Enhancement effect of asymmetry on the thermal conductivity of double-stranded chain systems*

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Using nonequilibrium molecular dynamics simulations, we study the thermal conductivity of asymmetric double chains. We couple two different single chains through interchain coupling to build three kinds of asymmetric double-stranded chain system: intrachain interaction, external potential, and mass asymmetric double chains. It is reported that asymmetry is helpful in improving the thermal conductivity of the system. We first propose double-heat flux channels to explain the influence of asymmetric structures on the thermal conductivity. The phonon spectral behaviour and finite size effect are also included.

Keywords: thermal conductivity, double-stranded chain, asymmetric structures, inter-chain flux

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1. Introduction

When it comes to transporting energy, Nature has two vital tools at her disposal: conduction by heat and by electricity.[1] However, we have never treated these phenomena equally. In the history of science development we have paid a lot of attention to electrical conduction but little to thermal conduction.[1] Since Fourier introduced the law bearing his name almost 200 years ago, a first-principles derivation of this simple law from statistical mechanics is still lacking. Worse still, the validity of this law in low dimensions has recently been called into question.[2−10] Terraneo *et al.*[11] proposed a theoretical mechanism realizing a heat rectifier. This mechanism attracted increasing attention to the thermal conductance of a one-dimensional single-chain system. An encouraging advance was made in 2006 when a carbon nanotube heat rectifier was realized in the laboratory.[12] The Frenkel–Kontorova (FK) model is often used to study one-dimensional single-chain systems. In 1938, the FK model was first proposed to study surface phenomena.[2] Since then this model, which consists of a nonlinear potential, has found applications in a wide variety of physical systems, such as adsorbed monolayers, Josephson junctions, charge density waves, magnetic spirals, tribology, and DNA denaturation.[13−16]

A typical thermal diode consists of two segments of FK lattices with different parameters.[2,17] However, a real one-dimensional single-chain structure in experimental implementation is rare. Double-chain systems such as the DNA molecule structure are more common.[18] Therefore, research on heat transport properties for double-stranded chain molecular structures is necessary. In this paper we build three kinds of asymmetric double-stranded chain structures, and study the influence of asymmetry on the thermal conductivity of the system. Our work provides a deep understanding of the thermal properties and energy transport problems of DNA and relevant biological molecular structures, which has many potential applications in biological thermal devices.

In recent years, the asymmetric heat conduction in one-dimensional inhomogeneous chains has been reported.[5,19−23] So far we have obtained many significant results, such as the thermal diode, thermal rectifier, thermal switch, thermal triode, thermal logic gates, and thermal computer. These theoretical and experimental studies are based on the concept of the thermal diode. The system of the thermal diode acts like a good thermal conductor in one direction but a good thermal insulator in the other when the po-

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sitions of the heat baths are reversed. An explanation of this phenomenon is phonon spectra of different chains changing from overlap to separation.[24−26] For a double-chain system, whether the phonon spectral explanation holds true is still uncertain. In this paper, we address the phonon spectral behaviour of the double-chain system.

2. Model and method

We consider the heat conductance in a double-chain system, a non-integrable model called the FK model. The Hamiltonian of the whole system is

$$H = H_{\rm A} + H_{\rm B} + H_{\rm int(A,B)}. \tag{1}$$

As shown in Fig. 1, we connect the i-th particle of the A-chain with the same order particles of the B-chain via a harmonic spring $k_{\rm ab}$, which is called inter-chain interaction. The coupling Hamiltonian of the two chains is

$$H_{\rm int(A,B)} = \sum_{i=1}^{N} \left[k_{\rm ab} \left(x_{{\rm A},i} - x_{{\rm B},i} \right)^2 \right]. \tag{2}$$

The Hamiltonian of the A-chain or B-chain is

$$H_M = \sum_{i=1}^{N} \left\{ \frac{p_{M,i}^2}{2m} + \frac{k_M}{2} \left(x_{M,i+1} - x_{M,i} \right)^2 + \frac{V_M}{(2\pi)^2} \left[1 - \cos(2\pi x_{M,i}) \right] \right\}, \tag{3}$$

where m is the mass of the particle, and the system size N is the number of the particles of the A-chain or B-chain. M denotes A or B. $x_{M,i}$ and $p_{M,i}$ are respectively the displacement from equilibrium position and the conjugate momentum of the i-th particle in chain M. k_M and V_M are the strength of the intrachain interaction and the external potential in the M-chain, respectively. We set m=1 and adjust the main parameters N, k_M, $k_{\rm ab}$, and V_M.

