Heat conduction in simple networks: The effect of interchain coupling

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Heat conduction in simple networks consisting of different one dimensional nonlinear chains is studied. We find that the coupling between chains has a different function in heat conduction from that in electric network (circuit). The two coupled particles form an interface and introduce an interface thermal resistance which reduces the heat current. The reduction of heat current depends sensitively on the position and strength of the coupling. This might find application in controlling heat flow in complex networks.

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I. INTRODUCTION

Energy and information transports in networks, such as the metabolism network, neuronal network, porous material network, and oil production network, etc., have been studied for a long time [1], and are attracting increasing attention in recent years from different fields such as biology, social science, computer science, and physical science [2–8]. It is found that the electric transport changes linearly with the number of added bonds [3,4]. The whole electric resistance of a network can be figured out by the Kirchhoff second law for the complicated parallel and serial electric circuit [5]. However, little is known about heat conduction in the complex networks, although some progress has been achieved for single one dimensional (1D) chains (see Ref. [9] and the references therein).

The fundamental question for heat conduction in one dimensional chains is what is the necessary and/or sufficient condition for the heat conduction to obey the Fourier law? From computer simulations, it is found that in 1D nonlinear lattices with on-site potential such as the Frenkel-Kontorova (FK) model and the ϕ^4 model, the heat conduction obeys Fourier's law, namely, the heat conductivity is size independent [10], which is also called normal heat conduction. Whereas in other nonlinear lattices without on-site potential, thus momentum is conserved, such as the Fermi-Pasta-Ulam (FPU) and similar models, the heat conduction exhibits anomalous behavior [11], namely, the heat conductivity κ diverges with the system size N as $\kappa \sim N^{\delta}$. A great effort has been devoted to understand the physical origin and the value of δ [12]. It is found that the anomalous heat conduction is due to the anomalous diffusion and a quantitative connection between them has been established [13]. Most recently, we found that both the normal and anomalous heat conduction can be described by an effective phonon theory under the same framework [14].

More importantly, it is found that a single 1D chain consisting of two segments of different nonlinear lattices exhibits very interesting physical phenomena such as thermal rectification [15] and negative differential thermal resistance [16]. The classical model of thermal rectification has been extended to a quantum system [17]. The essential ingredients to make thermal rectification (whether it is classical or quantum) are (i) the spatial symmetry breaking, and (ii) the introduction of nonlinearity. The study or rectification has been extended to the mass graded anharmonic lattice [19].

A recent experiment has demonstrated the thermal rectification in a heterogeneous nanotube [18], in which half of the tube has been gradually mass-loaded on the surface with heavy molecules. The result is quite similar to that from mass graded anharmonic lattice [19].

The study on the 1D single chain can be regarded as the first step towards the understanding of heat conduction in realistic physical systems, i.e., complex networks. The second step should be the study of heat conduction on a simple and small network [20,21] and in networks with fractal geometry [22,23], which represent an experimentally testable example of polymer network with fractal geometry.

In general, a complex network consists of many 1D (or quasi-1D) chains with diverse couplings among them. Therefore the key to understand the heat conduction in networks is to understand the influence of coupling to heat fluxes in simple networks, i.e., coupled chains. In this paper, we will first study the case of two coupled chains with both the same and different lengths and then study the case of multiple coupled chains. After that, we study the effect of the self-coupled loop, which appears in the complex networks very often. Our principle results are as follows: (i) The coupling will introduce an interface thermal resistance and thus reduces the heat current. The Kirchhoff second law is applicable only after considering the induced interface resistance, which is different from the situation of electric network (circuit) where no interface resistance is induced and the Kirchhoff second law can be directly applied. (ii) The reduction of heat current depends sensitively on the position and strength of the coupling, which can be figured out by the equivalent thermal circuit. (iii) In the case of single chain with self-coupled loop, the reduction of heat current decreases with the increase of the length of loop. (iv) There is a saturation effect for the coupling strength, which is related to the correlation between the two coupled particles.

The paper is organized as follows. Section II gives the model of coupled chains and presents the numerical simulations. Section III presents the model of a single chain with self-coupled loop and the numerical simulations. Finally, Sec. IV includes the discussion and the conclusions.

