Multimode quantized thermal conductance tuned by electric field in a composite polymer

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In this paper, we demonstrate theoretically that an electric-field-dependent multimode quantized thermal conductance can be achieved in a composite polymer in the frame of ballistic phonon transport. The composite polymer consists of three segments, where an ionic polymer is introduced as its central part and the nonpolar polymers are designed on the left and right parts, respectively. By increasing the applied electric field, the dispersion relation of phononic torsion mode is tuned, hence multiple phononic channels are adjusted one by one in the composite polymer. As a result, multiple-step quantized thermal conductance can be manipulated by external electric field. The analysis based on Landauer formula is in good agreement with both the numerical calculations with transfer-matrix method and molecular dynamics simulations. By designing such a three-segment composite polymer, multimode quantized thermal conductance tuned by external electric field becomes an exact analog to multistep quantized electrical conductance tuned by external magnetic field in the quantum Hall effect. The investigations may have potential applications in thermal manipulation and information transfer in mesoscopic phonon systems.

I. INTRODUCTION

Quantized thermal conductance can be achieved when the coherence length of phonons becomes comparable to sample size, which is often analogized to quantized electrical conductance[1,2] in mesoscopic electronic systems. It is well known that, due to the quantum confinement in mesoscopic systems, there exist discrete channels for electron transport, and each ballistic channel contributes a quantum $G_e = 2e^2/h$ to the electrical conductance. Similarly, in mesoscopic phonon systems, thermal conductance of a single channel for phonon transport is limited by its universal thermal conductance quantum $G_Q = \pi^2 k_B^2 T/(3h)$,[3,4] which has been experimentally verified in some nanostructures.[5,6] In the past decades, quite a few investigations on phononoic transport and thermal conductance in mesoscopic systems have been reported.[7–16] However, thermal conductance quantization has two obvious differences compared to electric conductance quantization. First, thermal conductance quantum depends linearly on temperature,[4] whereas the electrical conductance quantum is temperature independent. Second, electrical conductance quantization is demonstrated by a series of conductance steps. For example, in the case of quantum Hall effect, the electrons are confined in a number of discrete Landau levels. The external field (e.g. magnetic field) may change Landau levels of the system. By tuning the external field, multiple Landau levels are reached, and quantum channels are opened sequentially. For phonons, however, thermal conductance quantization is featured by only one plateau of conductance at low-temperature regime,[4,5] i.e. the thermal transport is restricted to acoustic phonon channels. Is it possible to open multiple phononic channels with the help of external fields so we can manipulate heat flux as we do for electrical conductance? The simplest way might be tuning the temperature. However, changing temperature fails to open phononic channels sequentially, since phonons are bosons, and a broader Bose distribution cannot be used to control the occupation of the channels one by one.[17,18] Clearly, alternative approaches have to be explored in order to open multiple phononic channels.

Recently, Cao *et al.*[19] have proposed an approach to realize field-dependent multimode quantized thermal conductance by introducing both harmonic and anharmonic couplings[20–22] to a quantum wire. By stretching or compressing the wire, phononic band structures are tuned and multiple phononic channels are opened one by one. However, practically, it remains challenging to stretch a nanowire homogeneously in a controllable way.

So far, it has been well established that a single polymeric molecule is an attractive system for exploiting thermal conduction in one-dimensional (1D) phononic systems.[23,24] Although bulk polyethylene is a thermal insulator, the thermal conductivity of a single polymer chain can be very high.[25] Very recently, Menezes *et al.*[26] have demonstrated the coupling between high ionic polymers and electric field and proposed a single-molecule field-effect transistor for phonons. Motivated by the fact that an external electric field can influence the lattice vibration in ionic polymers, in this paper, we propose a composite polymer to achieve an electric-field-dependent multimode quantized thermal conductance. The proposed composite polymer consists of three segments, where an ionic polymer is introduced as its central part and the nonpolar polymers are designed on the left and right parts, respectively. We demonstrate theoretically that, by applying external electric field, multimode quantized thermal conductance can be achieved in this composite polymer. It is shown that, when an external electric field is applied to the composite polymer, the dispersion curve of phononic torsion mode is tuned; thereafter, multiple phononic channels are shut down one by one with increasing external electric field. As a result, the multiple-step quantized thermal conductance tuned by external electric field is realized. By designing such a three-segment composite polymer, multimode quantized thermal conductance tuned by external electric field becomes an exact analog to multistep

quantized electrical conductance tuned by external magnetic field in the quantum Hall effect. These investigations may have potential applications in thermal manipulation and information transfer in mesoscopic phonon systems.

In this paper, we start from ballistic phonon transport in the composite polymer and analytically deduce the thermal conductance in the polymer based on Landauer formula in Sec. II. Then by using the transfer-matrix method, we calculate the phononic transmission and the heat current as a function of electric field in the composite polymer in Sec. III. In order to further give direct results, we carry out numerical simulations based on molecular dynamics. The power spectral density of phonons and the heat current vs electric field in the composite polymer are presented in Sec. IV. Finally, a summary is given in Sec. V.

