Double negative differential thermal resistance induced by nonlinear on-site potentials

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We study heat conduction through one-dimensional homogeneous lattices in the presence of the nonlinear on-site potentials containing the bounded and unbounded parts, and the harmonic interaction potential. We observe the occurrence of double negative differential thermal resistance (NDTR); namely, there exist two regions of temperature difference, where the heat flux decreases as the applied temperature difference increases. The nonlinearity of the bounded part contributes to NDTR at low temperatures and NDTR at high temperatures is induced by the nonlinearity of the unbounded part. The nonlinearity of the on-site potentials is necessary to obtain NDTR for the harmonic interaction homogeneous lattices. However, for the anharmonic homogeneous lattices, NDTR even occurs in the absence of the on-site potentials, for example, the rotator model.

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Heat conduction in low-dimensional systems has become the subject of a large number of theoretical and experimental studies in recent years [1]. The theoretical interest in this field lies in the rapid progress in probing and manipulating thermal properties of nanoscale systems, which presents the possibility of designing thermal devices with optimized performance at the atomic scale. As we all know, devices that control the transport of electrons, such as the electrical diode and transistor, have been extensively studied and have led to widespread applications in modern electronics. However, it is far less studied for their thermal counterparts as to control the transport of phonons (heat flux), possibly because controlling phonons is more difficult than controlling electrons. Recently, it has been revealed by theoretical studies in model systems, such as electrons and photons, that phonons can also perform interesting functions [2], which sheds light on the possible designs of thermal devices. For example, heat conduction in asymmetric nonlinear lattices demonstrates rectification phenomenon; namely, the heat flux can flow preferably in a certain direction [3–10]. Remarkably, a thermal rectifier has been experimentally realized by using gradual mass-loaded carbon and boron nitride nanotubes [11]. The nonlinear systems with structural asymmetry can exhibit thermal rectification, which has triggered model designs of various types of thermal devices such as thermal transistors [8], thermal logic gates [12], and thermal memory [13]. It is worth pointing out that most of these studies are relevant to heat conduction in the nonlinear response regime, where the counterintuitive phenomenon of double negative differential thermal resistance (NDTR) may be observed and plays an important role in the operation of those devices.

NDTR refers to the phenomenon where the resulting heat flux decreases as the applied temperature difference (or gradient) increases. It can be seen that a comprehensive understanding of the phenomenon of NDTR, which is lacking at the moment, would be conducive to further developments in the designing and fabrication of thermal devices. The existing studies on NDTR have been on models with structural inhomogeneity, such as the two-segment Frenkel-Kontorova model [8,14], the weakly coupled two-segment ϕ^4 model [15], and the anharmonic graded mass model [6]. However, structural asymmetry is not a necessary condition for NDTR. In the nonlinear response regime, NDTR can occur in absolutely symmetric structures where there exists nonlinearity in the on-site potential of the lattice model [16]. However, it is still not clear whether multiple NDTR can occur in symmetric structures. In this Brief Report, we study the exhibition of double NDTR in the absolutely symmetric structures and find the occurrence of double NDTR. Furthermore, we also find that NDTR can also occur in the coupled rotator model where the on-site potential is absent.

In this study, the homogeneous lattice models are each described by a Hamiltonian of the form

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

where p_i is the momentum of the ith particle and x_i its displacement from equilibrium position. m is the mass of the particles. $V(x)$ is the nearest-neighbor interaction potential, and the harmonic potential is used,

$$V(x) = \tfrac{1}{2}kx^2, \tag{2}$$

where k is the coupling constant. As for the on-site potential $U(x)$, we consider two cases shown in Fig. 1. For case A (ϕ^4 model) [1],