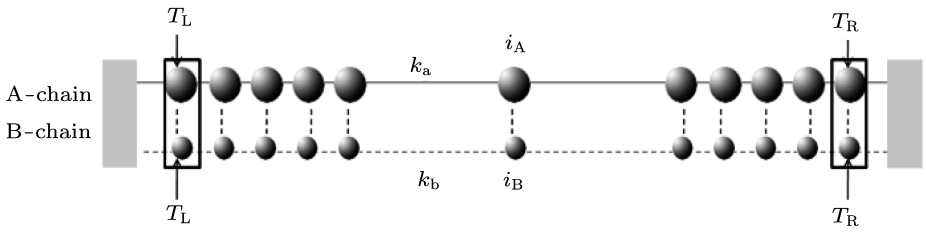


Fig. 1. Diagram of an asymmetric double-stranded chain structure.

In our simulations we use fixed boundary conditions, i.e., $x_{M,0} = x_{M,N+1} = 0$. The first particle and the last particle of the A-chain and B-chain are connected to heat baths. The temperatures of the left and the right heat baths are, respectively, $T_{\rm L} = 0.25$ and $T_{\rm R} = 0.10$. We use a Langevin thermostat and integrate the equations of motion using the fourth-order Runge–Kutta algorithm.[27] We choose a step size of the simulation $\triangle t = 0.01$ and average over 2×10^9 time steps. We have checked that our results do not depend on the particular thermostat realization, for example, the Nose–Hoover thermostat.[28,29] The local temperature is defined as $T_i = \langle p_i^2 \rangle / m k_{\rm B}$, where $\langle\ \rangle$ means time average, and the Boltzmann constant $k_{\rm B}$ is set to unity. The local heat flux in double chains is defined as[26]

$$\begin{aligned} j_i =\ & k_{\rm a} \langle p_{{\rm A},i} (x_{{\rm A},i} - x_{{\rm A},i-1}) \rangle \\ & + k_{\rm b} \langle p_{{\rm B},i} (x_{{\rm B},i} - x_{{\rm B},i-1}) \rangle \\ & + k_{\rm ab} \langle p_{{\rm A},i} (x_{{\rm A},i} - x_{{\rm B},i}) \rangle \\ & + k_{\rm ab} \langle p_{{\rm B},i} (x_{{\rm B},i} - x_{{\rm A},i}) \rangle. \end{aligned} \tag{4}$$

The local heat flux in the A-chain or B-chain is defined as

$$\begin{aligned} j_{{\rm a}i} =\ & k_{\rm a} \langle p_{{\rm A},i} (x_{{\rm A},i} - x_{{\rm A},i-1}) \rangle \\ & + k_{\rm ab} \langle p_{{\rm A},i} (x_{{\rm A},i} - x_{{\rm B},i}) \rangle, \end{aligned} \tag{5}$$

$$\begin{aligned} j_{{\rm b}i} =\ & k_{\rm b} \langle p_{{\rm B},i} (x_{{\rm B},i} - x_{{\rm B},i-1}) \rangle \\ & + k_{\rm ab} \langle p_{{\rm B},i} (x_{{\rm B},i} - x_{{\rm A},i}) \rangle. \end{aligned} \tag{6}$$

The simulations are performed long enough to allow the system to reach a steady state in which the local heat flux is constant along the double-stranded lattice. The thermal conductivity is defined as $K = Nj/\triangle T$, where $\triangle T = T_{\rm L} - T_{\rm R}$, $J = Nj_i$ is the total heat flux. $J_{\rm a} = Nj_{{\rm a}i}$ and $J_{\rm b} = Nj_{{\rm b}i}$ are the heat flux in the A-chain and B-chain, respectively.

3. Results and discussion

3.1. Asymmetric intrachain interaction

In order to study the effect of the non-symmetric intrachain interaction on the thermal conductance of the system, we first keep the external potentials in the A-chain and B-chain equal. Under the condition of the sum of intrachain interaction remaining unchanged, i.e., $k_a + k_b = 1.8$, we increase k_a and decrease k_b to obtain an increasing asymmetric ratio of the double chains.

As shown in Fig. 2, the thermal conductivity of the system increases with increasing asymmetric ratio k_a/k_b. The asymmetry of intrachain interaction has a positive influence on the thermal conductivity of the double-chain system.

