Multimode quantized thermal conductance tuned by external field in a quantum wire

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In this work, we propose an approach to realize field-dependent multimode quantized thermal conductance by introducing both harmonic and anharmonic couplings to a quantum wire. It is demonstrated theoretically that by stretching (or compressing) the wire, phononic band structures are tuned and multiple phononic channels are opened one by one. In this way, multiple-step quantized thermal conductance is realized. The research opens a way to manipulate heat transfer in mesoscopic phonon systems. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2956673]

Quantum transport in low dimension has attracted much attention in the past two decades. One of the remarkable achievements is the quantization of electrical conduction discovered by von Wees *et al.*[1] and Wharam *et al.*[2] Due to the quantum confinement in mesoscopic systems, electronic eigenstates become discrete, which is called the channels for electron transport. Each ballistic channel contributes a quantum to the electrical conductance. Similar phenomena occur in phononic transport and thermal transfer in mesoscopic phonon systems. The thermal conductance of a single channel is limited by its universal thermal conductance quantum, which was predicted in Refs. 3 and 4 and later demonstrated in nanostructures.[5] The single-mode photon-assisted thermal conductance has recently been observed,[6] and thermal rectifiers[7–10] are realized to modulate heat flux. The in-depth understanding of microscopic laws of heat transfer is important in designing thermoelectronic systems[11,12] and for the development information theory.[13]

It has been established that anharmonic potential can induce anomalous scaling relation of heat flux in a chain,[14] and generate nonlinear normal modes, i.e., solitons.[15] The thermal diodes[8] and transistors[16] can be realized by coupling nonlinear lattices. In this letter, we introduce both harmonic and anharmonic potentials to a wire to realize the multimode quantized thermal conductance. This is an approach to open channels for phononic transport.

We propose a *n-mer* wire (NMW) model, which consists of three segments: left, right, and central segments [as shown in Fig. 1(a)]. The left (or right) segment is a random *n-mer* (RN) chain containing different particles *A* and *B*. Particles *A* and *B* are arranged in such a way that particle *A* and a cluster of *n* particles $B\cdots B$ are randomly assigned, known as RN model.[17] In this segment, all the interaction potentials are harmonic. The central segment of the NMW, in contrast, is a periodic chain composed of two kinds of particles *A* and *C* in format of $ACAC\ldots AC$. The connection *C*-*A* is harmonic, whereas the connection $A-C$ is weakly nonlinear. Following Feimi, Pasta, and Ulam (FPU),[15,18] we let the interaction *A*-*C* take cubic-interaction-term potential (β). In this way, the harmonic potential and FPU-β potential appear alternately in the central segment of the wire.

Now we consider phononic transport in the NMW, whose ends are acted by a stretching force. The Hamiltonian of the central segment in the NMW can be expressed as

$$H_C = \sum_i \frac{p_i^2}{2m_i} + \sum_{i\epsilon \mathrm{odd}} \frac{\alpha}{2}(\Delta\mu_i)^2 + \sum_{i\epsilon \mathrm{even}} V_{\mathrm{FPU}-\beta}(i), \qquad (1)$$

where m_i and p_i are the mass and the momentum of the *i*th particle, respectively. α is the strength of the harmonic coupling of particles, and $\Delta\mu_i = \mu_i - \mu_{i-1}$ denotes the relative displacement between the neighboring particles. The FPU-β potential is described as[18]

$$V_{\mathrm{FPU}-\beta}(i) = \frac{\alpha'}{2}(\Delta\mu_i)^2 + \frac{\beta}{4}(\Delta\mu_i)^4. \qquad (2)$$

Here α' and β represent the strength of the linear-interaction term and the cubic-interaction term in the interaction *A*-*C*,