II. MODEL OF COUPLED CHAINS

For simplicity, we consider m 1D FPU-β chains [11], with several couplings between any two of them. The two ends of each chain are contacted with the Nose-Hoover thermostat [24] with temperature T_h and T_l, respectively. Without coupling, each chain has a Hamiltonian $H=\sum_i[\frac{1}{2}p_i^2+V_i(x_i,x_{i+1})]$, where $V(x)=\frac{1}{2}x^2+\frac{1}{4}x^4$, x_i represents the displacement from the equilibrium position of the ith particle. The motion of the particles for $i=2,3,\ldots,N-1$ satisfies the canonical equations $\dot{x}_i=\frac{\partial H}{\partial p_i}$; $\dot{p}_i=-\frac{\partial H}{\partial x_i}$. The dynamical equations for the heat baths are $\dot{\xi}_h=\frac{\dot{x}_1^2}{T_h}-1$, $\dot{\xi}_l=\frac{\dot{x}_N^2}{T_l}-1$. The dynamical equations for the first and last particles are $\dot{p}_1=-\frac{\partial H}{\partial x_1}-\xi_h p_1$, $\dot{p}_N=-\frac{\partial H}{\partial x_N}-\xi_l p_N$.

The temperature is defined as $T(i)=\langle p_i^2\rangle$ and the heat flux along the chain is $J=\langle p_i\frac{\partial V}{\partial x_{i+1}}\rangle$. Suppose there is a coupling with strength k between the node i of one chain and the node j of another chain, then we have an additional new potential $V'_{ij}=\frac{k}{2}(x_i-x_j)^2+\frac{k}{4}(x_i-x_j)^4$. The equations of node i and node j become

$$\dot{p}_i=-\frac{\partial H}{\partial x_i}-\frac{\partial V'_{ij}}{\partial x_i}\quad \dot{p}_j=-\frac{\partial H}{\partial x_j}-\frac{\partial V'_{ij}}{\partial x_j}. \tag{1}$$

In our numerical simulations, we take $T_h=3.0$ and $T_l=2.0$ for all the chains and first consider the case of $m=2$, i.e., two coupled chains in this paper, but the results are not limited to $m=2$. The two chains are coupled at different nodes i,j. We find that both the temperature distribution and the total flux in the steady state are changed with the coupling positions and strengths.

Case I: Two chains of the same length coupled together

We consider two identical chains with the same length, $N=20$. Like all models of heat conduction, there are always temperature jumps at the two boundaries [25] which is clearly shown in Fig. 1(a). When two chains are coupled together, regardless of the coupling position (called the junction), there is also a temperature jump at the junction and the coupled particles have roughly the same temperature, see Figs. 1(b)–1(d).

In Fig. 2 we show the corresponding fluxes of Fig. 1 where the arrows denote the directions of fluxes. Figure 2(a) is easy to be understood from their identity, where two uncoupled chains have the same flux. However, Fig. 2(b) shows a very interesting result—the reduction of the heat current. This is completely different from the electric circuit. It is well known that a circuit of two chains with four equal resistance R connected by a conduction line at the middle is a symmetric circuit. Since there is no potential difference between the two connecting points, there is no current through the middle connection line, thus the current in the electric circuit does not change! It remains the same if the two chains are disconnected.

What makes the "thermal circuit" different from the electric circuit? To this end, we need to go to the definition of temperature. The temperature is a measure of the kinetics of the particle, i.e., it is an ensemble (time) average of the kinetic energy. Without coupling, the middle particle at each chain is connected only by its two nearest neighbors. After coupling, the middle particle is connected with three particles which changes its equation of motion. Even though the two particles in the middle have the same temperature (same average kinetic energy and same velocity distribution), it does not mean that the two particles always oscillate in the same way. This is the fundamental difference between the electric circuit and thermal circuit.