$$U(x) = -\frac{\alpha}{2}x^2 + \frac{\lambda}{4}x^4, \tag{3}$$

and for case B,

$$U(x) = -\frac{U_0}{(2\pi)^2}\cos(2\pi x) + \frac{\lambda}{4}x^4, \tag{4}$$

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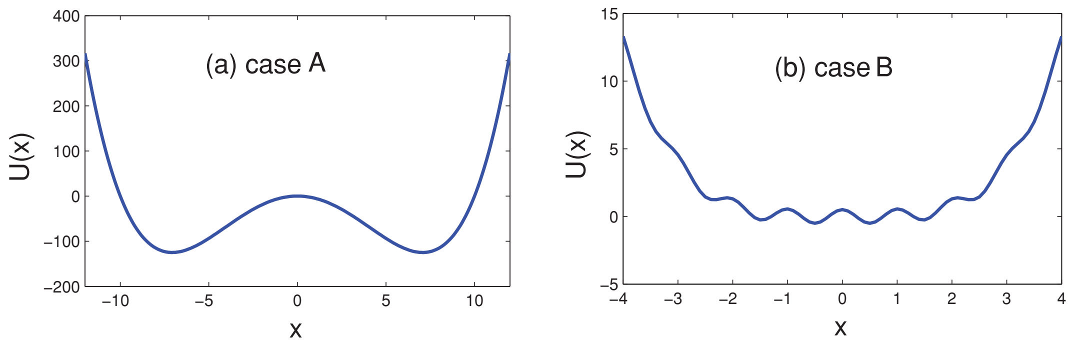

FIG. 1. (Color online) The shape of on-site potential. (a) Case A, $U(x) = -\frac{\alpha}{2}x^2 + \frac{\lambda}{4}x^4$ ($\alpha > 0$); (b) case B, $U(x) = \frac{U_0}{(2\pi)^2}\cos(2\pi x) + \frac{\lambda}{4}x^4$.

where α, U_0, and λ are the parameters that control the shape of the potential. The on-site potential contains the bounded and unbounded parts.

To obtain a stationary heat flux, the chain is connected to two heat baths at temperatures T_+ and T_-, respectively. Fixed boundary conditions are taken $x_0 = x_{N+1} = 0$. For each of the one-dimensional lattice models, the equation of motion takes the form

$$m\ddot{x}_i = -\frac{\partial H}{\partial x_i} - \gamma_i \dot{x}_i + \xi_i, \tag{5}$$

where $\gamma_i = \gamma(\delta_{i,1} + \delta_{i,N})$ and $\xi_i = \xi_+\delta_{i,1} + \xi_-\delta_{i,N}$. The noise terms $\xi_\pm(t)$ denote a Gaussian white noise that has a zero mean and a variance of $2\gamma k_B T_\pm$, where γ is the the friction coefficient and k_B is Boltzmann's constant. The dot stands for the derivative operator with respect to time t. The local heat flux is given by $j_i = \langle \dot{x}_i F(x_i - x_{i-1})\rangle$, where $F = -\frac{\partial V}{\partial x}$ and the notation $\langle\cdots\rangle$ denotes a steady-state average. The local temperature is defined as $T_i = \langle m\dot{x}_i{}^2\rangle$. After the system reaches a stationary state, j_i is independent of site position i, so that the flux can be denoted as j. In our simulations, the equations (5) of motion are integrated by using a second-order stochastic Runge-Kutta algorithm [17] with a small time step ($h = 0.001$). The simulations are performed long enough to allow the system to reach a nonequilibrium steady state in which the local heat flux is a constant along the chain.