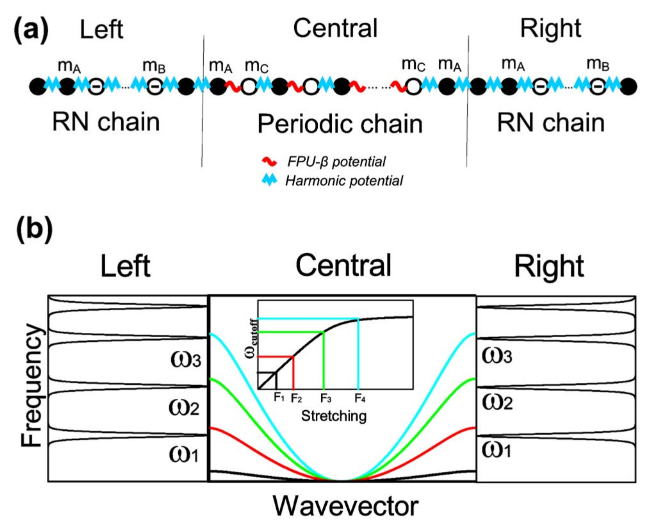

FIG. 1. (Color online) (a) Schematic diagram of an NMW, which consists of three segments as described in the text. (b) Schematic diagram of a tunable phononic band in the NMW. In the left and the right segments, some δ-function-like PBS levels locate at the resonant frequencies $\omega_j (j=1,2,3,\ldots)$ in the RN chain. While in the central segment, acoustic branch is tuned by stretching, and the curve with different colors corresponds to different stretching. The inset shows that the cutoff frequency ω_{cutoff} of the acoustic branch in central segment increases upon stretching the wire, where F_1, F_2, F_3, and F_4 refer to different stretching, respectively. By increasing the stretching, ω_{cutoff} gradually sweeps over $\omega_j (j=1,2,3,\ldots)$, hence multiple phononic channels are sequentially opened.

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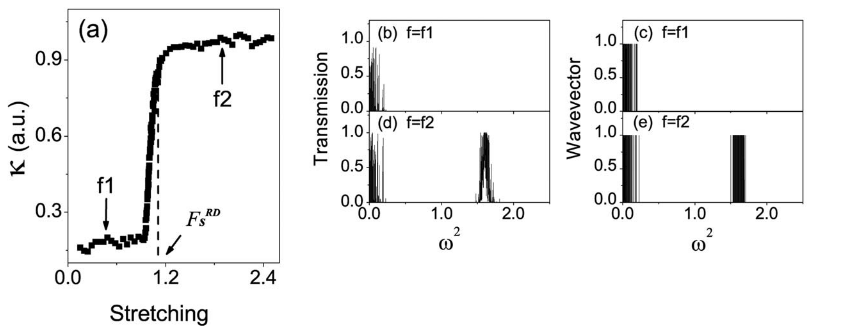

FIG. 2. (a) The thermal conductance κ as a function of the stretching (α_{eff}) in the *dimer* wire (i.e., the NMW with $n=2$), where the total number of atoms is $N=2113$. (b) and (d) illustrate the transmission coefficients of phonons in the same *dimer* wire at different stretching ($f_i, i=1,2$), which is marked in the curve of thermal conductance. (c) and (e) illustrate the frequency spectra of phonons in the same *dimer* wire at different stretching ($f_i, i=1,2$), respectively. The calculation parameters are set as $m_A=1.0$, $m_B=1.4$, $m_C=2.0$, $\alpha=2.0$, $T_H=\hbar\omega^*/k_B$, and $T_L=0.1T_H$, respectively. Here $\omega^* \sim 10^{13}\ \text{s}^{-1}$, which is the oscillator frequency of the typical atom.

respectively. Once stretching the NMW, the wire is elongate, i.e., $\Delta\mu_i$ adds a static term l (l stands for the displacement of particle away from the equilibrium position.) It is proved that when the FPU-β potential is sufficiently weak, the FPU-β potential can degenerate into a quasiharmonic one as $V_{\text{FPU}-\beta}(i) \cong V_0(i) + \alpha_{\text{eff}}/2(\Delta\mu_i)^2$, where $V_0(i)$ is a static potential, and α_{eff} is the strength of the effective harmonic potential as $\alpha_{\text{eff}}=\alpha' + 3\beta l^2$. Obviously, both l and α_{eff} can be controlled by stretching or compressing the wire. We will see that the external stretching can tune the phononic band structure (PBS) of the NMW.

The PBS of the whole NMW is determined by the phonons that can penetrate all three segments. On one hand, the central segment of NMW is a periodic chain composed of particles A and C, hence its PBS contains both an acoustic branch and an optical brance in the frame of the quasiharmonic approach. For the acoustic branch, the cutoff frequency of is given by $\omega_{\text{cutoff}}=(D-\sqrt{D^2-16\alpha\alpha_{\text{eff}}m_Am_C})/(2m_Am_C)$, where $D=(\alpha+\alpha_{\text{eff}})(m_A+m_c)$. By increasing the stretching, α_{eff} gradually increases; hence the cutoff frequency gradually increases in the central segment of NMW [as shown in the inset of Fig. 1(b)]. On the other hand, the left (or right) segment of NMW is the RN chain containing particles A and B. Due to the localization-delocalization transition of phonons in the RN chain, multiple resonant transmission can be obtained, thereafter, δ-function-like resonant modes can be achieved in the RN chain[17] [as shown in Fig. 1(b)]. Now the effective Hamiltonian of the whole NMW contains two parts: one is from the localized phonons (H_{loc}), and the other is from the delocalized phonons, i.e.,

