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Thermal rectification and negative differential thermal resistance in lattices with mass gradient

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We study thermal properties of one-dimensional (1D) harmonic and anharmonic lattices with a mass gradient. It is found that a temperature gradient can be built up in the 1D harmonic lattice with a mass gradient due to the existence of gradons. The heat flow is asymmetric in anharmonic lattices with a mass gradient. Moreover, in a certain temperature region, negative differential thermal resistance is observed. Possible applications in constructing thermal rectifiers and thermal transistors by using the graded material are discussed.

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Theoretical studies of heat conduction in low-dimensional anharmonic (nonlinear) lattices in recent years have not only enriched our understanding of the microscopic physical mechanism of heat conduction, but also suggested some useful thermal device models such as rectifiers or diodes[1] and thermal transistors[2] for controlling heat flow. More importantly, a two-segment thermal rectifier has been realized experimentally by using nanotubes,[3] which implies that phonons, like electrons, can be controlled and manipulated.

On the other hand, functional graded materials (FGMs) have attracted increasing attention in many fields ranging among aerospace engineering, electronics, optics, and biomaterials, etc., due to their intriguing properties.[4,5] FGMs are a kind of inhomogeneous materials whose compositions and/or structures change gradually in space, which results in corresponding changes in physical properties, such as electric, mechanical, thermal, and optical properties. FGMs are abundant in nature, and can be also purposely manufactured.[4,6]

However, compared with optical, mechanical, and many other properties, the thermal properties of graded materials have not yet been fully studied (see the recent review article[2] and the references therein).

In this paper, we study thermal properties of a FGM represented by one-dimensional (1D) harmonic and anharmonic lattices with a mass gradient. For convenience, we call the lattices mass-graded harmonic or anharmonic lattices. They can be used to model superlattice or layered structures. It will be seen that the 1D graded lattices exhibit different physics, such as asymmetric heat flow and negative differential thermal resistance, two essential properties used to construct thermal rectifiers and thermal transistors. Therefore, the graded material might find applications in heat control and management.

We consider a 1D mass-graded chain, which is equivalent to a chain with graded coupling constants.[7] Figure 1(a) shows the configuration. The mass of the ith particle is $M_i = M_{max} - (i-1)(M_{max} - M_{min})/(N-1)$, where M_{max} is the mass of the particle at the left end and M_{min} is that of the particle at the right end. N is the total number of the particles. The Hamiltonian of this model is

$$H = \sum_i \left(\frac{p_i^2}{2M_i} + V(x_i - x_{i-1}) \right); \qquad (1)$$

here x_i is the position of the ith particle. Without loss of generality, V takes an anharmonic form, namely, $(x_i - x_{i-1} - a)^2/2 + \beta(x_i - x_{i-1} - a)^4/4$, which is a Fermi-Pasta-Ulam (FPU) β potential. So the system is called a graded FPU lattice. The lattice constant $a = 1.0$ and the coupling constant $\beta = 1.0$. In the case of $\beta = 0$, this lattice reduces to a graded harmonic chain.

In our simulations we use both fixed and free boundary conditions. A stochastic heat bath with temperature T_L is put on the first and second particles, and a heat bath with temperature T_R is put on the $(N-1)$th and Nth particles. The