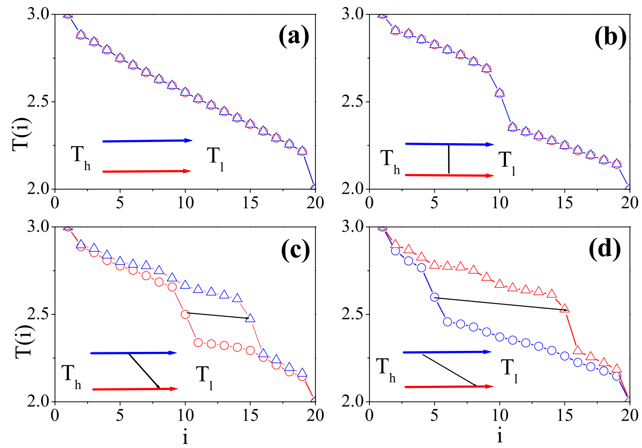

FIG. 1. (Color online) Temperature distributions of two coupled chains of length $N=20$ with $k=1$ and different coupling positions. The thin lines (black) denote the coupling. The insets are the schematic configurations of coupled chains, and the arrows label the direction of heat flow. (a) No coupling; (b) coupling at $i=j=10$; (c) coupling at $i=10$, $j=15$; (d) coupling at $i=5$, $j=15$.

Because the coupled particles subject to an additional force from its coupled partner in another chain, it oscillates differently from that of its neighbors in the same chain. In fact, this is equivalent to the introduction of an interface resistance at the junction. This resistance is also called the Kapitza resistance [26] which is defined as $R_{int}=\Delta T/J$, where ΔT is the temperature jump between the left and right particles of the interface (coupled particle in the middle). For the convenience of analysis, we divide R_{int} into three parts, i.e., R_{int}^l, R_{int}^r, and R_{int}^m which denote the interface resistances

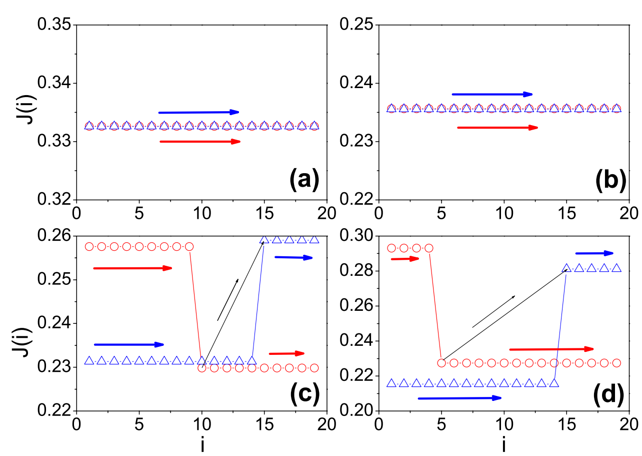

FIG. 2. (Color online) The corresponding fluxes of Fig. 1.

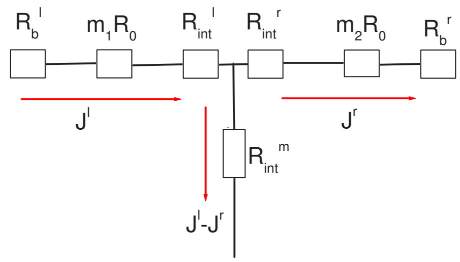

FIG. 3. (Color online) Schematic illustration of the heat resistance circuit in two coupled chains.

between the coupled particle and its three neighbors, respectively. The heat resistance circuit is shown in Fig. 3 where R_0 denotes the thermal resistance between two neighboring particles, $R_b^l = \frac{T_h - T(2)}{J}$ and $R_b^r = \frac{T(N-1)-T_l}{J}$ denote the boundary resistances at the two ends, m_1 and m_2 denote the numbers of free springs between the coupled particle and the two boundaries, respectively, and satisfy $m_1 + m_2 = N-5$. The heat fluxes J^l and J^r in Fig. 3 can be easily expressed as

$$J^l = \frac{T_h - T_c}{R_b^l + m_1 R_0 + R_{int}^l},$$

$$J^r = \frac{T_c - T_l}{R_b^r + m_2 R_0 + R_{int}^r}, \tag{2}$$

where T_c represents the temperature at the junction.

