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Delocalization of phonons and quantized thermal conductance in a random *n*-mer system

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In this paper we report the phononic transport and its influence on thermal conductance in a one-dimensional random *n*-mer system. Based on an elastic wave equation, we studied frequency spectrum, phononic transmission, and thermal conductivity of the system. Multiple resonant transmissions are observed, which originate from delocalization of phonons in the correlated disorder system. At each resonant mode, zero-Lyapunov exponent and undecayed vibration of atoms have been found through the whole chain. Meanwhile channels are opened for phonon transmission and heat transport. As a result, thermal conductance is significantly enhanced at each resonant mode, forming a quantized feature as frequency increases. These properties demonstrate the possibility of manipulating phonon propagation and thermal conductance in phononic bandgap materials and may have potential applications in designing filter and waveguide for acoustic waves.

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I. INTRODUCTION

The concept of electronic localization was initially proposed by Anderson in 1958 in dealing with electronic problem in one-dimensional (1D) disordered systems.[1] Since then, some interesting issues have been added into the localization problem. First, localization is found to be a common feature of any waves transporting in a disordered structure. It may exist in acoustic waves[2] and optical waves[3] in addition to the electron system. Second, localization of wave appears not only in disordered systems, but also in deterministic aperiodic systems, such as quasiperiodic structure,[4] incommensurate Aubry-Andre system,[5] and deterministic aperiodic Rudin-Shapiro system.[6] Third, localization demonstrates potential applications. For example, for last two decades, extensive studies have been carried out in photonic localization[7] and photonic band gaps in photonic crystals[8,9] with the aim to develop optoelectronic devices for future telecommunication.[10,11] Propagation of photons is forbidden in a photonic band gap (PBG), which makes it possible to manipulate photons by specific microstructure. Similarly, phononic band gap, in which propagation of phonons is forbidden, has attracted much attention in very recent years. Most of these studies focus on the elastic wave propagation in PBG materials, i.e., phononic crystals and quasicrystals, in order to control the propagation of acoustic waves and develop the phononic devices.[12–15]

The localization-delocalization transition of electron was first predicted by Dunlap *et al.* in 1D random-dimer (RD) model in 1990.[16] It was shown that extended states may exist in the system with correlated disorder. Recently, electronic delocalization has been experimentally demonstrated in RD GaAs-AlGaAs supperlattice.[17] Up to now, RD model has been generalized to twined disordered system, random trimer, random dimer-trimer, even random *n*-mer model.[18] Physically, electronic delocalization in RD-like systems originates from the internal structural symmetry of the impurity cluster. This short-range correlated disorder can make the localization length comparable to the length of the system at the resonant energy.[16,19] The RD-like model may also explain the high conductivity in some polymers.[19] Motivated by the localization-delocalization transition of electrons, we are interested in the property of phonons in PBG materials with correlated disorder. In this paper, we report phononic transport and its influence on thermal conductance in 1D random *n*-mer systems. It is shown that phononic delocalization indeed happens in random-dimer, random-trimer, and even random *n*-mer systems. The phononic delocalization induces the resonant transmission of acoustic waves in these systems with correlated disorder. At resonant frequencies, channels are opened for phonon transmission and heat transport. Thereafter, thermal conductance is enhanced at each resonant mode. Thermal conductance is finally quantized in the infinite random *n*-mer systems.

This paper is organized as follows. In Sec. II, a theoretical model based on elastic wave equation is presented. In Sec. III, phonon transmission and frequency spectra are given as an example in random-dimer (RD) system. The phononic delocalization is discussed based on undecayed vibration at the resonant mode. In Sec. IV, the RD model is generalized to random-trimer, random-tetramer, and random *n*-mer chains. Phonon transmission and thermal conductance are derived in these systems. The delocalization of phonons is discussed based on zero-Lyapunov exponent at the resonant modes. In Sec. V, finite-temperature effect of thermal conductivity is discussed. Finally, a summary is given in Sec. VI.