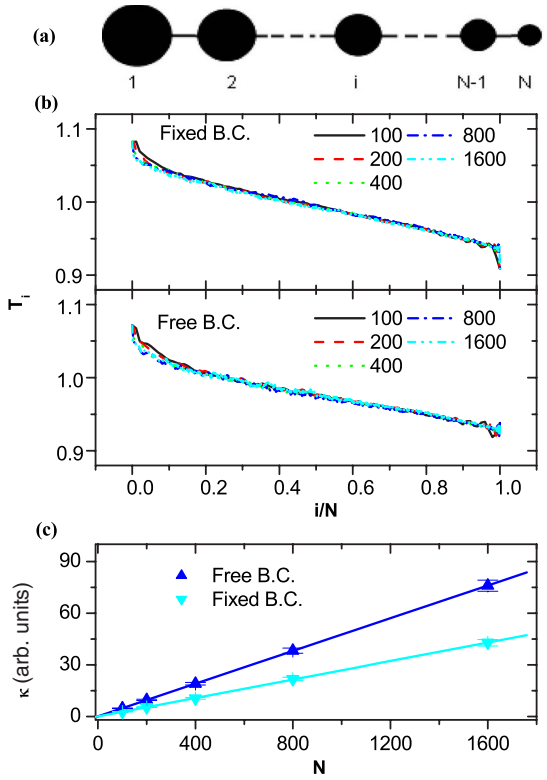

FIG. 1. (Color online) (a) Schematic picture of the mass-graded harmonic lattice. (b) Temperature profile for the lattice with fixed and free boundary conditions (B.C.). (c) Thermal conductivity κ versus system size N for the lattice with $M_{max} = 10$ and $M_{min} = 1$. $\kappa = AN$, where $A = 0.048$ and 0.027 for free and fixed boundary conditions, respectively. The temperatures of two baths are $T_L = 1.1$ and $T_R = 0.9$ for the left and right ends, respectively.

equations of motion (EOMs) of these four particles are described by the Langevin equations

$$M_i\ddot{x}_i = F(x_i - x_{i-1}) - F(x_{i+1} - x_i) - \begin{cases} \xi_L - \lambda_L\dot{x}_i, & i = 1,2, \\ \xi_R - \lambda_R\dot{x}_i, & i = N-1,N, \end{cases} \tag{2}$$

where $\xi_{L/R}$ are independent Wiener processes with zero mean, variance $2\lambda_{L/R}k_BT_{L/R}$, and force $F=-\partial V/\partial x$. To minimize the Kapitza resistance between the bath particle and its neighbor, we set $\lambda_{L/R}/M_i=0.1$. Both the fourth-order Runge-Kutta and the velocity Verlet algorithm are used to integrate the EOMs. Differences between the results of these two integration methods are negligible. Simulations are performed long enough ($>10^7$ time units) that the system reaches a stationary state where the local heat flux is constant along the chain.

We start with a mass-graded harmonic lattice, i.e., $\beta=0$ in the potential $V(x)$. Figure 1(b) shows the temperature profile with different lattice lengths N and different boundary conditions. M_{max} and M_{min} are fixed at 10 and 1, respectively. It is well known that no temperature gradient can be built up along a homogeneous harmonic lattice.[8] However, in the mass-graded harmonic lattice, the temperature gradient is clearly seen.

The local flux at site i is defined as

$$J_i = \frac{1}{2}a\langle(\dot{x}_{i+1} + \dot{x}_i)F(x_{i+1} - x_i)\rangle. \tag{3}$$

After the system reaches a stationary state, J_i is independent of site position i, so the flux can be denoted as J. The thermal conductivity is calculated as $\kappa=-J/(dT/dx)$. We should stress that, in calculating the temperature gradient, we get rid of temperature jumps at the two boundaries. In Fig. 1(c), the thermal conductivity versus N for different boundary conditions is plotted. For the same lattice length N, thermal conductivities with fixed boundaries are lower than those with free boundaries, because there is a limitation that all vibrational eigenmodes must vanish at the boundaries in fixed boundary cases. It is clearly seen that the thermal conductivity diverges linearly with length N. This linear property is independent of boundary conditions. It is different from that of a disordered harmonic lattice where the thermal conductivity diverges with system size as $\sqrt{N}$ and $1/\sqrt{N}$ for free and fixed boundary conditions, respectively.[9]

The linear divergence of thermal conductivity with system size is interesting, as we know that, in 1D homogeneous harmonic lattices, no temperature gradient can be built up and thus thermal conductivity cannot be defined.[10] In order to understand the underlying mechanism, we have to invoke the vibrational eigenmodes of the graded system. It is found in Ref. 7 that there is a critical frequency ω_c, which is the maximum eigenfrequency of the corresponding homogeneous harmonic lattice with $M_i=M_{max}$, where M_{max} is the maximal mass in the graded harmonic lattice. The modes with $\omega<\omega_c$ can be well extended over the whole chain, whereas those with $\omega>\omega_c$ (called gradons) are localized at the side with lighter masses. Therefore, the formation of a temperature gradient in the graded harmonic lattice is attributed to the localization of the gradons.