For the special case of symmetric coupling, we have $J^l = J^r \equiv J$, thus the heat current through each chain becomes

$$J = \frac{T_h - T_l}{R_b^l + R_b^r + (N-5)R_0 + R_{int}}, \tag{3}$$

where $R_{int} = R_{int}^l + R_{int}^r$. Obviously, J is less than $J_0 = \frac{T_h - T_l}{R_b^l + R_b^r + (N-3)R_0}$ for the uncoupled chain, $R_{int} > 2R_0$. The physical mechanism of $R_{int} > 2R_0$ can be understood from the following. The coupling is equivalent to adding another load to the oscillator, the oscillator will thus oscillate in smaller amplitude than before.

With the increase of coupling strength k, the disturbance between coupled particles will be larger and results in a larger R_{int}, which leads to more reduction of the flux J.

Without any coupling, the temperature of the ith particle inside the FPU chain is

$$T_i \approx T(2) - \frac{i-2}{N-3}[T(2) - T(N-1)], \tag{4}$$

where $i = 2, \ldots, N-1$. However, with coupling, the temperature distribution becomes

$$T_i \approx T(2) - \frac{i-2}{i_c - 3}[T(2) - T(i_c - 1)], \tag{5}$$

for $i = 2, \ldots, i_c - 1$ and

$$T_i \approx T(i_c + 1) - \frac{i - i_c - 1}{N - i_c - 2}[T(i_c + 1) - T(N-1)], \tag{6}$$

for $i = i_c + 1, \ldots, N-1$, where i_c denotes the coupling position.

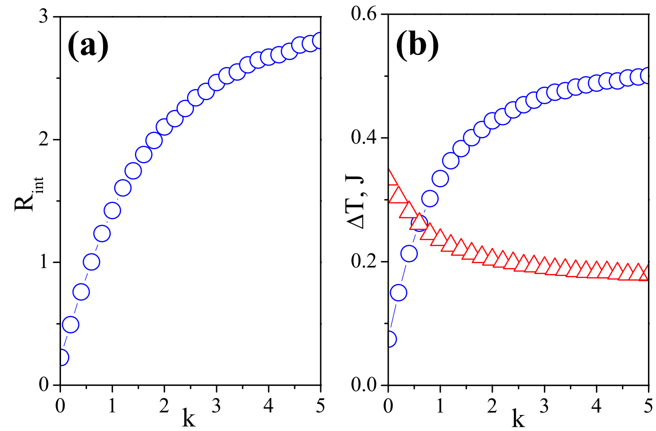

FIG. 4. (Color online) (a) Interface thermal resistance R_{int} vs spring constant k; (b) heat current J and temperature jump ΔT vs k. The circles and triangles denote ΔT and J, respectively. The results are for two identical coupled chains with coupling at the center where parameters are the same as in Fig. 1(b).

The heat current flows at the junction can be understood from Eqs. (4)–(6). For instance, the particle at $i = 10$ has higher temperature than the particle of $i = 15$. Heat always flows from high temperature to low temperature, therefore if one connects the particle $i = 10$ in the upper chain to particle $i = 15$ in the lower chain, there will be a heat current flow from the particle $i = 10$ (higher temperature) in the upper chain to particle $i = 15$ (low temperature) in the lower chain. As the coupling tries to make the connected particles have the approximate same temperature, this will drag the temperature of particle $i = 10$ down a little bit, thus we see the increase of the heat current in the part of $i \in [2, 10]$ in the upper chain in Fig. 2(c) compared with the case in Fig. 2(b). In contrast, as the heat current flows to particle $i = 15$ at the lower chain, the temperature at $i = 15$ is increased, thus the increase of the temperature difference between $i = 15$ and $i = 20$, which leads to the increase of heat current in segment of $i \in [15, 20]$ in lower chain. The exchanged flow at the junction equals the difference of fluxes between the two sides of the junction. This is what we observe in Figs. 1(c) and 2(c). The same mechanism applies also to Figs. 1(d) and 2(d).

To demonstrate the dependence of R_{int} on the coupling strength, we draw R_{int} vs k in Fig. 4(a) where R_{int} increases with k and then it is saturated for large k. The saturation is also reflected in J and ΔT, see Fig. 4(b).

