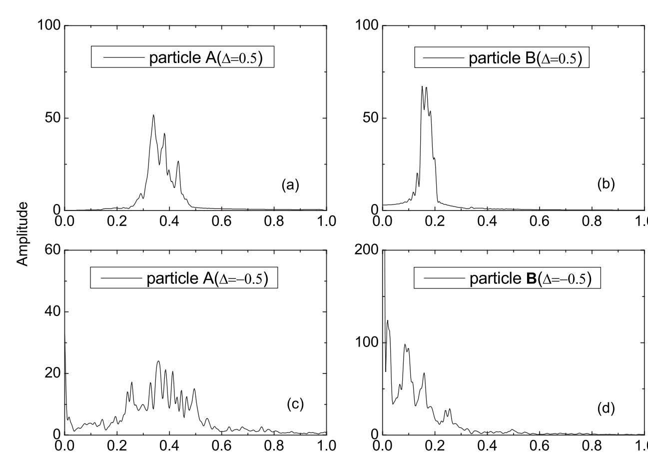

FIG. 7. The single-particle spectrum of interface particles A and B corresponding to Fig. 6(a) (Δ=0.5) are shown in (a) and (b). The phonon bands of A and B when Δ=−0.5 are given in (c) and (d). N=100, k_{int}=0.05 and T_0=0.02.

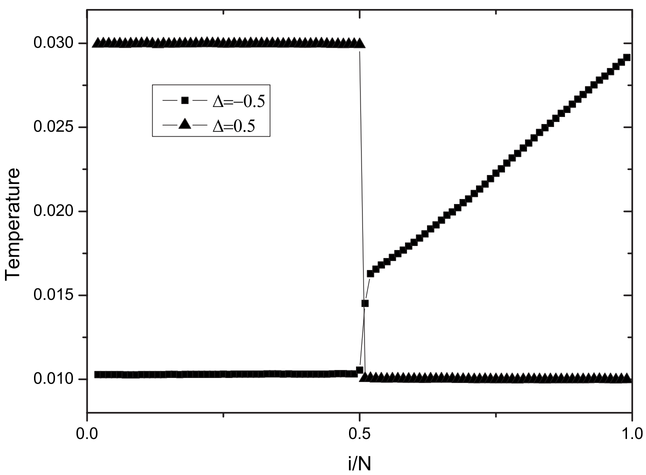

FIG. 8. Temperature profile for T_0=0.02 in the presence of collisions. Here, N=100 and k_{int}=0.05

lisions leads to the mixing of phonon bands. As a result, the system becomes a thermal conductor for $\Delta < 0$.

Figure 8 shows the temperature profile along the lattice size when T_0=0.02. If Δ=0.5, there exit a large temperature jump at the interface and the temperature gradient is very small inside the segment. As a result, the heat current is almost vanishing. While in the case of Δ=−0.5, the temperature gradient in the right segment is more larger than the left segment, which confirm the different dynamical behaviors between A and B shown in 6(b).

V. DEPENDENCE OF THERMAL RECTIFICATION EFFECT ON THE SYSTEM TEMPERATURE AND SIZE

The RTD effect is the result of the competition between thermal fluctuation and particle localization. When the system temperature T_0 is increasing, the RTD will disappear. Figure 9 shows the heat current $J_+(\Delta=0.5)$ and $J_-(\Delta=-0.5)$ against T_0 by squares and circles. It can be found that $|J_-|$ increases with T_0 because of the increasing frequency of

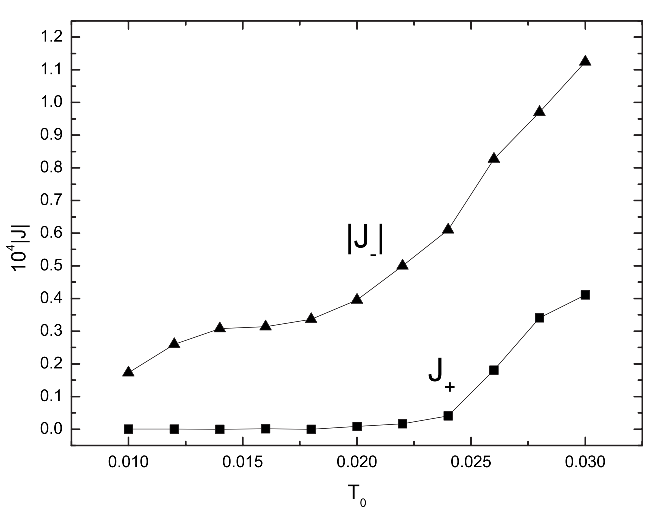

FIG. 9. The heat flow J_+ (denoted by squares) and the flow $|J_-|$ (denoted by triangles) versus the system temperature T_0.