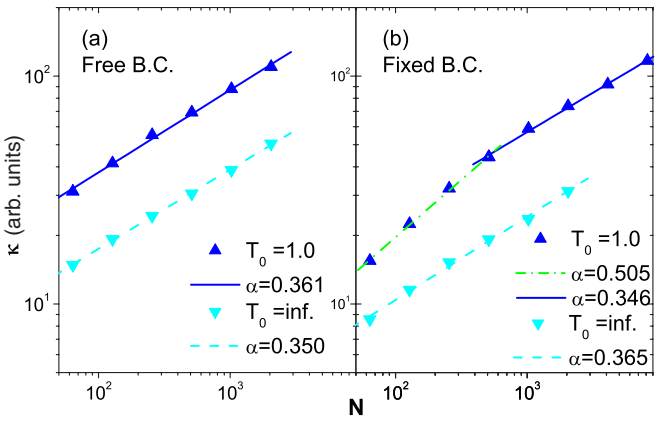

FIG. 2. (Color online) Thermal conductivity κ versus system size N for the mass-graded FPU lattice under free (a) and fixed (b) boundary conditions (B.C.) with $M_{max}=10$ and $M_{min}=1$. In all cases, $\kappa\propto N^{\alpha}$. The values of α are given in the figure.

In the following, we focus on the mass-graded anharmonic lattice. We first examine the size effect of thermal conductivity and its dependence on temperature. It is found that the thermal conductivity diverges with system size as $\kappa\sim N^{\alpha}$. Figure 2(a) shows the temperature effect of the divergent exponent under free boundary conditions. The value of α does not change too much; it keeps almost the same value of 0.36 (0.35) when the average temperature T_0 is increased from 1.0 to infinity. The value of the divergence exponent is very close to the results from the renormalization group for 1D hydrodynamic systems,[11] and that for the hard core model.[12] The calculation for infinite T_0 is actually realized by discarding the quadratic term (of potential) in the Hamiltonian, since this term is negligible compared with the quartic term in the infinite-temperature limit.

Figure 2(b) shows the temperature effect of the divergent exponent under fixed boundary conditions. In the case of $T_0=1$, the best fitting with all available data up to $N=512$ gives rise to $\alpha=0.51$. However, the best fitting for values of the largest five N ($512\leqslant N\leqslant 8192$) gives rise to $\alpha=0.35$, which is very close to the value at infinite temperature. The value $\alpha=0.51$ might be a finite-size effect.

The value of α for free boundary conditions is quite close to the value for fixed boundary conditions. Therefore, this result seems to be very similar to that for the homogeneous FPU β lattice, namely, the divergent exponent α seems to be independent of the boundary conditions.

As for the disordered FPU β lattice, it is observed that the value of β depends on the boundary conditions.[13] However, this result needs to be further checked, as the authors in Ref. 13 used a very short lattice, $N\leq 20$.

We should point out that the above results may not be very conclusive as we have a relatively small system size N. In order to get a more convincing conclusion, one might need to go to much larger N, say $N>10^5$, which is very difficult for current computer facilities. However, this is not the main purpose of the paper.