$$H = H_{\text{loc}} + \sum_{\omega_j<\omega_{\text{cutoff}}} \hbar\omega_j a_j^+ a_j, \tag{3}$$

where $a_j^+a_j$ is the number of delocalized phonons, and ω_j is the resonant frequency[17] given by $\omega_j^2=2\alpha/m_B(1-\cos j\pi/n)$, where $j=1,2,\ldots,n-1$. This Hamiltonian decides the heat current in the NMW.

Connect the NMW to two heat reservoirs with temperature T_H and T_L, respectively. By taking Eq. (3) to Landauer formula,[4] the heat current J through the NMW is

$$J = \sum_j \int_0^{\omega_{\text{cutoff}}} d\omega \cdot \hbar\omega\delta(\omega-\omega_j)T(\omega)[\eta_{\text{hot}}(\omega) - \eta_{\text{cold}}(\omega)], \tag{4}$$

where $\eta_{\text{hot(cold)}}$ is the Bose–Einstein distribution of two heat reservoirs, $T(\omega)$ is the phonon transmission coefficient, which depends on phonon scattering in the NMW. Hence, the thermal conductance can be expressed as

$$\kappa = \lim_{\Delta T\to 0}\frac{J}{\Delta T} = \sum_j \kappa_q \cdot \theta(\omega_j - \omega_{\text{cutoff}}), \tag{5}$$

where $\theta(x)$ is a step function [note: $\theta(x)=1$ if $x\geqslant 0$, or $\theta(x)=0$ if $x<0$], and κ_q is the quantum of thermal conductance. It is proved that κ_q is given by

$$\kappa_q = \frac{k_B^2 T}{\hbar}\frac{x_j^2 e^{x_j}}{(e^{x_j}-1)^2}, \tag{6}$$

where $x_j=\hbar\omega_j/k_BT$, and k_B is the Boltzmann constant. Obviously according to Eq. (5), the thermal conductance in the NMW is shown by a series of conductance steps.

It should be pointed out that by increasing the stretching on the NMW, the cutoff frequency ω_{cutoff} in the central segment gradually sweeps over all the resonant frequencies in the left and right segments [as shown in Fig. 1(b)]. Accurately, once the stretching is stronger than the resonant stretching (F_s), i.e., $\alpha_{\text{eff}}\geqslant F_s=[\alpha(m_A+m_C)\omega_j^2 - m_Am_C\omega_j^4]/[4\alpha-(m_A+m_C)\omega_j^2$, the cutoff frequency sweeps a resonant frequency ω_j, hence a phononic channel is opened. Therefore, by stretching the NMW, multiple phononic channels are opened sequentially, and multiple-step thermal conductivity is achieved [as shown in Eqs.(5) and (6)]. Interestingly, the phononic behavior in the NMW is exactly imitative of the electronic one in quantum Hall effect. The δ-function-like phononic levels in the NMW are analog to Landau levels. Meanwhile, external stretching on the NMW, which tunes the occupation of phononic levels, is analog to the magnetic field tuning Landau levels in quantum Hall effect. The cutoff frequency acts in the NMW just like a "gate voltage" in electronic scenario. In this way, multiple-step quantized thermal conductance can be achieved by tuning the external field.

The above analytical analysis can be demonstrated by the numerical calculation. Based on the transfer-matrix method in a quantum wire,[17] we first calculate frequency spectrum and transmission coefficient of phonons in the NMW under different stretchings. The fix-boundary condition is applied in the calculation. Then we calculate the heat current and the thermal conductance in the NMW according to Eqs. (4) and (5). Figure 2(a) presents the thermal conductance as a function of the stretching (α_{eff}) in a *dimer* wire ($n=2$ in NMW). It is shown that when the stretching is weak enough, the thermal conductance keeps stable on a low level. By increasing the stretching up to around the resonant stretching F_s^{RD}, the thermal conductance jumps. (Here F_s^{RD} is the resonant stretching corresponding to the delocalized frequency $\omega_j=\omega_{\text{RD}}=\sqrt{2\alpha/m_B}$ in the *dimer* wire.) Further increasing the stretching, thermal conductance remains stable on the higher level. Actually, when the stretching is far below

