Heat transport in coupled inhomogeneous chains*

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We first investigate the heat transport in a network model consisting of two coupled dimerized chains. Results indicate that the thermal resistance of each chain increases with the decrease of the mass ratio γ of the two types of atoms. Then, we find, when a light impurity or a heavy one is added in the two coupled homogeneous chains and coupled with a particle of another chain, the interface thermal resistances $R^l_{\rm int}$ and $R^r_{\rm int}$ present different dependences on the mass ratio γ'. Finally, a persistent circulation of energy current is observed in coupled inhomogeneous chains with two pairs of interchain coupling.

Keywords: heat transport, thermal resistance

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1. Introduction

In recent years, the problem of heat transport in low-dimensional systems has received a lot of interest not only from a theoretical point of view but also from a practical viewpoint.[1,2] Many numerical simulations have shown that Fourier's law in low-dimensional systems is violated and some of these systems exhibit anomalous heat conduction, especially the "length-dependent" thermal conductivity.[1,3,4] On the other hand, some interesting and promising models, such as the thermal rectifier,[5] thermal diode,[6] thermal transistor,[7] and thermal logic gates,[8] have been designed by coupling with different nonlinear lattice chains for controlling the heat flow. With the promotion of nanotechnology, most recently, Chang *et al.*[2] have experimentally realized a nanoscale solid-state thermal rectification by using gradual mass-loaded carbon and boron-nitride nanotubes based on the two-segment model proposed in Refs. [6] and [9]. These studies can be considered as the first step. Next, a complicated and realistic case will be considered. As is well known, electric circuits have been widely used in our lives. The whole electric resistance of the system can be dealt with as an understandable parallel and serial electric circuit and can be described by the Kirchhoff second law. However, unfortunately, little is known about the thermal transport in a composite or integrated case (e.g., in the thermal circuit[7,10]).

Generally, one-dimensional (1D) lattice models exhibiting some physical counterparts have been extensively used to study heat conduction. Based on previous studies, it is known that in a 1D integrable system, such as the homogeneous harmonic chain[11] and the monoatomic Toda chain,[12] the thermal conductivity κ diverges in the thermodynamic limit and no temperature gradient is formed, because the dominating energy carriers are not scattered and they propagate ballistically. In addition, in some 1D nonintegrable systems, such as the ding-a-ling model,[13] the Frenkel–Kontorova (FK) chain[14] and the discrete ϕ^4 model,[12,15] the thermal conductivity is proved to be finite and heat conduction obeys the Fourier's law. Some numerical calculations suggested that the external substrate potential is extremely significant for normal heat conduction.[16,17] While in some other nonintegrable systems, such as the FPU-β chain[18] and the diatomic Toda model,[19] despite the temperature gradient being built up, the total heat flux along the chains is proportional to N^α, where $0 < \alpha < 1$. They exhibit anomalous heat conduction behaviours. Although the complete understanding of the heat conduction in a low-dimensional system has not been obtained at present, with the contribution of the 1D lattice models many interesting and promising models are constructed[5−8] and an elementary exploration about the heat current flowing in coupled chains is performed by Liu and Li.[20] The model devised by Liu and Li is composed of two coupled homogeneous FPU-β chains. It may serve as a subsystem (or subnetwork) of a realistic complex system (or complex network). The numerical results show that the interface thermal resistance is induced by arbitrary two cou-

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pled particles and reduces the heat currents through the two chains. It is also found that the heat current depends on the position and the strength of the coupling. These results indicate that the behaviour of heat current is very different from electric current. Another simple and nontrivial network model consisting of two coupled inhomogeneous chains is also of both theoretical interest and practical importance. It is well known that the dynamical behaviour of the dimerized chain is different from that of the uniform one.[21] And currently, many 1D materials such as polyacetylene,[22] metallic atomic wires,[23] inorganic compound $CuGeO_3$,[24] display the dimerized configuration, i.e. inhomogeneous structure. Therefore, to make clear the effect of interchain coupling of the network model with coupled inhomogeneous chains will be a guide to further design the thermal circuits and control of heat current. In this paper, the properties of heat transport of coupled inhomogeneous chains are systemically investigated.