II. THEORETICAL MODEL

We consider the ballistic phonon transport in a three-segment polymer as shown in Fig. 1(a). To couple the external electric field and the system, we select a high ionic polymer as the central one of the three segments, while the left (or right) segment is a random n-mer (RN) chain consisting of nonpolar particles **A** and **B**. Particles **A** and **B** are arranged in such a way that particle **A** and a cluster of n particles **B**...**B** are randomly assigned, known as the RN model.[27] In contrast, the central segment is a single monomer periodic chain composed of highly polar particles **C**.[26] When an electric field is applied to the composite polymer, the coupling between the field and the polar particles **C** breaks the full rotational symmetry of the chain, thus transforming the phononic torsion branch from an acoustic to an optical one. As a result, the transport of the torsion-mode phonons through the whole chain is changed due to its transformed phononic band. This feature makes it possible for us to manipulate phonon-assisted thermal transfer via tuning external electric field.

Now we consider the heat flow carried by phonons in the system. For simplicity, we describe the system analogous to the Kirkwood model.[28] All interaction potentials are chosen to be harmonic, and there are two kinds of interactions, i.e. translation and torsion interactions, respectively. Suppose each monomer unit i has dipole moment $\vec{p}_i$ perpendicular to the chain and a moment of inertia I_i with respect to the chain axis [as shown in Fig. 1(a)]. The Hamiltonian of the system can be expressed as

$$H = \frac{1}{2}\sum_{i \in L,R,C} I_i \dot{\theta}_i^2 + \frac{1}{2}\sum_{i \in L,R,C} K(\theta_{i+1} - \theta_i)^2$$
$$+ \frac{1}{2}\sum_{i \in L,R,C} m_i \dot{x}_i^2 + \frac{1}{2}\sum_{i \in L,R,C} V(x_{i+1} - x_i) + \sum_{i \in C} \vec{p}_i \cdot \vec{E}$$

(1)

where K is the angular restoring force constant in the harmonic approximation, $\vec{E}$ is the applied electric field, and L, R, and C correspond to the left, right, and central segments, respectively. The first two terms are the Hamiltonian of the torsion mode, where θ_i is the torsion angle, and the next two terms correspond to the Hamiltonian of the translation mode, where m_i, x_i, and
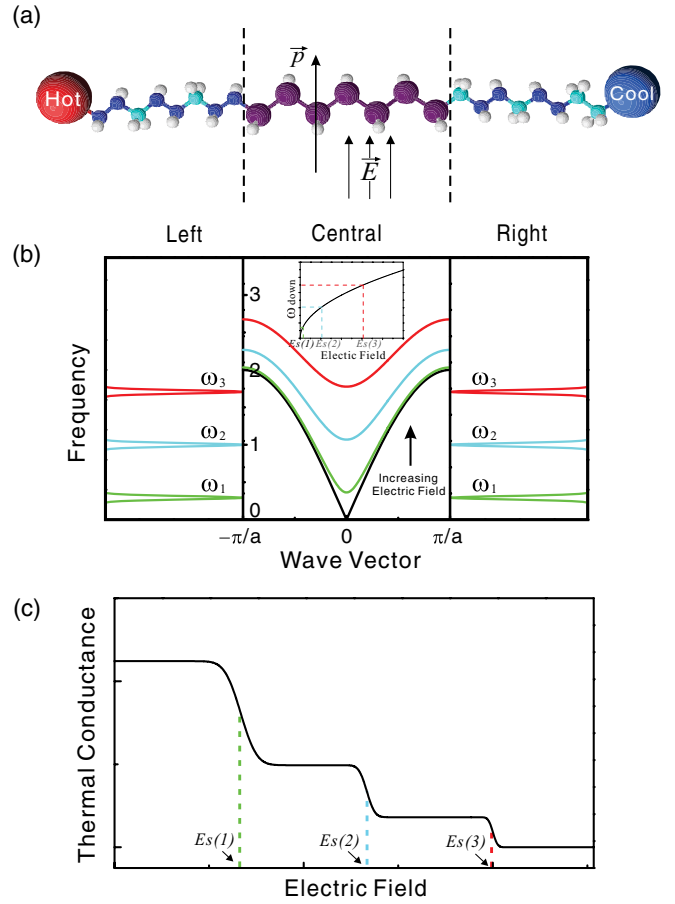

FIG. 1. (Color online) (a) Schematic diagram of a composite polymer (CP), which consists of three segments: the left (or right) segment is a random n-mer (RN) chain consisting of different nonpolar particles **A** and **B**; and the central segment is a single monomer periodic chain composed of highly polar particles **C**. (b) Schematic diagram of tunable phononic transmission modes in the CP. In the left and right segments, multidiscrete resonant modes can be identified around the resonant frequencies ω_j, while in the central segment, phononic band structure (PBS) is tuned by applied electric field, where the down-cutoff frequency ω_{down} moves up by increasing the electric field. The inset shows the relationship of the down-cutoff frequency ω_{down} as a function of the applied electric field. Here, $E_S(j)$ ($j = 1,2,3$) are the resonant fields which correspond to resonant frequency ω_j. (c) Schematic diagram of multimode thermal conductance tuned by external electric field.

