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Phonon transmission and thermal conductance in one-dimensional system with on-site potential disorder

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ABSTRACT

The role of on-site potential disorder on phonon transmission and thermal conductance of one-dimensional system is investigated. We found that the on-site potential disorder can lead to the localization of phonons, and has great effect on the phonon transmission and thermal conductance of the system. As on-site potential disorder W increases, the transmission coefficients decrease, and approach zero at the band edges. Corresponding, the thermal conductance decreases drastically, and the curves for thermal conductance exhibit a series of steps and plateaus. Meanwhile, when the on-site potential disorder W is strong enough, the thermal conductance decreases dramatically with the increase of system size N. We also found that the efficiency of reducing thermal conductance by increasing the on-site potential disorder strength is much better than that by increasing the on-site potential's amplitude.

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1. Introduction

In recent years, potential applications of nanotechnology have generated widespread interest in studying the electronic transport of one-dimensional systems, including carbon nanotubes, nanowires, and conducting molecules [1–3]. As is known that there is a nice correspondence between the phonon and electron properties. The understanding of the thermal transport of one-dimensional systems will become a significant factor in the development of future nanoelectronic circuits because of the importance of the thermal management among nanoelements. Meanwhile, the thermal conduction property of one-dimensional systems is also of particular interest in several possible applications of phononics [4], wherein phonons can be used to carry and process information. The manipulation and control of phonon transport have been proposed to design thermal devices models such as thermal diodes [5–7], thermal transistor [8], thermal logic gates [9], thermal memories [10] and thermoelectric power generation [11–13]. And experimental works such as thermal rectifier [14] and nanotube phonon waveguide [15] have been carried out. Therefore, the physics of the thermal transport in one-dimensional systems has attracted a great deal of attention [16–22].

Despite great progress in nanofabrication, the disorder is hard to get rid of. Along with the study of electron transport in disordered systems, heat conduction in one-dimensional disordered system has been studied for decades. It is well known that the electron eigenstates in a one-dimensional disordered potential are localized [23]. The electrical current thus decays exponentially with wire length, making it an insulator. However, in phononic systems, for example, a disordered harmonic chain, long wavelength modes are extended and a significant amount of heat can be conducted. According to Fourier's law, we expect that the heat current is proportional to the local temperature gradient, and the dependence of the heat current J on system size N is $J \sim N^{-1}$; while a large number of studies suggest that the thermal transport of one-dimensional systems is a non-Fourier process [16,24–26], the dependence of the heat current J on system size N is $J \sim N^{\alpha-1}$ (α is an exponent depending on different cases) [25,26]. However, most of the studies concentrated on isotopically disordered harmonic chain, where the disorder was introduced by a random distribution of the lattice mass [19–21]. As we know, expect for the defects during the production process of nanostructures (such as nanotubes and nanowires), there is an unavoidable source of additional disorder, the on-site potential disorder, which is used to model the effects of the environment on the sites. For example, in DNA molecule, which is the promising materials for nanotechnology [27–29], the on-site potential describes the interaction between two bases in a pair including several contributions such as the hydrogen bonds linking the two bases and the repulsion of the charged phosphate groups belonging to the backbone, and the on-site potential can be modulated [30,31]. Can on-site potential disorder lead to

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phonon's localization? How does the on-site potential disorder affect the thermal conductance? Although some studies have explored the effect of on-site potential on thermal transport [22,32], the role of on-site potential disorder on thermal transfer has rarely been studied. Accordingly, a better understanding of the role of on-site potential disorder on thermal transport may also lead to potential applications based on the possibility to manipulate and control the heat flow. In this Letter, we studied the phonon transmission and thermal conductance in one-dimensional systems with on-site potential disorder which simulates the environmental complications. The transfer-matrix method was used to calculate the phonon transmission and the thermal conductance in one-dimensional systems with on-site potential disorder.

The Letter is organized as follows. In the next section, we presented the lattice dynamics model of one-dimensional systems with on-site potential disorder. In Section 3 we focused on the role of on-site potential disorder on phonon localization. In Section 4 we calculated the transmission of phonons as a function of frequency. In Section 5 we described the calculated results of thermal conductance in one-dimensional systems with on-site potential disorder. Finally, the conclusions of this work were presented in Section 6.