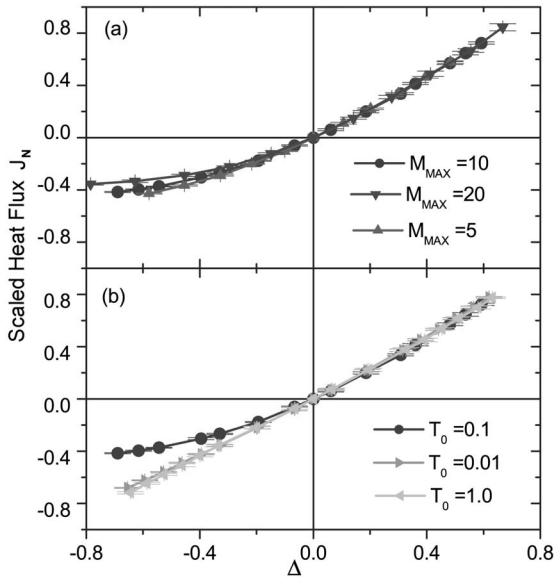

FIG. 3. (a) Scaled heat flux J_N versus Δ for three different mass gradients. $N=200$, $T_0=0.1$, $M_{min}=1$, and $M_{max}=20$, 10, and 5. $J_N=J/C$, where $C=0.0045$, 0.0080, and 0.0145 for $M_{max}=20$, 10, and 5, respectively. (b) Scaled heat flux J_N versus Δ for $T_0=1.0$, 0.1, and 0.01. $N=200$, $M_{min}=1$, $M_{max}=10$. $J_N=J/C$, where $C=0.072$, 0.008, and 0.0005 for $T_0=1.0$, 0.1, and 0.01, respectively.

In the following, we study thermal rectification in the mass-graded anharmonic lattice. In order to avoid the effect of the Kapitza resistance at the boundary, we record the temperatures of the closest particles to the bath particles at the two ends, namely, the third and the 198th for $N=200$, as $T_{l,r}$. For convenience, we set the temperature of the heavy-mass end $T_l=T_0(1+\Delta)$ and that of the light-mass end $T_r=T_0(1-\Delta)$, where T_0 is the average temperature of the system.

For comparison, we show the scaled heat flux J_N ($\equiv J/C$) versus Δ in Fig. 3(a) for three different mass gradients, where C is a constant. For different mass gradients, when $\Delta>0$, the heat flux increases steeply with the increase of Δ. However, in the case of $\Delta<0$, the heat flux changes a little when Δ changes. This asymmetry of heat flux with respect to Δ is called *thermal rectification*. We study the dependence of the rectification on the mass gradient (fix $M_{min}=1$ and change $M_{max}=20$, 10, and 5). It is shown in Fig. 3(a) that the larger the mass gradient, the more obvious the rectification.

To find the temperature dependence of rectification, we calculate the normalized heat flux J_N versus Δ for different temperatures, $T_0=0.01$, 0.1, and 1.0 [Fig. 3(b)]. From this figure, we can see that the thermal rectification vanishes in both the high- and low-temperature limits. In the low-temperature limit, the graded anharmonic lattice reduces to the graded harmonic lattice in which no rectification exists. In the high-temperature limit, the low-frequency vibration modes, which dominate the heat conduction, at both ends can be excited; therefore no rectification is found either. In the case of $T_0=0.1$, the low-temperature end is harmonic, while the high-temperature end is strongly anharmonic; thus the vibrational spectra are strongly mismatched, which leads to thermal rectification.

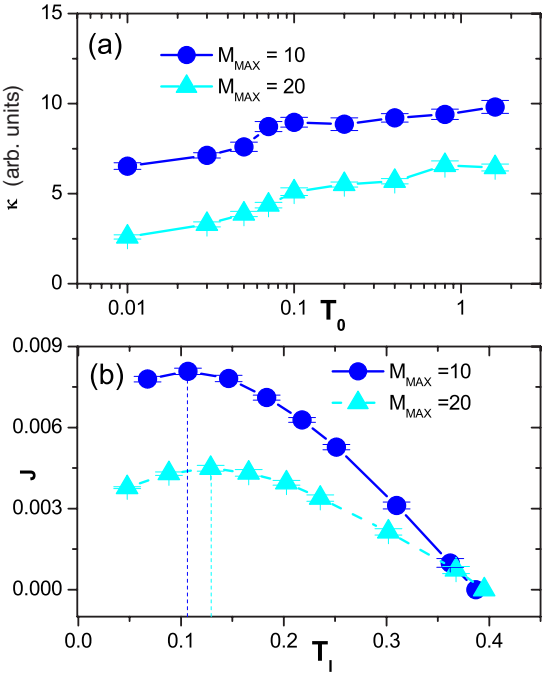

FIG. 4. (Color online) (a) Thermal conductivity κ versus temperature T_0. $\Delta=0.1$. (b) Heat flux J versus T_l. T_r is fixed at 0.4. $N=200$, $M_{min}=1$, and $M_{max}=20$ and 10. The negative differential thermal resistance ($R<0$) appears when $T_l<0.14$ and 0.11 for $M_{max}=20$ and 10, respectively.

Finally, we should stress that the rectification is sensitive to boundary conditions. The effect can be observed only for fixed boundary conditions, because the low-frequency mode cannot be restrained for free boundary conditions.