II. THE THEORETICAL MODEL

Consider a harmonic chain that contains two types of atoms A and B with masses m_A and m_B, respectively. The atoms A and B are arranged sequentially and connected by spring in the chain. The equation of atomic motion can be expressed as

$$-m_i\omega^2\mu_i = k_{i+1,i}(\mu_{i+1}-\mu_i) + k_{i,i-1}(\mu_{i-1}-\mu_i), \qquad (1)$$

where μ_i is the vibration displacement of the ith atom from its equilibrium, m_i is the mass of the ith atom, ω is the vibration frequency, and $k_{i+1,i}$ is the strength of the harmonic coupling between neighbor atoms. In this paper, we focus on the on-site model where $k_{i+1,i}$ is set as a constant, i.e., $k_{i+1,i}=k$, and $m_i=m_A$ (or m_B) if atom A (or B) occupies the ith site in the chain. Equation (1) can be expressed in a matrix form as

$$\begin{pmatrix} \mu_{i+1} \\ \mu_i \end{pmatrix} = P_i \begin{pmatrix} \mu_i \\ \mu_{i-1} \end{pmatrix}, \tag{2}$$

with

$$P_i = \begin{pmatrix} 2 - m_i\omega^2/k & -1 \\ 1 & 0 \end{pmatrix}, \tag{3}$$

where P_i is the transfer matrix that correlates the vibration displacements of adjacent sites μ_i and $\mu_{i\pm1}$. Therefore, atomic vibration in the whole chain is determined by a product matrix, i.e., a global transfer matrix

$$G(N,\omega) = \Pi_{i=1}^{N} P_i \equiv \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}, \tag{4}$$

where N is the number of atoms in the chain.

Let us define the trace of global transfer matrix G as TrG. The allowed region of phonons in the frequency spectrum satisfies

$$\left| \frac{1}{2} TrG \right| \leqslant 1. \tag{5}$$

Using unitary condition $\det|G|=1$, we can obtain the transmission coefficient of phonon through the whole chain. The transmission coefficient $t(N,\omega)$ can be expressed as

$$t(N,\omega) = \frac{4}{\sum_{i,j=1}^{2} g_{ij}^2 + 2}. \tag{6}$$

Based on Eqs. (3)–(6), frequency spectrum and transmission of phonons in the harmonic chain can be numerically obtained.

It has been established that phononic transmission directly determines the heat transport in a harmonic chain. In a macroscopic system, thermal conductivity κ is related to heat transport J by Fourier's law as $\kappa=J/\nabla T$, where ∇T is gradient of temperature in the system. Fourier's law is well established in the macroscopic system, but remains ambiguous on the microscopic scale. Yet it provides an adequate phenomenological description of heat transport in the system.[20,14] In a harmonic chain, Fourier's law takes the form in the "global" sense as[21]

$$\kappa = \frac{J}{c\Delta T}, \tag{7}$$

where ΔT is the temperature difference between two heat reservoirs connected by the chain, and c is a factor measuring the time interval between collisions in the reservoirs and is much smaller than unity. Thermal conductivity κ is contributed by different modes of energy transport, i.e.,

$$\kappa = \sum_{\gamma} (\xi_{\gamma,1}^{-2} + \xi_{\gamma,N}^{-2})^{-1}, \tag{8}$$

where $\xi_{\gamma,n}=\sqrt{m_n}U_{\gamma,n}$, $U_{\gamma,1}$ and $U_{\gamma,N}$ are amplitudes of the γth mode at both ends of the chain, respectively. Obviously, thermal conductivity is related to the transmission coefficient of each mode and the vibration amplitude of atom at the ends of the chain.

III. THE CASE OF RANDOM-DIMER (RD)

Now we consider a random-dimer (RD) chain, where atom A and paired atoms BB are randomly assigned in a chain as

$$\underbrace{A\ldots A}_{X_1}\underbrace{BB\ldots BB}_{Y_1}\underbrace{A\ldots A}_{X_2}\underbrace{BB\ldots BB}_{Y_2}\ldots\underbrace{A\ldots A}_{X_i}\underbrace{BB\ldots BB}_{Y_i}\ldots\underbrace{A\ldots A}_{X_m}\underbrace{BB\ldots BB}_{Y_m}. \tag{9}$$