Figure 2(a) shows the dependence of the heat flux j on temperature difference ΔT for ϕ^4 model with $\alpha > 0$ (case A). It is found that there exist two regions of ΔT, in which the larger the temperature difference the less heat flux there is through the system; namely, double NDTR occurs. The presence of the nonlinear on-site potential facilitates the occurrence of phonon-lattice scattering, which generally becomes more significant for increasing temperature and can therefore contribute to a decrease in the thermal conductivity. For low temperatures (small temperature difference), the bounded part of the on-site potential dominates the system. For this case, the phonon-lattice scattering is important only at sufficiently low temperatures where the dynamics of the particles is much influenced by the bounded on-site potential. As the applied temperature difference ΔT increases from zero with T_- being fixed, the increase in the thermodynamic driving force will drive an increase in the heat flux. For higher values of ΔT, however, the effect of phonon-lattice scattering becomes so significant that the first NDTR occurs. However, with a further increase in ΔT, the average temperature of the system has become sufficiently high that the particles can overcome the bounded part of the on-site potential, the phonon-lattice scattering becomes not significant, and the first NDTR disappears.

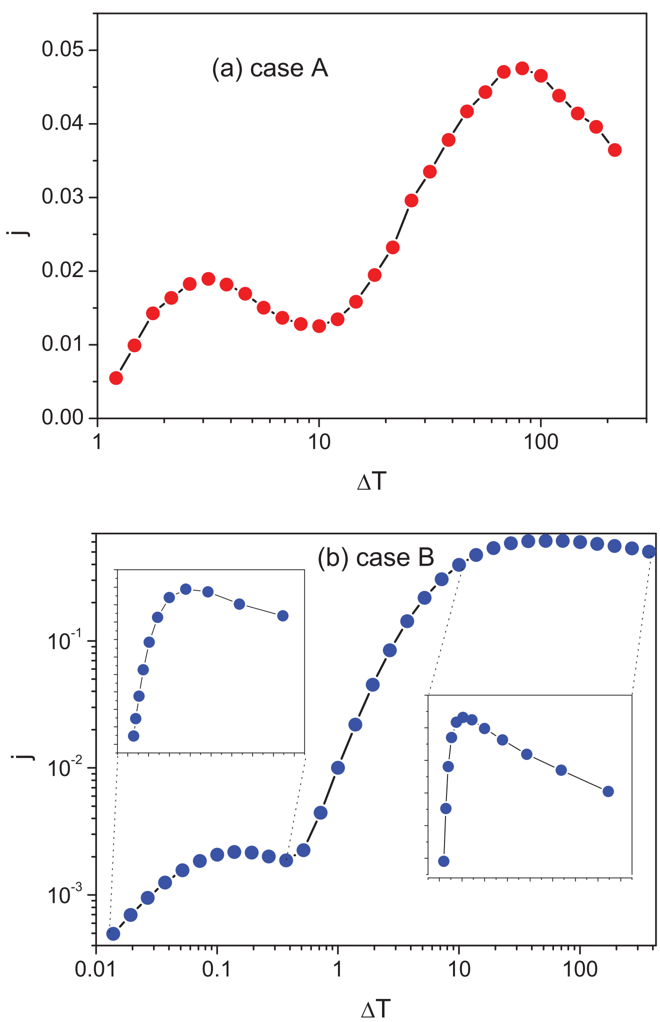

FIG. 2. (Color online) Heat flux j as a function of temperature difference ΔT for cases A and B. (a) For case A, $\alpha = 10$, $\lambda = 2.0$, and $T_- = 0.01$; (b) for case B, $U_0 = 10.0$, $\lambda = 0.2$, $T_- = 0.001$, and $N = 32$. The insets in (b) give enlarged views of the NDTR. The other parameters are $k = 1.0$, $N = 32$, and $T_+ = T_- + \Delta T$.