The effect of saturation can be understood from the correlation. Suppose the motion of two neighboring particles are correlated in the absence of coupling (with another chain). The coupling, acting as an external perturbation, will reduce this correlation and hence reduce the flow. When the coupling strength is too strong, the two coupled particles in different chains will become correlated. Therefore the coupling cannot be considered as a pure external perturbation and further increase of k will not affect the correlation anymore. We find that the variation of the relative distance between two neighboring particles may partially reflect this correlation. The possible reason might be that the transfer of heat energy

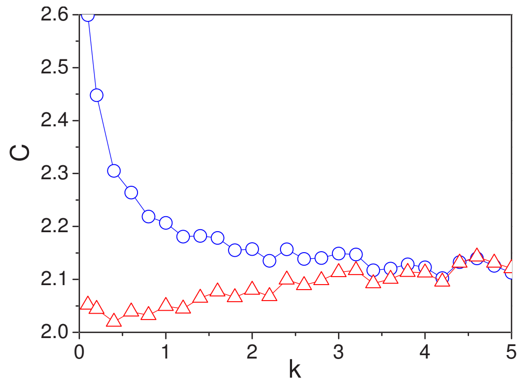

FIG. 5. (Color online) The displacement correlation of two particles in the same chain (circles) and displacement correlation of two particles in two different chains (triangles). The results are for two identical coupled chains with coupling at the center where parameters are the same as in Fig. 1(b).

or flow is through the impact of neighboring particles, i.e., the variation of potential. The flow will reach its maximum when the positions of the neighboring particles have their largest variation at the same time. Therefore we introduce the displacement correlation (for the two particles in the same chain) as follows:

$$C = \langle |x_{i_{c-1}} x_{i_c}| \rangle, \tag{7}$$

where "$\langle \cdots \rangle$" means the time average. We find that C has a similar behavior with the heat flow J (see the circles in Fig. 5). For the two coupled particles in different chains, we use

$$C = \langle |x_{i_c} y_{i_c}| \rangle, \tag{8}$$

to calculate their displacement correlation where x_{i_c} and y_{i_c} are the displacements of the coupled particles in two different chains. The triangles in Fig. 5 shows the result. It is easy to see that the correlation between the two coupled particles becomes saturated for strong coupling and is almost the same value with the correlation from Eq. (7), indicating the further increase of coupling cannot reduce the correlation between the neighboring particles or flow. The reason is that when k is larger than a certain value, the two coupled particles oscillate approximately in the same way.

Case II: Two chains of different lengths coupled together

We extend our study to the more general case, namely, one or multiple couplings in two chains of different lengths. It is found that the reduction of heat flux by couplings is quite general. Figure 6 shows the temperature distribution of two coupled chains with different lengths $N_1=20$ and $N_2=30$, respectively (see Fig. 6 caption for more information). We can see some common features between Figs. 6 and 1, i.e., there are temperature jumps at the coupled particles and the coupled particles have the approximate same temperature. Another interesting thing is that the crossing couplings in Fig. 6(d) make the middle part of the coupled chains appear a temperature plateau which might be useful in heat control.

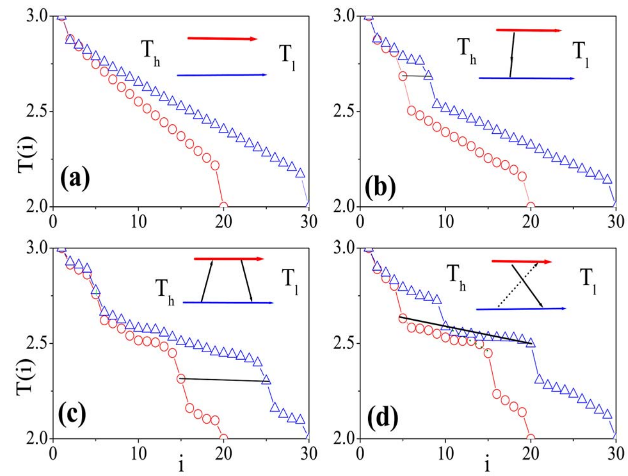

FIG. 6. (Color online) Temperature distributions of two coupled chains with different lengths $N_1=20$ and $N_2=30$ with $k=1$ and different coupling positions. The (thin and dotted) black lines denote the coupling. The insets are the schematic configurations of coupling chains, and the arrows indicate the direction of heat flow. (a) No coupling; (b) one coupling at $i=5$, $j=8$; (c) two couplings at $i_1=5$, $j_1=5$ and $i_2=15$, $j_2=25$; (d) two crossing couplings at $i_1=5$, $j_1=20$ and $i_2=15$, $j_2=10$.