2. Model and numerical method

In our study we consider a one-dimensional chain coupled at its ends (left and right) to some kind of inexhaustible heat reservoirs which are maintained at temperatures T_L and T_R. The Hamiltonian of the system is

$$H = \sum_{l=1}^{N}\left[\frac{p_l^2}{2m_l} - V_l\right] + \sum_{l=0}^{N}\frac{k}{2}(x_{l+1} - x_l)^2, \tag{1}$$

where N is the number of the atoms in the system, p_l and x_l are the momentum and the displacements of the atoms from their equilibrium position, m_l are the mass of atoms, k is the strength of the harmonic coupling between neighbor atoms, and V_l are the strength of the on-site potential, which are employed to model the effects of the environment on the sites. V_l are taken to be randomly distributed with in range $[V_0 - W/2, V_0 + W/2]$, where V_0 is the center of the potential region and W is the disorder degree. We apply the boundary condition of $x_0 = x_{N+1} = 0$.

The system has N normal modes $[x_1(t), x_2(t), \ldots, x_N(t)]$, and $x_l(t) = u_l e^{i\omega t}$, where ω is the vibration eigenfrequency. Then the eigenfrequency and eigenvector can be obtained by the following equation,

$$\begin{bmatrix} 2k + V_1 - m_1\omega^2 & -k & 0 & 0 & 0 \\ -k & 2k + V_2 - m_2\omega^2 & -k & 0 & 0 \\ 0 & -k & . & . & 0 \\ 0 & 0 & . & . & -k \\ 0 & 0 & 0 & -k & 2k + V_N - m_N\omega^2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_N \end{bmatrix} = 0. \tag{2}$$

Based on Dean and Martin's negative eigenvalue theory [33] as well as Wu and Zheng's infinite order perturbation theory [34], the eigenfrequencies and eigenvectors of the system can be obtained.

The dynamic equation of the system can also be expressed as

$$-m_l\omega^2 u_l = k(u_{l+1} - u_l) + k(u_{l-1} - u_l) + V_l u_l. \tag{3}$$

Making use of the transfer-matrix formalism, Eq. (3) can be expressed in a matrix form

$$\begin{pmatrix} u_{l+1} \\ u_l \end{pmatrix} = \begin{pmatrix} \frac{a_l}{k} & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_l \\ u_{l-1} \end{pmatrix} \equiv G_l \begin{pmatrix} u_l \\ u_{l-1} \end{pmatrix}, \tag{4}$$

where $a_l = 2k + V_l - m_l\omega^2$, and M_l is the transfer matrix that correlates the vibration displacement of adjacent sites u_l and $u_{l\pm1}$. Therefore, the global transfer matrix can be expressed as

$$G(N) = \prod_{l=1}^{N} G_l = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix}. \tag{5}$$

The allowed regions of the frequency spectrum are determined from the usual spectral condition [35,36] $|\mathrm{Tr}\, G(N,\omega)| \leqslant 2$. To calculate the transmission coefficients of an incoming plane wave with frequency ω, we only need to find a solution of the equations of motion which to the left of the segment $1, 2, \ldots, N$ is combination of an incoming and a reflected wave and to the right is a pure outgoing wave, i.e.,

$$\begin{aligned} &u_l = Ae^{iql} + Be^{-iql}, \quad l \leqslant 0, \\ &u_l = Ce^{iql}, \quad l \geqslant N+1, \end{aligned} \tag{6}$$

where $\omega = \omega(q) = \sqrt{4/m}\sin(q/2)$, q is wave vector which is related to the frequency via the dispersion relation of heat bath. Using the transfer matrix approach, the transmission coefficient $T(N,\omega)$ of phonon passing through the whole system can be expressed as [32]

$$T(N,\omega) = \left|\frac{C}{A}\right|^2 = \frac{4\sin^2 q}{|-G_{11}e^{-iq} + G_{21} - G_{12} + G_{22}e^{iq}|^2} = \frac{4\sin^2 q}{[G_{12} - G_{21} + (G_{11} - G_{22})\cos q]^2 + (G_{11} + G_{22})^2\sin^2 q}, \tag{7}$$

where $\sin^2 q = \frac{m\omega^2}{k}(1 - \frac{m\omega^2}{4k})$ and $\cos q = 1 - \frac{m\omega^2}{2k}$.

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