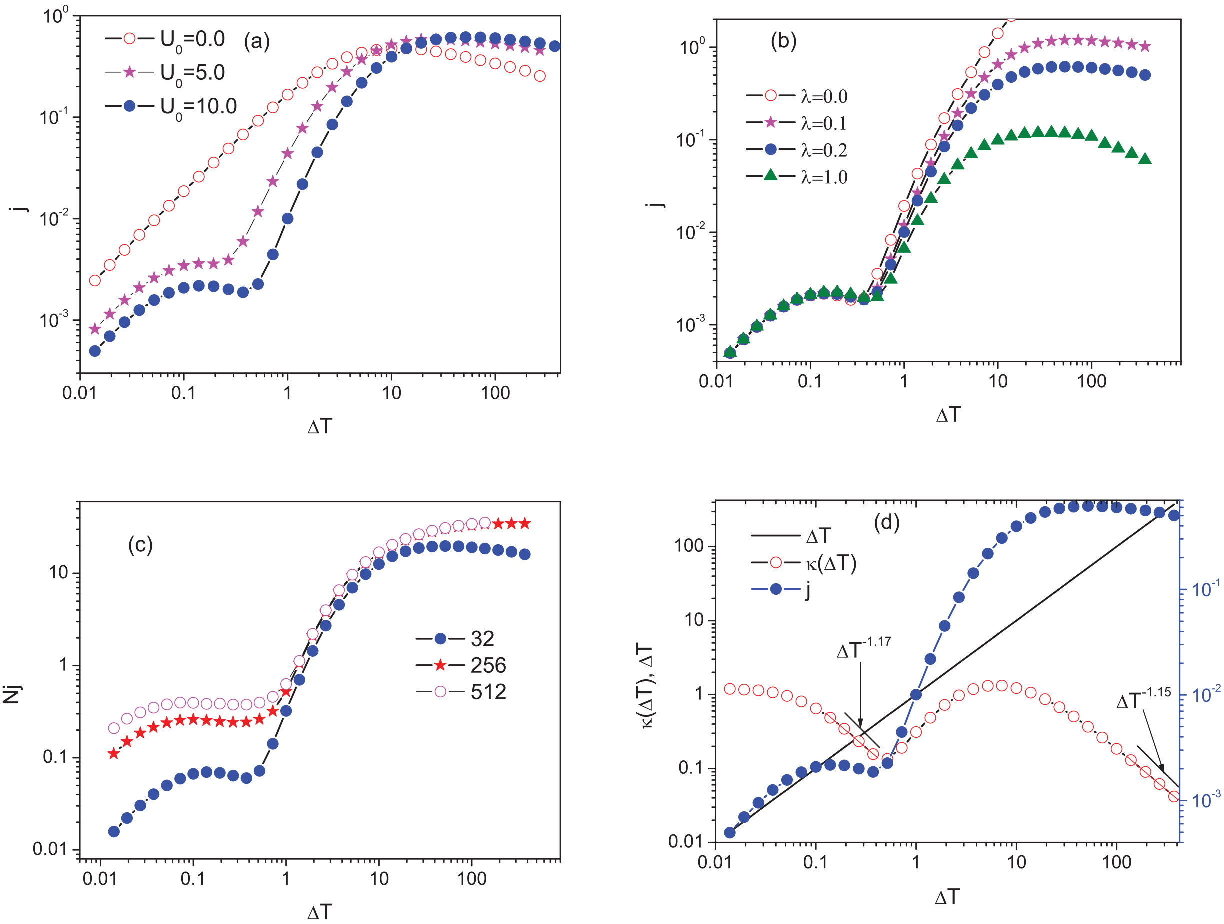

FIG. 3. (Color online) (a) Heat flux j as a function of ΔT for different values of U_0 at $k = 1.0$, $\lambda = 0.2$, and $N = 32$. (b) Heat flux j as a function of ΔT for different values of λ at $k = 1.0$, $U_0 = 10.0$, and $N = 32$. (c) The total heat flux Nj as a function of ΔT for $N = 32, 256$, and 512 at $U_0 = 10.0$, $k = 1.0$, and $\lambda = 0.2$. (d) $\kappa(\Delta T)$, ΔT, and heat flux j as a function of ΔT at $U_0 = 10.0$, $k = 1.0$, $\lambda = 0.2$, and $N = 32$. The other parameters are $T_- = 0.001$ and $T_+ = T_- + \Delta T$.