2. Model and method

Let us consider a simple model which consists of two parallel coupled 1D dimerized chains with the same length and there may be a coupling between any two particles in different chains (see Fig. 1). Two Nosé–Hoover thermal reservoirs at temperatures T_+ and T_- are adopted and acting on the two ends of each chain. Fixed boundary conditions are assumed for each chain. The Hamiltonian of each isolated (uncoupled) chain is

$$H = \sum_i \left[\frac{p_i^2}{2m_i} + V(x_i - x_{i-1})\right], \tag{1}$$

$$V(x) = \frac{1}{2}x^2 + \frac{\beta}{4}x^4, \tag{2}$$

where p_i denotes the momentum of the i-th particle, x_i is the displacement of the i-th particle from its equilibrium position, m_i denotes the mass of alternate two different particles with $m_{2i} = m$, $m_{2i-1} = \gamma m$, where γ is the mass ratio. $V(x)$ is the quartic Fermi–Pasta–Ulam (FPU) potential, namely FPU-β potential. The single chain represents the simplest anharmonic approximation of the dimerized solid. Then the equations of motion for the oscillators of each chain are given by (without coupling in two chains)

$$\dot{x}_i = p_i/m_i,$$

$$\dot{p}_i = \begin{cases} -\zeta_+\dot{q}_1 + f_1, & i = 1, \\ f_i - f_{i+1}, & 2 \le i \le N-1, \\ -\zeta_-\dot{q}_N + f_N, & i = N, \end{cases}$$
$$f_i = -V'(x_i - x_{i-1}), \tag{3}$$

and $\dot{\zeta}_{\rm L} = M_1\dot{q}_1^2/T_{\rm L} - 1$ and $\dot{\zeta}_{\rm R} = M_N\dot{q}_N^2/T_{\rm R} - 1$ are dynamical equations of heat baths. Then a new coupling between the node i of one chain (chain 1) and the node j of another chain (chain 2) is given. Thus we have a potential

$$V'_{ij} = \frac{k}{2}(x_i - x_j)^2 + \frac{k}{4}(x_i - x_j)^4,$$

where k is the strength of the coupling. For simplicity, in what follows, we will use the subscript index notation: 1 for index of chain 1, 2 for index of chain 2 and i for index of the sequence number of particles in each chain. The average kinetic temperature of a particle is given by $T_1(i) = \langle p_{1,i}^2/m_{1,i}\rangle$, $T_2(i) = \langle p_{2,i}^2/m_{2,i}\rangle$ and the heat flux through the chain is given by $J_1 = j_1(i) = \langle(1/2)(\dot{x}_{1,i+1} + \dot{x}_{1,i})f_{1,i+1}\rangle$, $J_2 = j_2(i) = \langle(1/2)(\dot{x}_{2,i+1} + \dot{x}_{2,i})f_{2,i+1}\rangle$ in steady state, where $\langle\ \rangle$ denotes the ensemble average. Here, the heat flux is equivalent to the energy flux. In computation, we use the time average instead of the ensemble average. The fourth-order Runge–Kutta algorithm is used to solve the differential equations and we take m =1, $\beta = 0.5$, $k = 1$, $T_+ = 0.3$, and $T_- = 0.2$ through this paper except special explanation.

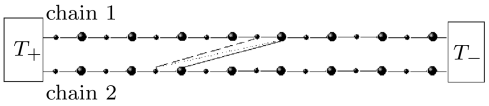


Fig. 1. A schematic model which consists of two coupled 1D diatomic chain and two Nosé–Hoover thermal reservoirs at temperatures T_+ and T_- acting on the two ends of each chain, respectively. Solid line, dashed line and dotted line denote three different coupling forms between the two chains.

3. Simulations and results

We first study the heat transport in the model with mass ratio $\gamma = 0.5$ in the case of three different coupled modes, i.e., coupling between two light particles (L_1L_2, dashed line in Fig. 1), coupling between two heavy particles (H_1H_2, solid line in Fig. 1) and coupling between a heavy particle and a light one (H_1L_2, dotted line in Fig. 1). Figures 2(b)–2(d) show the kinetic temperature profiles of the model with these three different coupled modes, respectively