X_j in Eq. (9) is the number of atom A in the jth cluster of A, which is random. $Y_j=2Z_j$ is the number of atom B in the jth cluster of B, which is even because atom B exists in pairs in the RD chain. According to Eqs. (3)–(6), frequency spectrum and transmission coefficient of phonons can be numerically calculated in the RD chain. In the calculation, the masses of atom A and B are set as $m_A=1$ and $m_B=2$, respectively, the strength of harmonic coupling between neighboring atoms is set as $k_{i+1,i}=k=2$. Figures 1(a) and 1(b) show, respectively, the phononic transmission and the frequency spectrum in the RD chain. The nonzero transmission coefficient (shown in Fig. 1(a)) corresponds to the allowed "band" of phonons [shown in Fig. 1(b)]; while zero transmission corresponds to the forbidden zone, i.e., the phononic bandgap. It is well known that in a random chain, phonon cannot propagate in high-frequency region [as shown in Fig. 1(c)]. By comparing to Figs. 1(b) and 1(c), it is obvious that a new phononic "band" appears in frequency spectrum of the random-dimer (RD) chain. Actually, this new band will be reduced to be a single mode in an infinite RD chain. For a finite RD chain, however, there exist multiple extended states in this frequency zone. Therefore, the new band appears in the frequency spectrum. This feature indicates that the localization-delocalization transition of phonons may take place at specific frequencies in a RD chain.

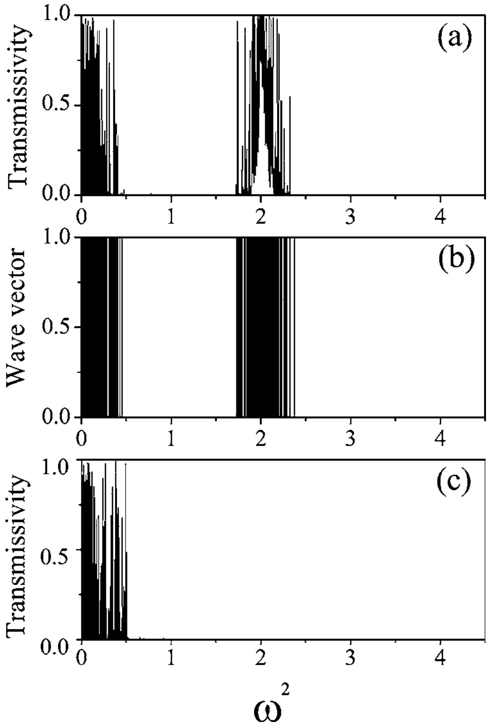

FIG. 1. (a) The transmission coefficient in a random-dimer (RD) chain. (b)The frequency spectrum for the same RD chain. (c) The transmission coefficient in a random chain. Here, $m_A=1$, $m_B=2$, $k_{n+1,n}=k=2$, and the total number of atoms $N=1550$ in each chain.

Actually in RD case, the global transfer matrix can be rewritten as

$$G(N,\omega)=(P_A)^{X_1}(P_B)^{Y_1}(P_A)^{X_2}(P_B)^{Y_2}\cdots (P_A)^{X_i}(P_B)^{Y_i}\cdots(P_A)^{X_m}(P_B)^{Y_m}. \tag{10}$$

Here P_A (or P_B) is the matrix P_i in Eq. (3) when m_i equals to m_A (or m_B), and $Y_i=2Z_i$ ($i=1,2,\ldots,n$ and Z_j is an integer). According to the matrices theory, the qth power of 2×2 unimodular matrix P_B can be simplified as[22]

$$(P_B)^q=c_{q-1}(\chi)P_B-c_{q-2}I, \tag{11}$$

where

$$\chi\equiv\tfrac{1}{2}Tr(P_B)=\tfrac{1}{2}(2-m_B\omega^2/k). \tag{12}$$

I is the unit matrix, and c_q is the qth Chebyshev polynomial of the second order. If $|\chi|\leqslant1$, c_q can be expressed as

$$c_q=\sin(q+1)\theta/\sin\theta \quad (\theta=\arccos\chi). \tag{13}$$

For $q\geqslant2$, if

$$\chi=\chi_p=\cos\left(\frac{p}{q}\pi\right),\quad p=1,2,\cdots,q-1, \tag{14}$$

we obtain $c_{q-1}(\chi_p)=0$ and $c_{q-2}(\chi_p)=(-1)^{p+1}$. In this case, Eq. (11) turns to

$$(P_B)^q=(-1)^pI,\quad p=1,2,\cdots,q-1. \tag{15}$$

Because atom B appears in pairs in the RD chain, we have

$$(P_B)^{Y_j}=[(P_B)^2]^{Z_j}. \tag{16}$$

Based on the above matrix theory, we can simplify the second power of 2×2 unimodular matrix P_B, i.e., $(P_B)^2$ in the globe matrix. It follows that when

$$\omega^2=\omega_{RD}^2=2k/m_B, \tag{17}$$

the matrix $(P_B)^{Y_j}$ satisfies

$$(P_B)^{Y_j}=[(P_B)^2]^{Z_j}=(-1)^{Z_j}I. \tag{18}$$

Therefore, global transfer matrix becomes

$$G(N,\omega)=(P_A)^{\Sigma_iX_i}\text{ or }-(P_A)^{\Sigma_iX_i} \tag{19}$$

Physically, once the frequency of phonon satisfies Eq. (17), the phonon can propagate through the whole RD chain. Meanwhile the behavior of phonon in the RD chain is similar to that in a homogeneous atom chain of atom A. From this point of view, localization-delocalization transition of phonons indeed takes place at the resonant frequency given by Eq. (17).