We show the temperature dependence of thermal conductivity in Fig. 4(a) for the graded anharmonic lattice. Another important feature found in this 1D graded chain is *negative differential thermal resistance* (NDTR),[2] namely, the larger the temperature difference the less the heat flux through the system. In order to illustrate the NDTR, we fix the temperature of the right (light-mass) end at $T_r=0.4$ and plot the heat flux J versus temperature T_l in Fig. 4(b). The differential thermal resistance is defined as $R=-(\partial J/\partial T_l)^{-1}_{T_r=const}$. The NDTR is seen on the left part of the vertical line, where J increases as T_l is increased.

To understand the mechanism of rectification and NDTR, we calculate the power spectra of the particles close to the two ends, and then compare their spectra with each other (Fig. 5). When the temperature is high enough, the quartic term in the FPU potential is the dominant term in the whole chain. So the coupling among modes is strong, and low-frequency modes, which contribute to the heat conduction most, are abundant in the spectrum. Then the flux depends mainly on the temperature difference. So the quartic term is dominant only at the end with high temperature, and the quadratic term plays the main role at the low-temperature end; therefore, the low-frequency modes cannot go through the system. The heat current is controlled by two competing effects: temperature gradients and overlaps of vibrational spectra. In the presence of a mass gradient, there is a big

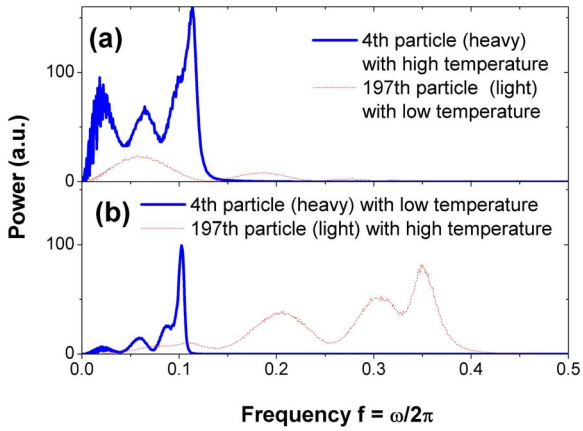

FIG. 5. (Color online) Spectra of the two end particles for system $N=200$, $T_0=0.1$, $M_{min}=1$, and $M_{max}=10$. (a) Heavy-mass end (left) contact with high-temperature bath ($\Delta=0.6$). (b) Light-mass end (right) contact with high-temperature bath ($\Delta=-0.7$).

difference between $\Delta>0$ and $\Delta<0$ in the spectra. As shown in Fig. 5(a), where the left end (heavy mass) contacts with the high-temperature bath ($\Delta>0$), the spectra of the two particles overlap in a wide range of frequencies; thus the heat can easily go through the lattice along the direction of the temperature gradient. However, when the right end (light mass) contacts with the high-temperature bath [$\Delta<0$, Fig. 5(b)], the spectra separate from each other. It can be seen that the light-mass particle with high temperature oscillates mainly at high frequency; however the heavy-mass particle at low temperature oscillates at low frequency. As a result, it is difficult for heat to go through the system, although there is a temperature gradient. When T_0 goes to the low-temperature limit, the graded chain can be regarded as a graded harmonic lattice whose thermal properties are like those of the homogeneous harmonic lattice; then the flux depends only on the temperature difference.

In summary, we have studied thermal properties of 1D mass-graded harmonic and anharmonic lattices in this paper. It is found that a temperature gradient can be built up in the 1D graded harmonic lattice chain due to the localization of high-frequency gradon modes. The thermal conductivity diverges with the system size linearly, $\kappa \propto N$. In graded anharmonic lattices, the thermal conductivity diverges with system size as $\kappa \sim N^{\alpha}$; the value of α seems to be independent of temperature and boundary conditions.

Thermal rectification and negative differential thermal resistance have been observed in the graded anharmonic lattice. This is quite similar to the recent nanotube experiment,[3] in which half of the tube was gradually mass loaded on the surface with heavy molecules. Our results suggest that graded materials might be used as thermal rectifiers and thermal transistors.

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