Figure 7 shows the corresponding fluxes of Fig. 6. The longer chain with $N_2=30$ has smaller heat current. In fact, like in the previous cases shown in Figs. 1 and 2, the heat current flow in the (multi)coupled chains of different lengths can be also understood from Eqs. (4)–(6).

We have also checked the heat conduction in multiple chains with a diversity of couplings, such as in the three coupled chains with different lengths, and observed the similar results as in the case of two coupled chains. We conclude that, in general, the coupling will introduce an interface resistance at the junction, thus affect the heat flow through the whole system.

III. MODEL OF SINGLE CHAIN WITH SELF-COUPLED LOOP

Another interesting question is how do the self-coupling or a shortcut in a single chain affect the heat current? This

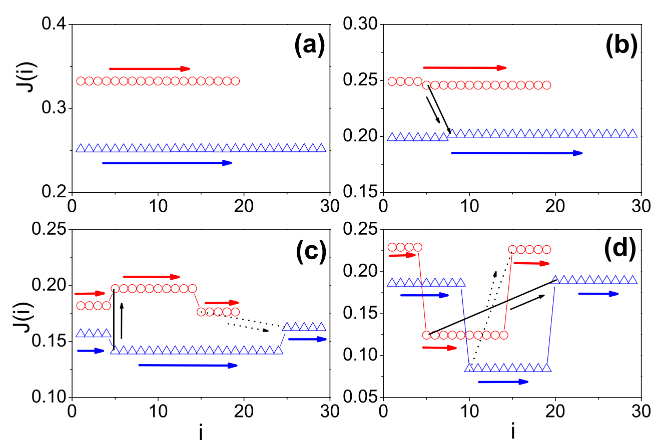

FIG. 7. (Color online) The corresponding fluxes of Fig. 6.

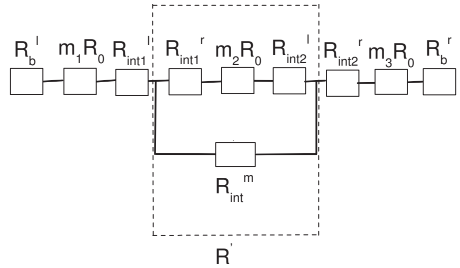

FIG. 8. Schematic illustration of the heat resistance circuit in a chain with self-coupled loop.

may happen in the polymer chain and biological networks [27]. For example, if there is a shortcut between the particle i_1 and the particle i_2 of a chain, does this shortcut reduce the flux? To solve this problem, we first draw the heat resistance circuit as in Fig. 8 where $m_1+m_2+m_3=N-7$. The equivalent resistance R' is given by

$$R' = \frac{R_{int}^m(R_{int1}^r + m_2R_0 + R_{int2}^l)}{R_{int}^m + R_{int1}^r + m_2R_0 + R_{int2}^l}, \tag{9}$$

and the flux can be calculated by

$$J = \frac{T_h - T_l}{R_b^l + (m_1+m_3)R_0 + R_{int1}^l + R' + R_{int2}^r + R_b^r}. \tag{10}$$

From Eq. (10) it is easy to see that the interface resistances induced by the self-coupling will also reduce the heat flux in the single chain. Our numerical simulations have confirmed the prediction, see Fig. 9(a). The "triangles" in Fig. 9(a) is the result with $N=20$, $k=1$, $i=5$, and $j=15$. Comparing it with Fig. 2(a) of no coupling, the flux is significantly reduced. Circles, triangles, and squares in Fig. 9(a) denote