In order to demonstrate localization-delocalization transition of phonons in a RD chain, spatial distribution of vibration amplitudes is obtained by using triangular matrix.[23] Figure 2 illustrates the vibration amplitude of atom at each site of a RD chain. It turns out that when phonon possesses a frequency close to $\omega_{RD}=\sqrt{2k/m_B}$, the vibration amplitude is extendedly distributed in RD chain and vibration propagates through the whole RD chain without decay [as shown in Figs. 2(a) and 2(b)]. Figure 2 also provides critical amplitude distributions [as shown in Figs. 2(c) and 2(d)] and localized amplitude distributions [as shown in Figs. 2(e) and 2(f)] when the frequency of phonon deviates from the resonant frequency ω_{RD}. In those cases, vibration cannot propagate in the whole chain [as indicated in Figs. 2(c) and 2(f)]. Therefore, at the resonant frequency ω_{RD}, the localization-delocalization transition of phonons occurs indeed in the RD chain.

Delocalization of phonons inevitably affects the thermal conductivity in the RD chain. Figure 3 illustrates thermal conductivity as a function of frequency through a random chain and a random-dimer (RD) chain, respectively. Comparing to the thermal conductivity in a random chain [shown in Fig. 3(a)], an enhancement of thermal conductance around resonant frequency $\omega_{RD}=\sqrt{2k/m_B}$ in RD chain [shown in Fig. 3(b)] can be identified. According to Eq. (8), thermal conductivity relates to the vibration state of atoms. Actually, only the extended state contributes to the heat transfer. In the RD case, localization-delocalization transition of phonons occurs at the resonant frequency, around which the extended state appears in the chain [as shown in Figs. 2(a) and 2(b)]. As a result, thermal conductance is enhanced at the zone of resonance. According to Eqs. (1)–(8), enhancement of κ can be estimated as

$$\Delta\kappa=\int_{\omega_{RD}-\Delta\omega/2}^{\omega_{RD}+\Delta\omega/2}\frac{t^2(\omega)}{t^2(\omega)+1}U_1^2(\omega)d\omega\cong\frac{1}{2}U_1^2(\omega_{RD})\cdot\Delta\omega,$$

where $\Delta\omega$ is the zone of resonance, $U_1(\omega_{RD})$ is the amplitude of the first atom in the chain at resonant frequency and