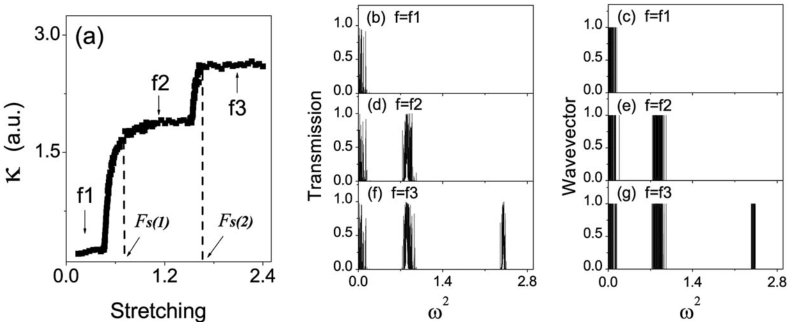

FIG. 3. (a) The thermal conductance κ as a function of the stretching (α_{eff}) in the *trimer* wire (i.e., the NMW with $n=3$), where the total number of atoms is $N=3255$. (b), (d), and (f) illustrate the transmission coefficients of phonons in the same *trimer* wire at different stretching ($f_i, i=1,2,3$), which is marked in the curve of thermal conductance. (c), (e), and (g) illustrate the frequency spectra of phonons in the same *trimer* wire at different stretching ($f_i, i=1,2,3$), respectively. The calculation parameters are the same as those in Fig. 2.

F_s^{RD}, phonons in the wire exists at low frequency only [as shown in Figs. 2(b) and 2(c)]. Once the stretching becomes as large as F_s^{RD}, the cutoff frequency ω_{cutoff} in the central segment reaches the resonant frequency ω_{RD} in the left and right segments. Consequently an additional phononic channel is indeed opened and the quantized heat transfer is achieved [as shown in Figs. 2(d) and 2(e)].

In order to open multiple phononic channels by the stretching, we come to the NMW with larger n. Figure 3(a) presents the thermal conductance versus the stretching in a *trimer* wire ($n=3$). By increasing the stretching, thermal conductance jumps twice around the resonant stretching $F_s(1)$ and $F_s(2)$, respectively [as shown in Fig. 3(a)]. It is known that in the *trimer* wire, there are two localization-delocalization transitions of phonons,[17] which happen around the phononic frequencies $\omega_{\text{RT}}(1)=\sqrt{\alpha/m_B}$ and $\omega_{\text{RT}}(2)=\sqrt{3\alpha/m_B}$, respectively. These two delocalized frequencies correspond to the resonant stretching $F_s(1)$ and $F_s(2)$, respectively. When the stretching is far below $F_s(1)$, phonons exist at low frequency only [as shown in Figs. 3(b) and 3(c)]. When the stretching becomes stronger than $F_s(1)$, the first phononic band occurs in the high-frequency region [as shown in Figs. 3(d) and 3(e)]. This phononic band originates from phononic delocalization at $\omega_{\text{RT}}(1)$ in *trimer* wire, which means that the first phononic channel is opened, and the thermal conductance has the first jump. Further increasing the stretching to $F_s(2)$, the second delocalization of phonons happens at $\omega_{\text{RT}}(2)$, then the second channel of phonons is opened [as shown in Figs. 3(f) and 3(g)], and the thermal conductance has the second jump. Similarly, external stretching can open sequentially three phononic channels in the *quadramer* wire ($n=4$), where thermal conductance presents three steps. In principle, $n-1$ steps of thermal conductance can be found in the NMW by increasing the stretching. Therefore, by increasing the stretching, $n-1$ channels for thermal transfer are opened sequentially in the NMW, and multimode quantized thermal conductance is achieved.

It is possible to find an experimental system with both harmonic and anharmonic potentials, which can also be tuned by stretching or compressing. One of the candidates is a double-stranded DNA,[19] where both harmonic and anharmonic potentials exist simultaneously. Furthermore, DNA molecules are stretchable.[20] We expect that in such a system multimode quantized thermal conductance can be realized by external stretching.

In summary, we have demonstrated theoretically the field-dependent multimode quantized thermal conductance in a quantum wire. Our research presents a possibility to design a smart material that may tune the thermal conductance by itself upon thermal expansion, and hence manipulate heat transfer in the system. What is more interesting is that based on the system, where multiple phonon channels are tuned by external field, it is possible to design kinds of functional devices of phonons. Future studies may provide the in-depth understanding of microscopic laws of heat transfer, and contribute to design functional thermal-conductive materials and also develop information theory on heat.

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