At the same time, the dynamics of the particles is dominated by the unbounded part of the on-site potential. As the temperature increases, the increase in phonon-lattice scattering is reflected by the power-law decrease of the thermal conductivity and the second NDTR occurs. Therefore, we can obverse the double NDTR as the temperature difference increases from zero with T_- being fixed. From Fig. 2(b), we can see that the similar double NDTR can also occur for case B.

Since the results for case A are similar to those for case B, we only focus on case B for investigating the parameter dependence of double NDTR. The on-site potential of case B is composed of two parts: the bounded part $-\frac{U_0}{(2\pi)^2}\cos(2\pi x)$ and unbounded part $\frac{\lambda}{4}x^4$.

Figure 3(a) shows the heat flux j as a function of ΔT for different values of U_0 with λ being fixed. For decreasing U_0, the first NDTR region becomes smaller and finally disappears. Therefore, the bounded part of the on-site potential contributes to the occurrence of the first NDTR. From Fig. 3(b), one can find that the occurrence of the second NDTR is induced by the unbounded part of the on-site potential. Figure 3(c) shows that the two NDTR regimes generally become smaller as the system size N increases and eventually vanishes in the thermodynamic limit.

Figure 3(d) shows the effective thermal conductivity $\kappa(\Delta T)$, heat flux j, and ΔT as a function of ΔT at $U_0 = 10.0$, $k = 1.0$, $\lambda = 0.2$, and $N = 32$. As we know, $j = \kappa(\Delta T)\Delta T$. It is found that $\kappa(\Delta T) \propto \Delta T^{-1.17}$ for the first NDTR region and $\kappa(\Delta T) \propto \Delta T^{-1.15}$ for the second NDTR region, resulting in $j \propto T^{-0.17}$ for the first NDTR region and $j \propto T^{-0.15}$ for the second NDTR region.

Note that there is no definite relation between the shape of the on-site potentials and the occurrence of NDTR. For example, if the term x^4 in case B is replaced by the harmonic term (linear potential) x^2, the shape of the on-site potentials does not change essentially, while NDTR at high temperatures will disappear. Therefore, it is the nonlinearity, not the shape of the on-site potentials, that determines the occurrence of NDTR. The nonlinearity in the on-site potentials is necessary to obtain NDTR for the harmonic interaction homogeneous systems. Now we return to the anharmonic homogenous systems and check if NDTR can occur in the absence of the on-site potentials. From the previous work [16], one can find that NDTR cannot occur in pure harmonic and Fermi-Pasta-Ulam model. However, in that work, the rotator model was not considered. The simplest example of rotator model with nearest-neighbor interactions lies in the class (1): $V(x) =$

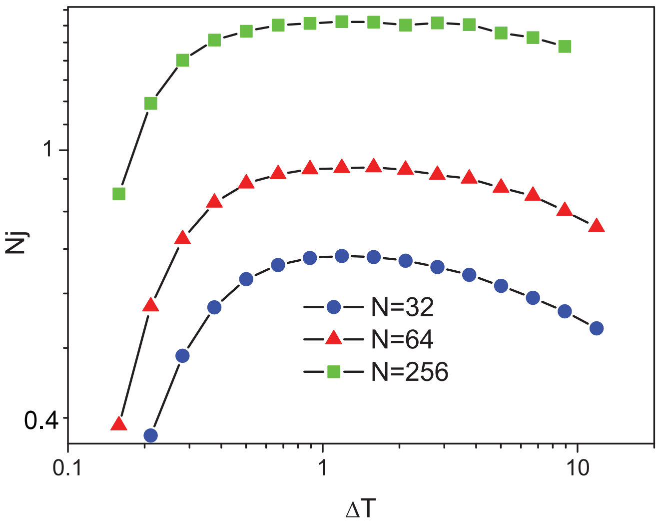

FIG. 4. (Color online) The total heat flux Nj as a function of temperature difference ΔT. The other parameters are $T_- = 0.1$ and $T_+ = T_- + \Delta T$.