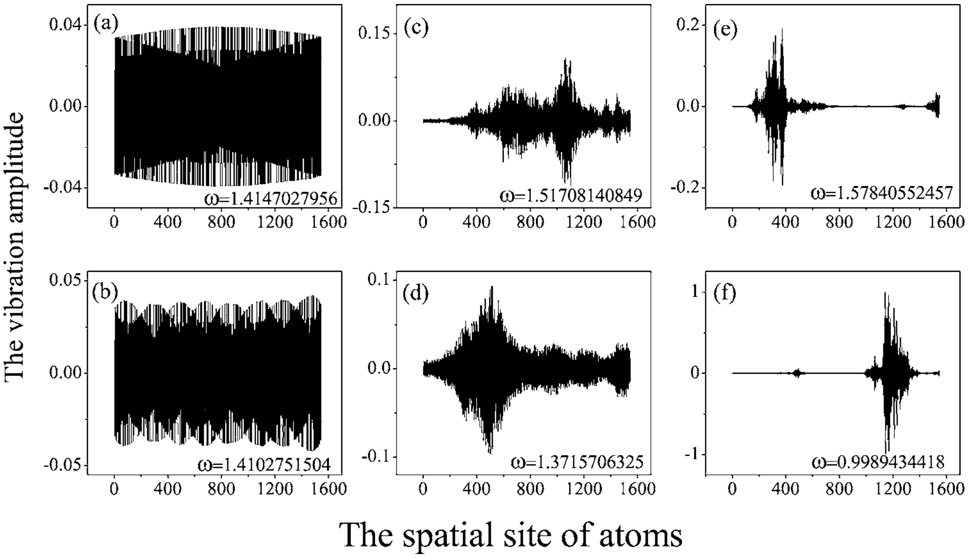

FIG. 2. The vibration amplitude of atom at each spatial site in a RD chain with $N=1550$. (a) and (b) the extended distributions around the resonant frequency $\omega_{RD}=\sqrt{2k/m_B}=\sqrt{2}$; (c) and (d) the amplitude distributions between the extended and the localized states away from the resonant frequency ω_{RD}; (e) and (f) the localized distributions away from the resonant frequency ω_{RD}. Here, $m_A=1$, $m_B=2$, and $k_{n+1,n}=k=2$.

$m_1=m_N=1$ is held. (Obviously, $\Delta\omega=\delta(\omega-\omega_{RD})$ in an infinite RD chain). Therefore, adjacent to the resonant frequency, a new channel is opened for phonon transmission and heat transfer.

IV. THE CASES OF RANDOM *n*-MER

To generalize the RD model, we construct random n-mer (RN) model, where atom A and atoms $B\ldots B$ (the number of atom B is n) are randomly assigned in the chain. The RN model can be described as Eq. (9), where X_j (or Y_j) is the number of atom A (or B) in the jth cluster of A (or B). Obviously, $Y_j=2Z_j$ in the random-dimer model, $Y_j=3Z_j$ in the random-trimer model, and in general $Y_j=nZ_j$ in the random n-mer (RN) model, respectively. Here Z_j is an integer. According to the matrix theory shown in Eqs. (10)–(15), localization-delocalization transition of phonons takes place in RN chain at resonant frequencies

$$\omega_R^2(n)=\frac{2k}{m_B}\left(1-\cos\frac{g\pi}{n}\right), \tag{20}$$

where $g=1,2,\ldots,n-1$. For example, there are two resonant frequencies in the random-trimer chain, i.e., $\omega_R^2=k/m_B$ and $\omega_R^2=3k/m_B$. There are three resonant frequencies in the random-tetramer chain, i.e., $\omega_R^2=(2-\sqrt{2})k/m_B$, $\omega_R^2=2k/m_B$, and $\omega_R^2=(2+\sqrt{2})k/m_B$, respectively. For random 5-*mer* chain, four resonant frequencies exist, which are $\omega_R^2=(3-\sqrt{5})k/2m_B$, $\omega_R^2=(5-\sqrt{5})k/2m_B$, $\omega_R^2=(3+\sqrt{5})k/2m_B$, and $\omega_R^2=(5+\sqrt{5})k/2m_B$, respectively. At these resonant frequencies, vibration of atoms can propagate through the whole RN chain and new channels are opened for phonon transmission and heat transport.

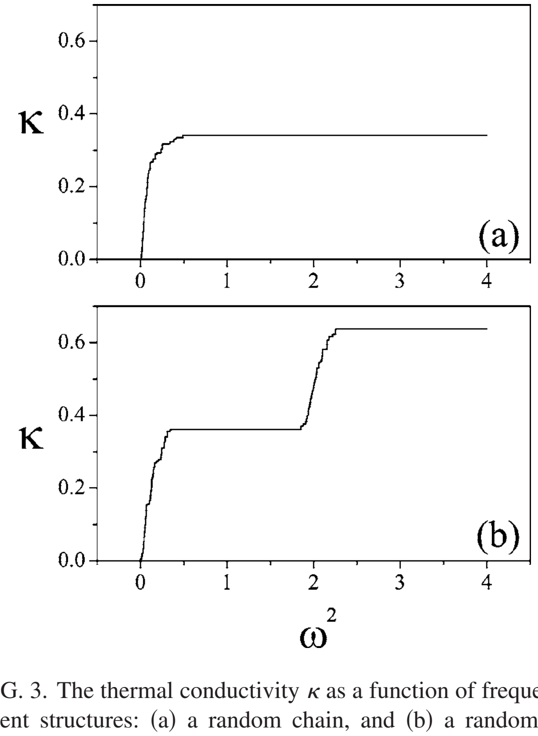

FIG. 3. The thermal conductivity κ as a function of frequency in different structures: (a) a random chain, and (b) a random-dimer chain. Here, $m_A=1$, $m_B=2$, $k_{n+1,n}=k=2$, and the total number of atoms $N=1550$ for each chain.