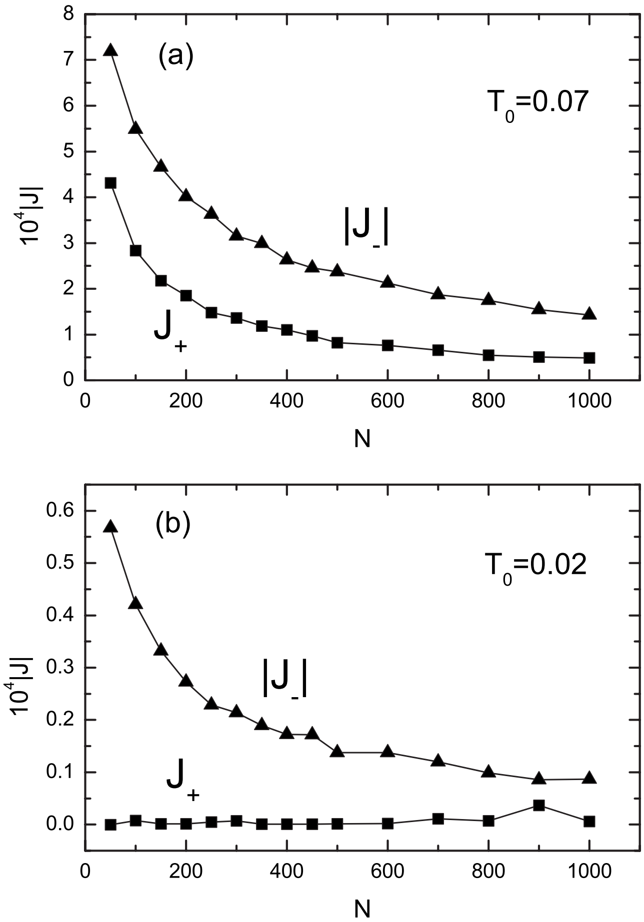

FIG. 10. The heat flow J_+ (denoted by squares) and the flow $|J_-|$ (denoted by circles) versus the system size N for (a) T_0=0.07 and (b) T_0=0.02.

thermal-fluctuation-activated collisions. For J_+, there is a critical point at $T_{cr} \approx 0.024$, where J_+ keeps almost zero when $T_0 < T_{cr}$. When $T_0 > T_{cr}$, particles in the right segment may get enough kinetic energy from the heat bath. Then they may overcome the substrate barrier and collide with the left-segment particles. This leads to a drastic increase of J_+. Although $|J_-| > J_+$, the ratio $|J_+/J_-|$ is not significant, while the thermal-diode effect is weaken and even disappears in the high-temperature regime.

Figure 10 shows the dependence of J_+ (Δ=0.5) and J_- (Δ=−0.5) on the system size N for different temperatures. For typical high temperature, T_0=0.07, both J_+ and J_- decreases with increasing N due to the decreasing temperature gradient. When T_0=0.02, J_+ keeps in a very low level and the system keeps in a thermal insulator state for $\Delta > 0$. J_- decreases with increasing N, which indicates that the rectification efficience decreases if we increase the system size.

VI. DISCUSSION AND CONCLUSIONS

In conclusion, we explore the important role of interfacial collisions on thermal conduction, especially on thermal rectification effect in the two-segment lattices in this paper. It is revealed that the heat transfer behavior can be drastically influenced by the collisions between the interfacial particles. In the high-average temperature regime, the thermal-diode effect may be significantly weaken and even annihilated; While at low temperature, where the thermal diode is inhibited in the collisionless case, an interesting reversed thermal diode is achieved. These behaviors are interpreted in terms of phonon-band mixing induced by interfacial collisions. At high temperatures, the mixing of phonon bands takes place no matter $\Delta > 0$ or $\Delta < 0$, so the thermal-diode effect disappears. At low average temperatures, we can get a reversed thermal diode because the phonon-band mixing induced by collisions appears only in the case of $\Delta < 0$ but it is invalid when $\Delta > 0$. The regime where a reversed thermal diode can be observed by resorting to the dependence of the heat current on T_0, and a critical temperature $T_0 = T_{cr}$ exists.

An appropriate interface is important for designing thermal devices, especially for implementing thermal rectifiers and thermal logic gates. The results proposed in this paper reveal that thermal-diode effect can be qualitatively changed when the interface collision effect could not be neglected. Interface collision is a simplification of high-order interactions at the interface for composites with multiple segments. In the higher-dimensional cases, collisions at the interface should also be very important and even prevail in the thermal rectification processes.

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