V are the atom mass, position displacement, and translation potential, respectively. The last term is the coupling of the applied electric field to the dipole moments of particles. The coupling breaks the full rotational symmetry of the chain, thus changing the dispersion relation of torsion-mode phonons.

Due to the fact that the external electric field does not influence the translation modes, the manipulation of thermal conductance in this composite polymer only relies on tuning the transmission of torsion phonons by the applied electric field. In the following paragraphs of this paper, we will focus on torsion modes. Assuming that the ground-state configuration corresponds to the case that all dipoles are in antiparallel direction of the electric field, the Hamiltonian of the torsion

mode in the harmonic approximation can be expressed as

$$
H_{\text{torsion}} = \frac{1}{2} \sum_{i \in L,R,C} I_i \dot{\theta}_i^2 + \frac{1}{2} \sum_{i \in L,R,C} K(\theta_{i+1} - \theta_i)^2
$$
$$
- \sum_{i \in C} p_C E \left(1 - \frac{\theta_i^2}{2} \right), \tag{2}
$$

where p_C is the dipole moment of the monomer unit in the central segment. For the left (or right) segment, the last term in Eq. (2) equals zero because of nonpolarity of the particles, but for the central segment, the polar particles are coupled with the electric field; then the last term in Eq. (2) becomes nonnull and depends on the applied electric field. It is obvious that this composite polymer can be considered as one-dimensional harmonic oscillators, and the dispersion relation of torsion-mode phonons in the central segment can be described as[26]

$$
\omega = \sqrt{\frac{p_C E + 2K(1 - \cos qa)}{I_C}}, \tag{3}
$$

where q is the wave vector, I_C is the moment of inertia of particle **C**, and a is the lattice constant of the polymer. For zero field, the torsion mode belongs to the acoustic branch with phonon velocity $v = (Ka/I_C)^{1/2}$; while for the positive electric field, the torsion mode has two cutoff frequencies, i.e. a down-cutoff frequency $\omega_{\text{down}} = (p_C E/I_C)^{1/2}$ at $q = 0$ and an up-cutoff frequency $\omega_{\text{up}} = [(p_C E + 4K)/I_C]^{1/2}$ at $qa = \pi$.

The phononic transmission of the whole polymer is determined by the phonons penetrating through all three segments. The left (or right) segment is the RN chain containing particle **A** and cluster **B**...**B**. Due to the localization-delocalization transition of phonons in the RN polymer, phononic transmission occurs at the modes denoted by $\omega_j^2 = 2K/I_B(1 - \cos j\pi/n)$, where $j = 1,2,\ldots,n-1$.[19,27] As a result, discrete multiple resonant modes can be achieved in the RN polymer as shown in the left (right) of Fig. 1(b). For the central segment, when the electric field is applied, there exist both a down-cutoff frequency ω_{down} and an up-cutoff frequency ω_{up}. By increasing the electric field, both cutoff frequencies move up simultaneously, as shown in the central part of Fig. 1(b). The dependence of the down-cutoff frequency ω_{down} as a function of the external electric field is given in the insert of Fig. 1(b). Subsequently, only the modes between these two cutoff frequencies can propagate through the whole polymer. Thus, the effective Hamiltonian of the whole composite polymer is contributed by three parts: translation phonons, localized phonons, and delocalized torsion phonons, i.e.

$$
H = H_{\text{trans}} + H_{\text{loc}} + \sum_{\omega_j \in Q} \hbar \omega_j a_j^+ a_j, \tag{4}
$$

where $a_j^+ a_j$ is the number of delocalized phonons, and ω_j is the resonant frequency given by $\omega_j^2 = 2K/I_B(1 - \cos j\pi/n)$, where $j = 1,2,\ldots,n-1$.[19,27] Here, Q corresponds to the propagating phononic band of the central segment, and Q is between the down-cutoff frequency (ω_{down}) and the up-cutoff frequency (ω_{up}). By increasing the applied electric field from zero to a positive value, the cutoff frequencies move upwards, and the phononic band structure is changed.