Figure 4 presents phononic transmission and thermal conductivity as a function of frequency through several RN chains. Because of delocalization of phonon at resonant frequencies, $n-1$ resonant peaks appear in the transmission spectrum of the RN chain [as shown in Figs. 4(a)–4(d)]. For instance, there is one transmission peak in the spectra of a random-dimer chain, two peaks in a random-trimer chain, three peaks in a random 4-*mer* chain, and four peaks in a random 5-*mer* chain, respectively. As discussed in Sec. III, adjacent to the resonant frequency, new channel is opened for phonon transmission and heat transport. Therefore, thermal conductivity has an enhancement around each resonant frequency [as shown in Figs. 4(a)–4(d)]. The enhancement of thermal conductivity can be estimated. The thermal conductivity comes from the contribution of different modes, at which phonon can propagate through the whole chain. According to Eq. (8), contribution of each extended state can be expressed as $\kappa_\gamma=(\xi_{\gamma,1}^{-2}+\xi_{\gamma,N}^{-2})^{-1}=[t^2/(t^2+1)]U_{\gamma,1}^2$ (here we assume $m_1=m_N=1$). If there are N_s extended states, thermal

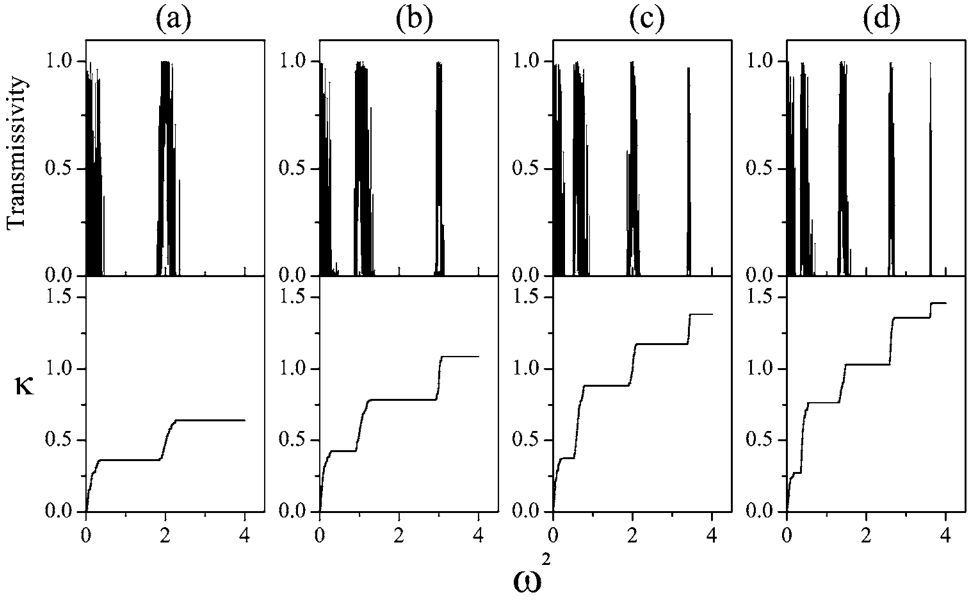

FIG. 4. The transmission coefficient and the thermal conductivity κ as a function of frequency in several random *n-mer* chains with $m_A=1$, $m_B=2$, and $k=2$. (a) A random-dimer (RD) chain with $N=1550$, where the resonant frequency satisfies $\omega_{RD}^2=2$; (b) A random-trimer chain with $N=2077$, where the resonant frequencies follow $\omega_R^2=1$ and 3, respectively; (c) A random-tetramer chain with $N=2604$, where the resonant frequencies follow $\omega_R^2=2-\sqrt{2}$, 2 and $2+\sqrt{2}$, respectively; (d) A random 5-mer chain with $N=3131$, where the resonant frequencies follow $\omega_R^2=(3-\sqrt{5})/2$, $(5-\sqrt{5})/2$, $(3+\sqrt{5})/2$, and $(5+\sqrt{5})/2$, respectively. Here, $m_A=1$, $m_B=2$, and $k_{n+1,n}=k=2$.

conductivity is approximately expressed as $\kappa \cong N_s\langle\kappa_\gamma\rangle$, where $\langle\kappa_\gamma\rangle$ is the average of κ_γ. Since the number of extended states around each resonant frequency does not change significantly, the increment of thermal conductance deviate only slightly at each resonant mode. Consequently, thermal conductivity seems "quantized" in the finite RN chain, as indicated in Figs. 4(a)–4(d). The "quantization" of thermal conductivity originates from multiple delocalization of phonons and multiple resonant modes in a random *n-mer* chain. Each delocalization of phonons opens a channel for phononic transport. Hence thermal conductivity enhances at each corresponding resonant frequency. As a result, thermal conductivity increases step by step as the frequency increases.