and in Fig. 2(a) the temperature profile of the system without any coupling between the two chains is also given. They all represent unusual oscillating figures and the lighter particles are hotter than the nearest neighbouring heavier ones in each chain. Comparing Figs. 2(b)–2(d) with Fig. 2(a) it is clear that the two coupled particles in different chains are dragged to have roughly the same temperature. Figures 3(a)–3(d) display the heat fluxes corresponding to Fig. 2 with uncoupling, L_1L_2 coupling, H_1H_2 coupling and H_1L_2 coupling, respectively, from which we know the heat current flows from high temperature to low temperature and the arrows represent the direction of flux. Then we alter the value of the mass ratio γ. The oscillating temperature profiles are also obtained if γ is not equal to unity. In Fig. 4 the heat fluxes are given in the case of γ equal to 0.3, 0.5, 0.7, and 1.0 (solid symbols). It is observed that the heat current always flows from particle 7_2 (high temperature) to particle 10_1 (low temperature). In order to further study the influence of mass ratio on heat flux, we calculate the heat fluxes of the model consisting of two homogeneous chains with a coupling between particle 7_2 and particle 10_1 (the hollow symbols in Fig. 4). The results indicate that decreasing the masses of all particles of the chains synchronously will increase the heat fluxes through the chains. Hence, from Fig. 4 we know that the smaller the mass ratio γ ($\gamma \leq 1$), the smaller the heat fluxes through each chain. In other words, the thermal resistance of each chain increases with the decreasing mass ratio γ.

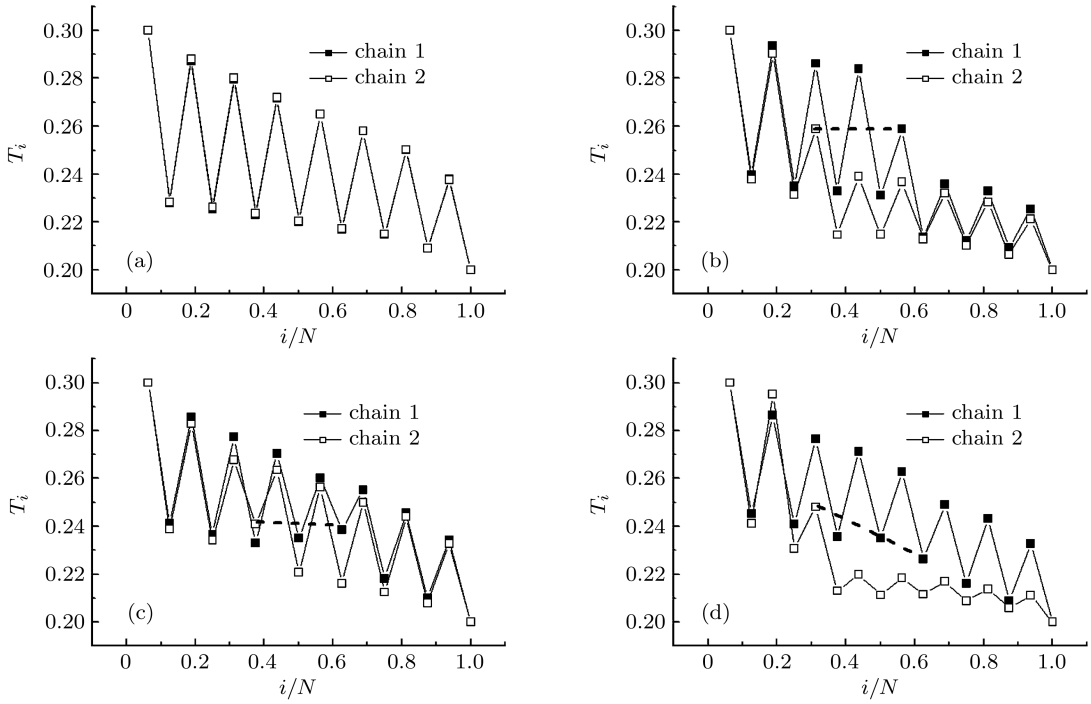
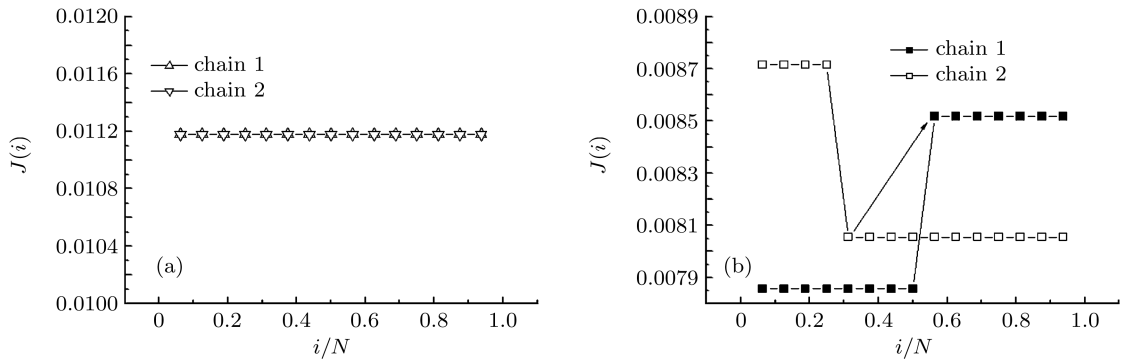