Now let us consider the scenario that the composite polymer (CP) is connected to two heat reservoirs with temperatures T_H and T_L, respectively. By taking Eq. (4) to the Landauer formula,[4] the heat current J through a composite polymer can be written as

$$
J = J_{\text{trans}} + \sum_j \int_{\omega_{\text{down}}}^{\omega_{\text{up}}} d\omega \cdot \hbar \omega \delta(\omega - \omega_j) T(\omega)
$$
$$
\times [\eta_{\text{hot}}(\omega) - \eta_{\text{cold}}(\omega)], \tag{5}
$$

where J_{trans} comes from the contribution of translation phonons, and $\eta_{\text{hot/cold}}(\omega)$ is the Bose–Einstein distribution of two heat reservoirs. Here, $T(\omega)$ is the transmission coefficient of the torsion phonon, which depends on phonon scattering in the multichannels. It follows that the thermal conductance can be expressed as

$$
\kappa = \lim_{\Delta T \to 0} \frac{J}{\Delta T} = \kappa_{\text{trans}} + \sum_j \kappa_q \cdot \theta(\omega_j - \omega_{\text{down}})
$$
$$
\cdot \theta(\omega_{\text{up}} - \omega_j), \tag{6}
$$

where κ_{trans} is the contribution coming from the translation phonons, $\theta(x)$ is a step function, [i.e. $\theta(x) = 1$ if $x \geqslant 0$, or $\theta(x) = 0$ if $x < 0$], and κ_q is the quantum of thermal conductance. We can deduce the quantum of thermal conductance as

$$
\kappa_q = \frac{k_B^2 T}{\hbar} \frac{x_j^2 e^{x_j}}{(e^{x_j} - 1)^2}, \tag{7}
$$

where $x_j = \hbar \omega_j / k_B T$, and k_B is the Boltzmann constant. Obviously, the thermal conductance in the composite polymer appears as a series of conductance steps, which can be tuned by the external electric field [as shown in Fig. 1(c)].

If the applied electric field approaches zero, the phononic band structure of the central segment tends to cover all the resonant frequencies of the left and right segments. When the electric field is increased, the down-cutoff frequency ω_{down} moves upward gradually. When the field exceeds the resonant field $Es(j) = I_C \omega_j^2 / p_C$, the down-cutoff frequency ω_{down} is beyond the corresponding resonant frequency ω_j. As a result, the phononic channel corresponding to ω_j is shut down, and the thermal conductance has a jump. Therefore, by increasing the electric field, multiple phononic channels are closed sequentially, and multiple-step thermal conductance is achieved [shown in Fig. 1(c)]. In this way, multiple-step quantized thermal conductance can be achieved by tuning the applied electric field.

III. NUMERICAL SIMULATIONS BASED ON THE TRANSFER-MATRIX METHOD

Numerical calculations have been carried out to verify the above analytical analysis. Based on the transfer-matrix method,[23] we first calculate the transmission coefficient of torsion-mode phonons in the composite polymer by increasing the applied electric field. The motion equation of torsion mode can be expressed as

$$
I_i \ddot{\theta}_i = K(\theta_{i+1} - \theta_i) + K(\theta_{i-1} - \theta_i) - \sum_{c \in C} \delta_{i,c} p_C E \theta_i, \tag{8}
$$

where the last term equals zero for the left and right segments in the composite polymer. Considering $\ddot{\theta}_i = -\omega^2 \theta_i$ in this
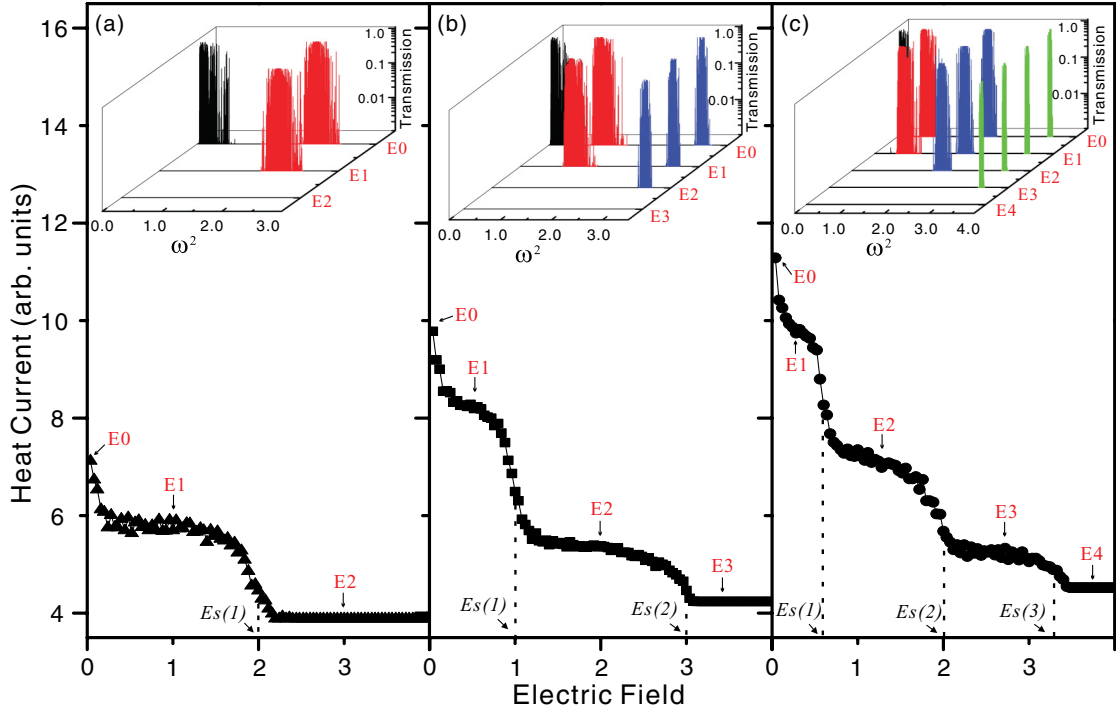
FIG. 2. (Color online) The heat current as a function of the electric field (E/Ec) in the composite polymer with different n. Here, $Ec = 10$ MV/cm. (a) The dimer polymer ($n = 2$). The total number of particles $N = 919$. (b) The trimer polymer ($n = 3$). The total number of particles $N = 1306$. (c) The quadramer polymer (n = 4). The total number of particles $N = 1640$. In all polymers, the number of particles in the central segment $N_C = 200$, and $I_A = 1.0$, $I_B = 2.0$, $I_C = 1.0$, $p_C = 1.0$, $K = 2.0$, the reduced temperature of heat baths as $T_H/T_0 = 0.01$ and $T_L/T_0 = 0.001$. The inserts illustrate the phonon transmission spectra at different applied electric fields which are marked in the curve of heat current.