In an infinite RN chain, localization-delocalization transitions of phonons take place exactly at $n-1$ resonant frequencies shown in Eq. (20). The extended state appears only at those resonant frequencies, and perfect transmission is achieved at corresponding frequencies. Therefore, thermal conductivity enhances at the resonant frequency, and its increment is exactly a quantum of thermal conductivity, $\kappa_q=\frac{1}{2}U_1^2(\omega_R)$, where $U_1^2(\omega_R)$ is the amplitude of the first atom of the chain at the resonant frequency. By increasing frequency, thermal conductivity increases exactly at $n-1$ resonant frequencies. Finally, quantization of thermal conductivity is demonstrated in the infinite RN chain, which originates from multiple delocalization of phonons in the system.

Actually, delocalization of phonons in RN system can also be characterized by zero-Lyapunov exponent at the resonant mode. It is known that one important parameter to characterize the physical nature of random matrices is Lyapunov coefficient.[24] In a harmonic chain, Lyapunov coefficient can be expressed as[14]

$$\Gamma = \frac{1}{N}\ln(g_{11}^2 + g_{12}^2 + g_{21}^2 + g_{22}^2), \tag{21}$$

where g_{ij} $(i,j=1,2)$ is the element of the global matrix $G(N,\omega)$. According to the Furstenberg theorem,[25] Lyapunov coefficient exists and converges to its mean value for sufficiently long chains. In fact, in a vibrational system, Lyapunov coefficient is inverse to the localization length of phonons. Once the length of the sample is sufficiently long, zero Lyapunov coefficient corresponds to delocalized states with infinite localized length. Therefore, based on the Lyapunov coefficient, we can obtain the overall behavior of the phonons, i.e., we can know whether they are localized or delocalized at specific frequencies in the system. Figure 5 shows Lyapunov coefficients as a function of phononic frequency in several RN chains. It can be seen that around resonant frequencies in each chain, Lyapunov coefficient approaches zero even though fluctuation exists [as shown in Figs. 5(a)–5(d)]. Actually, fluctuation can be eliminated when the length of the chain increases. Because the zero Lyapunov coefficient appears at the resonant frequencies, the localized length of phonons is infinite at these frequencies. At these modes, atomic vibration can not "feel" defects in the chain structure, and vibration can propagate through the chain without decay. Therefore, delocalization of phonons occurs at each resonant mode in RN chain, and total number of resonant modes in the system is $n-1$. Each delocalization of phonons opens a channel for phononic transport, which eventually leads to quantized thermal conductivity.

From the above analysis, it is possible to manipulate phonon propagation by introducing random n-mer model. By designing a random n-mer chain, we can select phonons of specific frequencies and obtain high transmission at desired