$1 - \cos(x)$ and $U(x) = 0$. From Fig. 4, we can see that NDTR occurs in the rotator model, which is related to excitation of nonlinear localized rotational modes of the chain [18]. In addition, NDTR can also occur in the anharmonic graded mass lattices [6]. Therefore, for the anharmonic systems, the on-site potential is not a necessary condition for NDTR.

In conclusion, we study heat conduction through the one-dimensional homogeneous lattices with the nonlinear on-site potentials. The on-site potentials are composed of two parts: the bounded and unbounded parts. From nonequilibrium molecular dynamics simulations, it is found that double NDTR occurs as the temperature difference increases. The occurrence of NDTR at low temperatures is caused by the nonlinearity of the bounded part, while the nonlinearity of the unbounded part induces the occurrence of NDTR at high temperatures. In addition, we also find that NDTR even occurs in anharmonic homogenous lattices without on-site potentials, for example, the rotator model. Therefore, the on-site potential is not necessary to obtain NDTR for the anharmonic lattices. It is also found that the regime of NDTR becomes smaller as the system size increases and eventually vanishes in the thermodynamic limit. The observation of double NDTR in homogeneous systems shows that the nonlinearity of the on-site potentials is very important for designing NDTR devices. It is possible to design the thermal devices with the more complex functions by using the occurrence of double NDTR.

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[1] S. Lepri, R. Livi, and A. Politi, Phys. Rep. **371**, 1 (2003); A. Dhar, Adv. Phys. **57**, 457 (2008).

[2] G. Casati, Nat. Nanotechnol. **2**, 23 (2007).

[3] M. Terraneo, M. Peyrard, and G. Casati, Phys. Rev. Lett. **88**, 094302 (2002).

[4] D. Segal and A. Nitzan, Phys. Rev. Lett. **94**, 034301 (2005).

[5] B. Li, L. Wang, and G. Casati, Phys. Rev. Lett. **93**, 184301 (2004).

[6] N. Yang, N. Li, L. Wang, and B. Li, Phys. Rev. B **76**, 020301(R) (2007); E. Pereira, Phys. Rev. E **82**, 040101(R) (2010).

[7] B. Hu and L. Yang, Chaos **15**, 015119 (2005).

[8] B. Li, L. Wang, and G. Casati, Appl. Phys. Lett. **88**, 143501 (2006).

[9] L. Wang and B. Li, Phys. Rev. Lett. **99**, 177208 (2007).

[10] B. Hu, L. Yang, and Y. Zhang, Phys. Rev. Lett. **97**, 124302 (2006).

[11] C. W. Chang, D. Okawa, A. Majumda, and A. Zettl, Science **314**, 1121 (2006).

[12] L. Wang and B. Li, Phys. Rev. Lett. **99**, 177208 (2007).

[13] L. Wang and B. Li, Phys. Rev. Lett. **101**, 267203 (2008).

[14] W. R. Zhong, P. Yang, B. Q. Ai, Z. G. Shao, and B. Hu, Phys. Rev. E **79**, 050103(R) (2009); Z. G. Shao, L. Yang, H. K. Chan, and B. Hu, *ibid.* **79**, 061119 (2009).

[15] D. He, S. Buyukdagli, and B. Hu, Phys. Rev. B **80**, 104302 (2009).

[16] D. He, B. Q. Ai, H. K. Chan, and B. Hu, Phys. Rev. E **81**, 041131 (2010).

[17] R. L. Honeycutt, Phys. Rev. A **45**, 600 (1992).

[18] O. V. Gendelman and A. V. Savin, Phys. Rev. Lett. **84**, 2381 (2000); C. Giardina, R. Livi, A. Politi, and M. Vassalli, *ibid.* **84**, 2144 (2000).