harmonic system, we can rewrite Eq. (8) in a matrix form as

$$\begin{pmatrix} \theta_{i+1} \\ \theta_i \end{pmatrix} = Q_i \begin{pmatrix} \theta_i \\ \theta_{i-1} \end{pmatrix}, \tag{9}$$

where Q_i is the transfer matrix that correlates with the adjacent rotation angles θ_i and $\theta_{i\pm1}$. For the left (or right) segment and the central segment, Q_i can be expressed as

$$Q_{i \in L,R} = \begin{pmatrix} 2 - I_i\omega^2/K & -1 \\ 1 & 0 \end{pmatrix} \tag{10}$$

and

$$Q_{i \in C} = \begin{pmatrix} (2K + p_C E - I_i\omega^2)/K & -1 \\ 1 & 0 \end{pmatrix}, \tag{11}$$

respectively. Thereafter, the torsion mode through the whole polymer is determined by a global transfer matrix

$$G(\omega) = \prod_{i=1}^{N} Q_i \equiv \begin{pmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{pmatrix}, \tag{12}$$

where N is the number of atoms in the composite polymer.

Based on the global transfer matrix, the transmission coefficient $T(\omega)$ can be expressed as[27]

$$T(\omega) = \frac{4}{\sum_{i,j=1}^{2} q_{ij}^2 + 2}. \tag{13}$$

Suppose the two boundaries of composite polymer are connected with two different fixed-temperature heat reservoirs.

We can numerically obtain $T(\omega)$ based on Eqs. (10)–(13). Then by using Eqs. (5) and (6), we can calculate the heat current and thermal conductance of the composite polymer. Please note that the central region in the system should be large enough in order to achieve continuous phonon modes [given by Eq. (3)] which may couple to the RN modes. Usually, there should be more than 100 particles in the central segment. Figure 2(a) presents the heat current as a function of the applied electric field in a dimer polymer ($n = 2$ in the composite polymer), where the insert illustrates the transmission spectra in different applied electric fields. While the applied field is zero, the heat current presents a comparatively high level. When the applied field is increased gradually, the heat current quickly jumps and then remains stable on a lower level. This quick jump of the heat current originates from the fact that long-wavelength phonons are blocked by the central polymer. By increasing the electric field up to around the resonant electric field $E_S(1)$, the heat current jumps again and remains stable on an even lower level with stronger electric field. Here, $E_S(1)$ is resonant electric field corresponding to the delocalized frequency $\omega_1 = (2K/I_B)^{1/2}$. Further increasing the electric field, the heat current remains stable. However, once the electric field becomes larger than $E_S(1)$, the down-cutoff frequency ω_{down} in the central polymer is beyond the corresponding resonant frequency ω_1. As a result, the phononic channel is shut down, and the heat current has a jump. This feature is essential to shut down the phononic channel and hence to achieve a reduced heat transfer.

In order to manipulate multiple phononic channels by applied electric field, we come to the RN chain with higher n. Figure 2(b) presents the heat current vs the electric field in a trimer polymer ($n = 3$ in the composite polymer), where the insert illustrates the transmission spectra in different applied electric fields. By increasing the electric field, the heat current jumps three times, where two happen around resonant electric fields $E_S(1)$ and $E_S(2)$, respectively. It is known that, in the trimer polymer, there are two localization-delocalization transitions of phonons, which happen around the phononic frequencies $\omega_1 = (K/I_B)^{1/2}$ and $\omega_2 = (3K/I_B)^{1/2}$, respectively. These two delocalized frequencies correspond to the resonant electric fields $E_S(1)$ and $E_S(2)$. When the electric field is nonzero but far below $E_S(1)$, the two channels are both allowed. When the electric field is stronger than $E_S(1)$, the first phononic channel is shut down, and thermal conductance has a jump. Further increasing the electric field to a value beyond $E_S(2)$, the second channel of phonons is shut down, and the heat current has another jump. Similarly, increasing the electric field can shut down sequentially three phononic channels in the quadramer polymer ($n = 4$ in the composite polymer), where the heat current presents three steps as shown in Fig. 2(c). In principle, n-1 steps of thermal conductance can be found in the composite polymer by increasing the electric field. Therefore, multimode quantized thermal conductance which can be tuned by electric field is achieved.