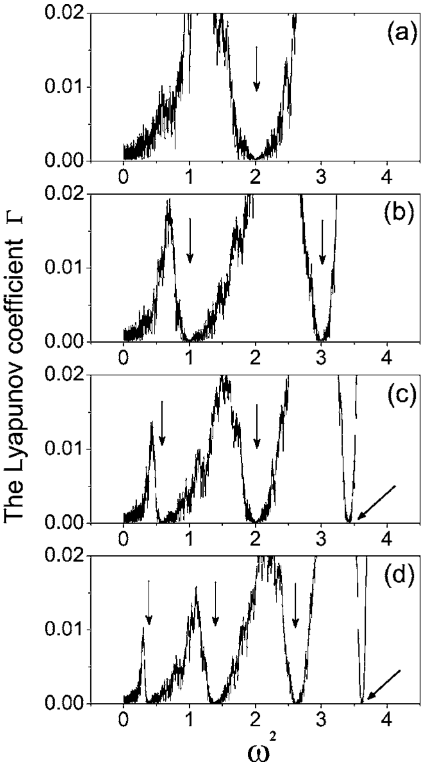

FIG. 5. The Lyapunov coefficient Γ as a function of the frequency in several random *n-mer* (RN) chains with $m_A=1$, $m_B=2$, and $k=2$. (a) A random-dimer (RD) chain with $N=1550$, where $\omega_{RD}^2=2$; (b) A random-trimer chain with $N=2077$, where $\omega_R^2=1$ and 3, respectively; (c) A random-tetramer chain with $N=2604$, where $\omega_R^2=2-\sqrt{2}$, 2, and $2+\sqrt{2}$, respectively; (d) A random 5-mer chain with $N=3131$, where $\omega_R^2=(3-\sqrt{5})/2$, $(5-\sqrt{5})/2$, $(3+\sqrt{5})/2$, and $(5+\sqrt{5})/2$, respectively. Note that zero-Lyapunov coefficient exists adjacent to each resonant frequency in these RN chains as indicated by the arrows.

frequencies. In this way we can tune quantized thermal conductance in the system. This feature implies potential application in designing filters of acoustic waves and developing phononic devices.

V. TEMPERATURE-DEPENDENT THERMAL CONDUCTIVITY

It is interesting to discuss the finite-temperature effect of thermal conductivity. Consider a chain where both ends connecting to thermal reservoir of free phonon gas. At finite temperature, free phonon gas follows Bose-Einstein distribution in thermal reservoir. Heat flow equals to the energy transmitted per unit time from the thermal reservoir to the end atom, which can expressed as[26]

$$J=\lambda(k_BT-m_a\overline{v_a^2}), \tag{22}$$

where T is temperature of the thermal reservoir, k_B is the Boltzmann constant, m_a is the mass of the end atom, $\overline{v_a^2}$ is the average velocity of the end atom, and λ is a coefficient related to the damping force. $\overline{v_a^2}$ can be expressed as $\overline{v_a^2}=k_B/m_a\sum_\gamma[(T_1U_{\gamma,1}^2+T_NU_{\gamma,N}^2)/(U_{\gamma,1}^2+U_{\gamma,N}^2)]U_{\gamma,a}^2$, where $U_{\gamma,a}$ is the vibration amplitude of the end atom at the γth mode. Consider an atomic chain with two ends connecting to the thermal reservoirs with temperature T_1 and T_N, respectively. The heat flow in the chain satisfies

$$J=\lambda k_B(T_1-T_N)\sum_\gamma\frac{U_{\gamma,1}^2U_{\gamma,N}^2}{U_{\gamma,1}^2+U_{\gamma,N}^2}. \tag{23}$$

We suggest that in a harmonic RN chain only those modes with high transmission coefficient contribute to the heat transport, and the amplitude of end atom satisfies $U_{\gamma,v}^2=cf_B(T_v,\gamma)$. Here, $v=1$ or N, $f_B(T,\gamma)$ is the Bose-Einstein distribution. For an infinite RN chain, we have

$$J=\frac{1}{2}\lambda k_B\sum_n\{T_1f_B[T_1,\omega_R(n)]-T_Nf_B[T_N,\omega_R(n)]\}, \tag{24}$$

where the sum covers all resonant modes in an infinite RN chain and transmission coefficient $t[N,\omega_R(n)]=1$ at each resonant mode. Finally, thermal conductivity takes the form of

$$\kappa=\lim_{\Delta T\to 0}\frac{J}{\Delta T}=\frac{1}{2}\lambda k_B\sum_n T\frac{df_B[T,\omega_R(n)]}{dT}\equiv\sum_n\kappa_q. \tag{25}$$

Therefore, the quantum of the thermal conductivity is expressed as $\kappa_q=\frac{1}{2}\lambda k_BTdf_B[T,\omega_R(n)]/dT$. Obviously, the quantum of the thermal conductivity is temperature dependent.

VI. SUMMARY

To summarize, we theoretically investigated the frequency spectrum, the phononic transmission and the thermal conductivity of a random n-mer $(n=2,3,4,\ldots)$. chain. Multiple resonant transmissions are observed, which originates from delocalization of phonons in the correlated disorder system. At each resonant mode, zero-Lyapunov exponent and undecayed vibration of atoms have been found through the whole chain. Meanwhile, channels are opened for phonon transmission and heat transfer. As a result, thermal conductance enhances significantly at each resonant mode, forming a quantized feature as the frequency increases. The phonon behavior presented here provides a possible way to manipulate phonon propagation and thermal conductance in phononic bandgap materials, and may have potential applications in designing filters and waveguide of acoustic waves.

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