Fig. 2. Temperature profiles of two coupled chains of length $N = 16$ with different coupling modes (dashed lines). The mass ratio γ is 0.5. (a) No coupling; (b) L_1L_2 coupling (particle 9_1 couples with particle 5_2); (c) H_1H_2 coupling (particle 10_1 couples with particle 6_2); and (d) H_1L_2 coupling (particle 10_1 couples with particle 5_2).



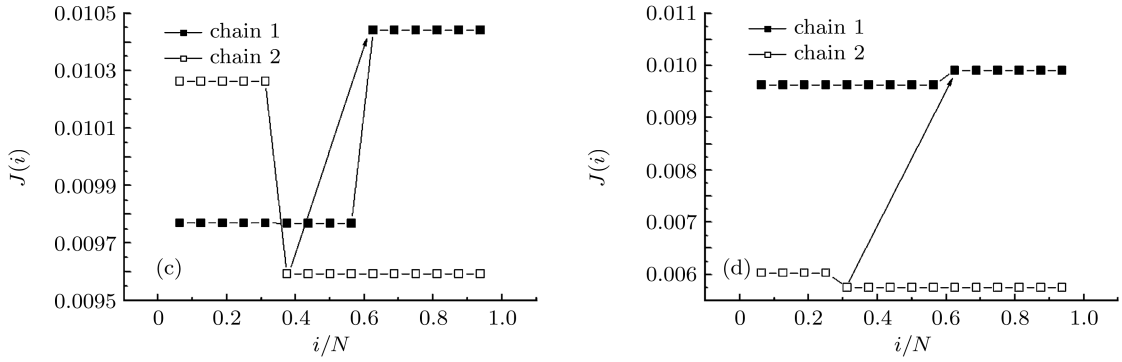


Fig. 3. The corresponding heat fluxes of two chains in Fig. 2 in the case of uncoupling (a), L_1L_2 coupling (b), H_1H_2 coupling (c), and H_1L_2 coupling (d). The arrows indicate the direction of heat flow.

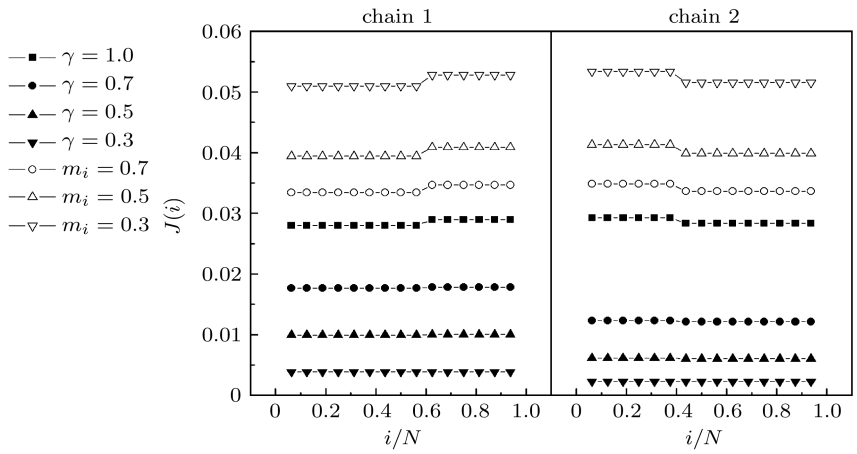


Fig. 4. The heat fluxes of two coupled chains of length $N = 16$ in the case of particle 10_1 couples with particle 7_2. The solid symbols show the heat fluxes in the case of mass ratio γ equal to 0.3, 0.5, 0.7 and 1.0. And the hollow symbols indicate the case of chains having homogeneous masses.