To show the presence of channels for phononic transport in the polymer more clearly, we have analyzed the transmission spectra of phonons vs the electric fields. For example, the phonon transmission spectra of the dimer polymer with different electric fields are shown in the insert of Fig. 2(a). When the electric field is E0, there exist two phononic transmission bands, i.e. the low-frequency band and the transmission band around ω_1 which offers one channel of torsion phonons for the thermal conductance. With the electric field increased to E1 but below $E_S(1)$, the low-frequency phonons are blocked, and only the transmission band exists around ω_1. When the electric field is beyond $E_S(1)$, the transmission is very limited, which means that there is no channel for torsion modes. As a result, the heat current jumps to a lower level. Therefore, we can conclude that, by increasing the electric field, the channels for thermal transfer can be shut down sequentially in the dimer polymer. Similar phenomena can also been observed in the trimer and quadramer polymers [shown in the inserts of Figs. 2(b) and 2(c)], and multimode quantized thermal conductance is finally achieved in the composite polymer by tuning the external electric field.

IV. NUMERICAL SIMULATIONS BASED ON MOLECULAR DYNAMICS

To further verifying the multimode quantized thermal conductance in the composite polymer, molecular dynamics (MD) simulations have also been explored. Compared with the transfer-matrix method, the MD simulation does not rely on the assumption of ballistic phonon transport and can give direct results. We have carried out the numerical simulations based on the dynamical equations of the particles. Firstly, we thermalize the first and last particles in the composite polymer at temperature T_H and T_L ($T_H > T_L$) by using Nosé–Hoover
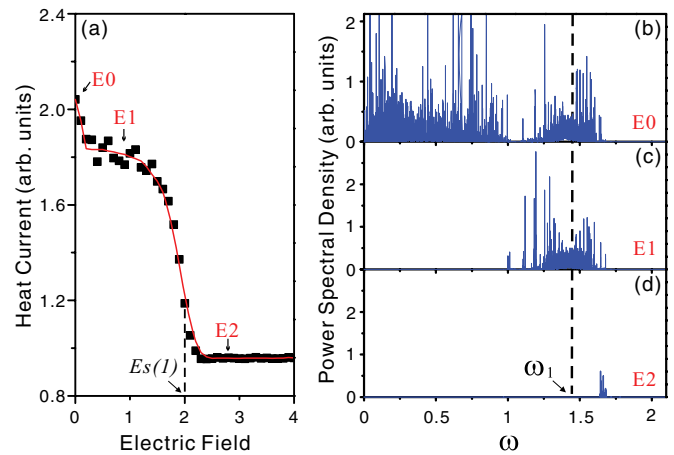

FIG. 3. (Color online) (a) The heat current vs the electric field (E/Ec) in the dimer polymer ($n = 2$) based on MD simulations. Here, $Ec = 10$ MV/cm. The total number of particles $N = 919$, and the number of particles in the central segment $N_C = 200$. Here, E0 = 0, E1 = 1.0, and E2 = 2.7, respectively. (b)–(d) correspond to numerical calculations of the power spectral density of torsion modes in the central segment with applied E0, E1, and E2 electric fields, respectively.

heat baths.[29–31] This heat bath is one kind of deterministic heat bath,[31] and it works as following. Firstly, the particles in the baths are coupled with external restoring forces. Whenever the kinetic temperature of the particles goes up or falls down away from the prescribed temperature, the restoring forces act as dissipation or enhancement, respectively, to make the temperature return to the prescribed one. This process represents a stabilizing feedback around the prescribed temperature. Under Nosé–Hoover heat baths, we integrate the dynamic equations with the fourth-order Runge–Kutta method[32] and achieve the information on phonon transport and the heat current in the system. By this way, the contributions of both torsion and translation modes to the heat current have been included in current MD simulation. However, with increasing the electric field, the contributions from translation modes do not change and give a constant part to the total heat current.