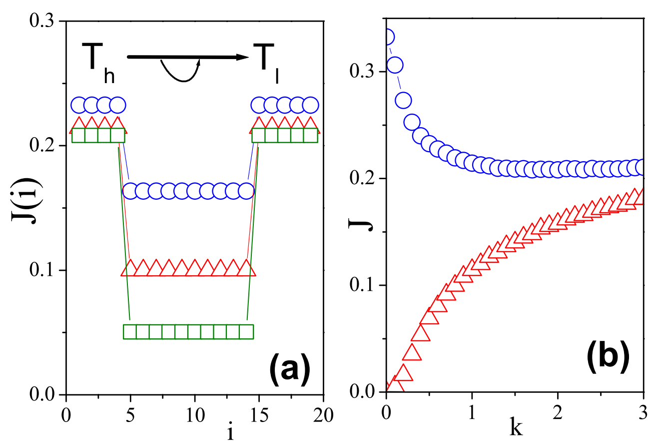

FIG. 9. (Color online) (a) The distributions of flux in a single chain with self-coupled loop. $N=20$, $i_1=5$, and $i_2=15$ where circles, triangles, and squares denote the cases of $k=0.5$, 1.0, and 2.0, respectively. The arrows in the inset of (a) indicate the direction of heat flow; (b) shows how the flux in (a) changes with the coupling strength k where the circles are the total flux and the triangles are the flux through the shortcut.

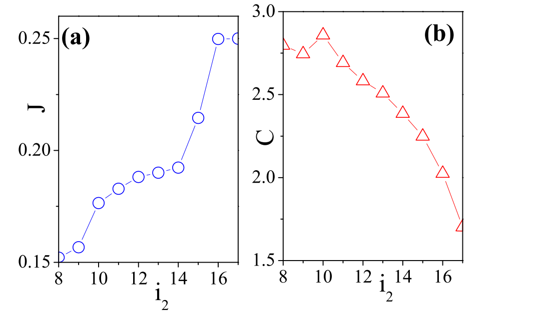

FIG. 10. (Color online) Influence of loop length m_2 for $k=1$ and $i_1=5$ where (a) J vs i_2 and (b) C vs i_2.

the cases of $k=0.5$, 1, and 2.0, respectively. From the middle parts of this figure, we see that large coupling makes less flux go through the original path.

In order to see the influence of coupling strength in more detail, we show flux vs coupling strength k in Fig. 9(b). The circles denote the total flux and the triangles denote the flux going through the shortcut. Obviously, the total flux becomes stabilized when $k>1$ and the flux through the shortcut increases monotonously with k, confirming the saturation effect revealed in Fig. 4.

Except the coupling strength, the length $m_2=i_2-i_1-2$ of the loop may also influence the flux J. For a fixed m_1, from Eq. (10) it is easy to find

$$\frac{dJ}{dm_2} > 0, \tag{11}$$

where $m_3=N-7-m_1-m_2$ is used. Therefore J will increase with m_2. Our numerical simulations have confirmed it, see Fig. 10(a) where i_1 is fixed at $i_1=5$ and i_2 is changed from 8 to 17.

The influence of m_2 on J may be also reflected by the displacement correlation. Here we define the correlation as

$$C = \langle |x_{i_1}x_{i_2}| \rangle. \tag{12}$$

Without coupling, i_1 is less correlated with i_2 for larger m_2. And with coupling, this decreasing relation should be kept although the value of correlation increases a lot because of the coupling. This has been confirmed by numerical simulations; see Fig. 10(b).

IV. DISCUSSIONS AND CONCLUSIONS

In this paper we have studied the influence of coupling in simple networks on the heat conduction. It is found that different from the electric circuit, the coupling affects very much the heat current flow in the thermal circuit. In electronic circuit, if two points have the same electric potential, then when these two points are connected, it will not affect the current through the system. However, in the thermal circuit, even if the two points in different chains have the same temperature, if these two points are connected, the current through the system will be reduced. The reason is that any introduction of coupling is equivalent to an introduction of an interface resistance and thus influences largely the heat current in the circuit. The interface resistance saturates for larger k.

The study given in the current paper, although it is very preliminary, provides an important message—the thermal circuit is very different from the electric circuit.

On the other hand, even though there exists difference between the electric circuit and thermal circuit, thermal diode, and thermal transistor which are similar to electric counterparts can be worked out to control heat flow like we do for electric flow. More importantly, a recent work on the thermal logic gate [28] might overturn a long believe perception that heat is useless and harmful for information transmission and processing. One day, heat can be used as an information carrier and can be processed like electrons and photos.

Therefore the study given in the current paper may shed light not only for studying heat conduction in complex networks and understanding heat conduction in complex material and biological systems, but also may stimulate us to think about how the heat "information" is transmitted in the complex networks.

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