Another problem is the dependence of the interface thermal resistance induced by the two coupled particles in different chains on the mass ratio γ'. Here, we restrict to a special case that only one of the mass of the coupled particles can be changed, and the masses of the other particles in each chain are fixed at unit (see Fig. 5). Then we define the interface thermal resistance as $R_{\rm int} = \Delta T/J$, where ΔT is the temperature difference between the left and right particles of the interface. Notice that the interface thermal resistance $R_{\rm int}$ is composed of three parts, i.e., $R^l_{\rm int}, R^r_{\rm int}$, and $R^m_{\rm int}$, which are induced by the coupled particle and its three neighbours. We numerically calculate the values of the interface thermal resistance $R_{\rm int}$ of chain 1 at various mass ratios γ' and give the dependence of $R^l_{\rm int}$, $R^r_{\rm int}$ and R^m_{in} on γ', respectively, in Fig. 6(a). It is displayed that when the mass ratio γ' of the coupled particles gets to 1.0, $R^l_{\rm int}$ and $R^r_{\rm int}$ both have a smallest interface thermal resistance, and when the mass ratio γ' far from 1.0 a very large interface thermal resistance will be introduced. The interface thermal resistance induced by the two coupled particles in different chains, i.e. $R^m_{\rm int}$, is larger than the corresponding $R^l_{\rm int}$ and $R^r_{\rm int}$. The particle with changeable mass can be considered as an isotopic impurity atom which causes the decrease of heat flow through the system.[25] It is found that the interface thermal resistance $R^l_{\rm int}$ and $R^r_{\rm int}$ decrease linearly with increasing mass ratio γ' if the mass of the impurity atom is lighter than the host particle (see Fig. 6(b)). However, when the mass of the impurity atom is heavier than the host particle, the interface thermal resistances $R^l_{\rm int}$ and $R^r_{\rm int}$ increase exponentially with increasing mass ratio γ' (see Fig. 6(c)).

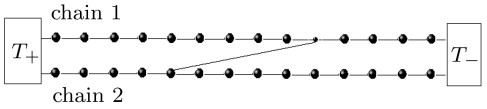


Fig. 5. A schematic model which consists of two coupled 1D chains and two Nosé–Hoover thermal reservoirs at temperature $T_+ = 0.3$ and $T_- = 0.2$, acting on the two ends of each chain, respectively. Particle 10_1 coupled with particle 5_2 and the mass of particle 10_1 can be altered. The masses of the other particles in each chain are fixed at unit.

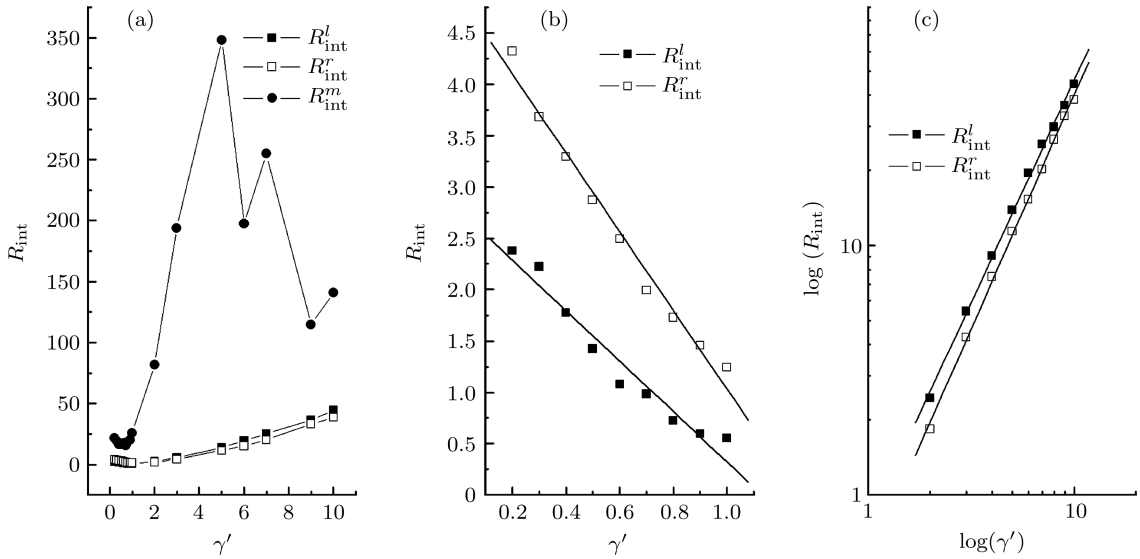


Fig. 6. The dependence of the interface thermal resistance $R_{\rm int}^l, R_{\rm int}^r$, and $R_{\rm int}^m$ on the mass ratio γ' was shown in panels (a)–(c), respectively. Other parameters are the same as those in Fig. 5.