Figures 3–5 present the heat current and the power spectral density of torsion phonons in the dimer, trimer, and quadramer polymers, respectively. For example, Fig. 3(a) presents the heat current as a function of the applied electric field in a dimer polymer ($n = 2$ in the composite polymer). It is obvious that the heat current jumps around the resonant electric field $Es(1) = I_C\omega_1^2/p_C$ and $\omega_1 = \sqrt{2K/I_B}$. As shown in Figs. 3(b)–3(d), we have also calculated the power spectral density of torsion modes in the central segment with applied electric field as E0, E1, and E2, respectively. Here, the power spectral density is obtained by carrying out the Fourier transform of the particle velocity in the central segment. When the applied electric field is E0, there exist both low-frequency band and torsion phonon band around ω_1 [as indicated with the dashed line in Figs. 3(b)–3(d)]. By increasing the applied electric field, the down-cutoff frequency ω_{down} firstly sweeps the low-frequency phonons, then the corresponding channel for low-frequency phonons is closed. Further increasing the applied electric field, ω_{down} sweeps the phonon band around resonant frequency ω_1, and the corresponding channel is closed. Thus, there are two plateaus
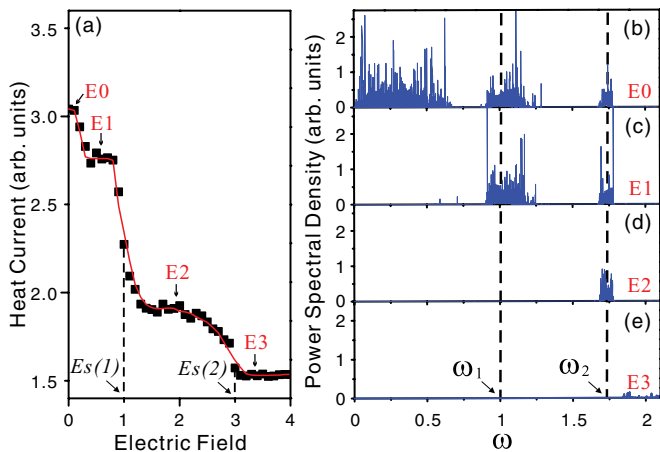
FIG. 4. (Color online) (a) The heat current vs the electric field (E/E_c) in the trimer polymer ($n = 3$) based on MD simulations. Here, $E_c = 10$ MV/cm. The total number of particles $N = 1306$, and the number of particles in the central segment $N_C = 200$. Here, E0 = 0, E1 = 0.5, E2 = 2.0, and E3 = 3.4, respectively. (b)–(e) correspond to numerical calculations of the power spectral density of torsion modes in the central segment with applied E0, E1, E2, and E3 electric fields, respectively.

and two jumps in the heat current curve of the dimer polymer [as shown in Fig. 3(a)].

Figures 4(a) and 5(a) present the heat current vs the electric field in a trimer polymer ($n = 3$ in the composite polymer) and a quadramer polymer ($n = 4$ in the composite polymer), respectively. In the trimer polymer, as shown in Fig. 4(a), the heat current has three plateaus and jumps three times around E0 and two resonant electric fields $E_s(j) = I_C \omega_j^2 / p_C$, where $j = 1, 2$. As shown in Figs. 4(b)–4(e), when the applied electric field is increased from E0 to E3, the phononic
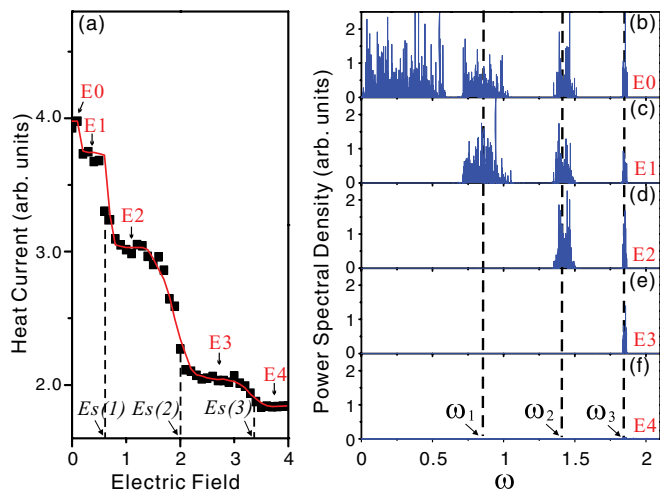

FIG. 5. (Color online) (a) The heat current vs the electric field (E/E_c) in the quadramer polymer ($n = 4$) based on MD simulations. Here, $E_c = 10$ MV/cm. The total number of particles $N = 1640$, and the number of particles in the central segment $N_C = 200$. Here, E0 = 0, E1 = 0.25, E2 = 1.4, E3 = 2.8, and E4 = 3.6, respectively. (b)–(e) correspond to numerical calculations of the power spectral density of torsion modes in the central segment with applied E0, E1, E2, E3, and E4 electric fields, respectively.

channels around the low-frequency regime and also around the resonant frequencies $\omega_1 = \sqrt{K/I_B}$ and $\omega_2 = \sqrt{3K/I_B}$ are shut down sequentially, which leads to three steps in heat current curve. In Fig. 5(a), the heat current of the quadramer polymer ($n = 4$ in the composite polymer) has four plateaus and jumps four times around the low-frequency regime and around three resonant electric fields, respectively. The phononic channels around the low-frequency regime and three resonant frequencies are shut down sequentially by increasing electric field as shown in Figs. 5(b)–5(f). Obviously, the MD simulations shown in Figs. 3–5 are in good agreement with the numerical calculations shown in Fig. 2, which are based on the transfer-matrix method in Sec. III. These two types of approaches have demonstrated that multimode quantized thermal conductance in the composite polymer can be tuned by electric field.