We also studied the case that there are two pairs of coupled particles. For simplicity, we take $N_1 = N_2 = 4$ and particle 2_1 coupled with particle 2_2, particle 3_1 coupled with particle 3_2. In chain 1, we thermalize at $T_+ = 10$ and $T_- = 8$ the first and the last particles by using Nosé–Hoover thermal reservoirs. Reversely, in chain 2, we thermalize at $T_- = 9.5$ and $T_+ = 9.8$ the first and the last particles. A schematic representation of the model is depicted in Fig. 7(a) and we assume the mass of the particle 3_1 can be altered but others not. By numerical simulation, it is validated that the energy flow is conserved, i.e., the sum of the energy fluxes in-flowing from thermal reservoirs in the two chains is equal to the sum of the energy fluxes out-flowing from thermal reservoirs. Then a nontrivial and persistent circulation of energy current is observed at steady state when the mass of the particle 3_1 is taken to be of some special values (see Fig. 7(b)). This may exist in some polymers and organisms.[26] The reason for the circulation is that altering the mass of the middle particle rebuilds the temperature distribution and two local "backward flux"[27] may be introduced at the same time, i.e. the energy current flows from the particle 2_2 (low temperature) to the particle 2_1 (high temperature) and from the particle 3_1 (low temperature) to the particle 3_2 (high temperature). The other heat current through each chain remains flowing from the high-temperature bath to the low-temperature one at the same time. As a result, a circulation of energy current is formed in the system.

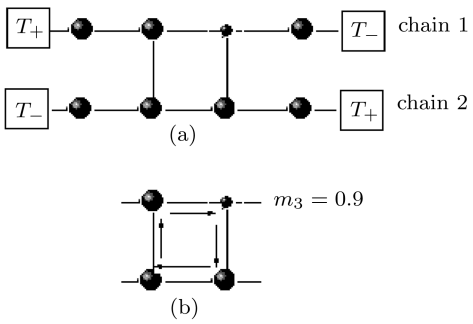


Fig. 7. (a) A schematic model of two coupled chains of length $N = 4$ with particle 2_1 coupled with particle 2_2 and particle 3_1 coupled with particle 3_2. In chain 1, the first and the last particles are thermalized at $T_+ = 10$ and $T_- = 8$, respectively. In chain 2, the first and the last particles are thermalized at $T_- = 9.5$ and $T_+ = 9.8$, respectively. The mass of particle 3_1 can be altered. (b) Schematic representation of a circulation of heat flow when the mass of particle 3_1 is taken to be 0.9. The arrows indicate the direction of heat flow.

4. Summary

In this paper, a simply coupled chains model with inhomogeneous masses has been explored. By nonequilibrium molecular dynamics simulation, it is found that the properties of heat transport in the model of two coupled FPU-β chains with alternate masses are different from those with homogeneous masses. The oscillating temperature profile can be built up in the dimerized model. When the mass ratio of the coupled particles in different chains becomes 1.0, there will be a smallest interface thermal resistance. In addition, when we add a light impurity atom to a homogeneous coupled FPU-β chains and intro-

duce a coupling between it and a particle in another chain, the interface thermal resistance $R^l_{\rm int}$ and $R^r_{\rm int}$ decrease linearly with increasing mass ratio γ' of them. Whereas, when a heavy impurity atom is added in the system, the interface thermal resistance $R^l_{\rm int}$ and $R^r_{\rm int}$ are increased exponentially with increasing mass ratio γ'. Then we studied the case that there are two pairs of coupled particles forming a closed loop circuit, in which a nontrivial and interesting circulation of energy current is observed in a steady state. Generally, it happened in some polymers and organisms. Our ultimate aims of this paper are to further reveal the properties of the heat transport in the simple network system and present an attempt of controlling the heat flow (or energy flow) by alter the masses of the coupled particles. In experiments, although, presently, it is difficult to deal with the mass of a single particle, with the promotion of the nanotechnology it will be accomplished.

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