It is interesting to mention that quantized thermal conductance in the composite polymer could be simulated by molecular dynamics which belongs to classical methods. Actually, in our composite-polymer model, due to the localization-delocalization transition of phonons in the RN polymer of the left and right segments, phononic transmission occurs at multiple discrete resonant modes[19] denoted by $\omega_j^2 = 2K/I_B(1 - \cos j\pi/n)$, where $j = 1, 2, \ldots, n - 1$. These resonant modes provide multiple discrete thermal channels, which leads to multimode quantized thermal conductance. This physical picture can be understood in either the quantum or classical point of view. Thereafter, by using the classical MD simulation, we can verify the multimode quantized thermal conductance in the composite polymer.

Actually, both phononic channels and the heat current are strongly influenced by temperature gradient. The opening up of phononic channels relies on the harmonic approximation approach, which only works at the low-temperature regime. By increasing the temperature of the heat baths, the amplitude of particle torsion increases until the harmonic approximation approach fails. Figures 6(a) and 6(b) show the heat current in dimer and trimer polymers with different temperature gradients, respectively. Here, we fix up the low bath temperature (T_L) and change the high one (T_H). When the temperature is low, the heat current has a jumplike response to the increasing electric field, and multiple steps are distinct. By increasing temperature, the jumps on the heat current are weakened, and the steps become unclear. By further increasing T_H, the heat current shows approximately a linear response to the electric field, where the harmonic approximation approach does not work, and the phononic channel becomes uncontrollable.

It is noteworthy that our model may be realized experimentally with high ionic polymers, such as PVDF ($[C_2H_2F_2]_n$), PVC($[C_2H_3Cl]_n$), and PPy($[C_5NH_3]_n$).[26] In high ionic polymers, lattice vibrations couple strongly to the external electric fields. Consequently, the thermal conductance can be effectively tuned by the external electric field. According to Ref. 26, the required electric field for tuning torsion phonons is about 10 MV/cm in the proposed high ionic polymers, which is a typical field for nanoscale field effect devices. Comparing with the stretching-nanowire model,[19] our present model possesses some distinct features. For example, electrical operation allows much faster switching rate and more precise control compared to the mechanical stretching. Furthermore, electric modulation
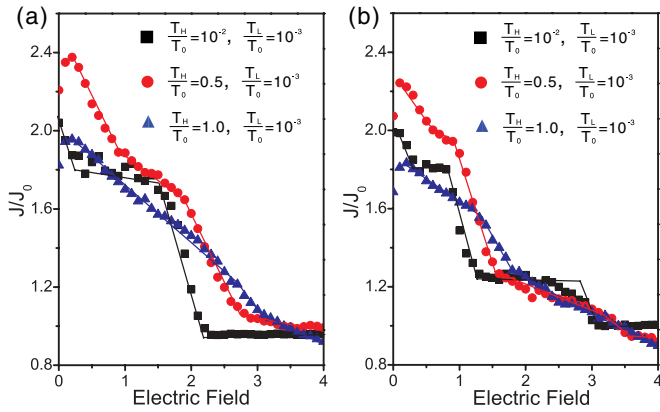
FIG. 6. (Color online) Heat current J vs the electric field (E/Ec) with different temperature gradients: (a) The dimer polymer ($n = 2$). The total number of particles $N = 919$. (b) The trimer polymer ($n = 3$). The total number of particles $N = 1306$. Here, $Ec = 10$ MV/cm, J_0 is the heat current when the applied electric field is 3.5, T_H/T_0 and T_L/T_0 are the reduced temperature of heat baths.

could be easier to manipulate than the mechanical stretching on nanoscale. More interestingly, multimode quantized thermal conductance tuned by external electric field in the composite polymer becomes an exact analog to multistep quantized electrical conductance tuned by external magnetic field in the quantum Hall effect.

V. SUMMARY

We have demonstrated theoretically the field-dependent multiple quantized thermal conductance in a composite polymer. By introducing ionic polymer, we could manipulate the torsion phonon band structure with an external electric field. Through tuning the down-cutoff frequency of the phononic band structure in the central segment by increasing the electric field, multiple phononic channels are shut down sequentially, and multiple quantized thermal conductance steps can be achieved. The analysis based on the Landauer formula is in good agreement with both the numerical calculations from the transfer-matrix method and the molecular dynamics simulations. Our results may have potential applications in nanoscalar thermal manipulation and phonon-assisted information transfer.

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