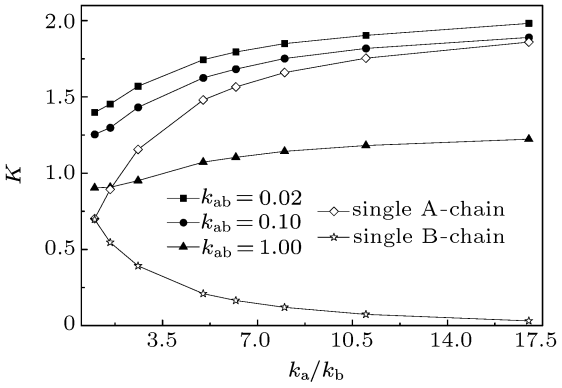


Fig. 2. Dependences of conductivity K on asymmetric ratio of the intrachain coupling k_a/k_b for various values of inter-chain interactions $k_{ab} = 0.02$, 0.10, 1.00, external potential $V_a = V_b = 4.0$, and mass of each particle $m = 1.0$.

Figure 3 shows the separated heat fluxes of the A-chain and B-chain, which helps us to understand the results of Fig. 2. As the value of k_a/k_b increases, the heat flux of the system, flowing along the strong intrachain interaction chain (A-chain), increases rapidly. Contrarily, the heat flux flowing along the weak intrachain interaction chain (B-chain) decreases with the increase of the asymmetric ratio. When the ratio k_a/k_b reaches a value larger than 16, we obtain the result: $J_a \to J$, and $J_b \to 0$. That means the heat flux going along the strong intrachain interaction chain (A-chain) increases rapidly. Contrarily, the heat flux flowing along the weak intrachain interaction chain (B-chain) decreases with the increase of the asymmetric ratio. When the ratio k_a/k_b reaches a value larger than 16, we obtain the result: $J_a \to J$ and $J_b \to 0$. That means all the heat fluxes go along the strong intrachain interaction chain.

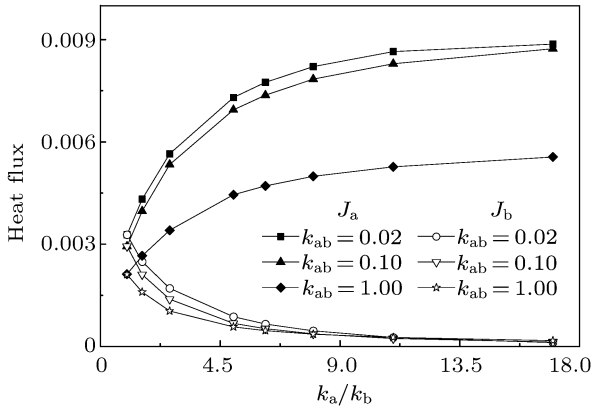


Fig. 3. Dependences of intrachain heat fluxes J_a and J_b on the value of k_a/k_b. The remaining parameters are the same as those for Fig. 2.

3.2. Asymmetric external potential

For comparison, we consider the asymmetry of the external potential and set the values of the intrachain interaction in the A-chain and B-chain as $k_a = k_b = 0.9$. We increase the asymmetric ratio of the external potential in the A-chain V_a to that in the B-chain V_b without changing the value of $V_a + V_b (= 8.0)$. As shown in Fig. 4, the thermal conductivity of the system increases with increasing potential asymmetric ratio V_a/V_b. Obviously, the asymmetry of the external potential also exerts a positive influence on the thermal conductivity of the double-chain system.

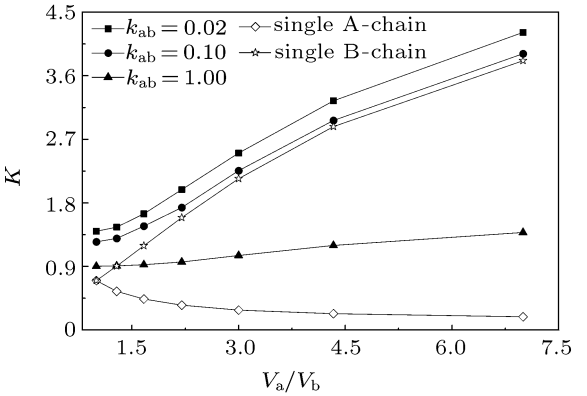


Fig. 4. Dependences of conductivity K on the value of V_a/V_b for various inter-chain interactions $k_{ab} = 0.02$, 0.10, 1.00, the intrachain interaction $k_a = k_b = 0.9$ and particle mass $m = 1.0$.

From Fig. 5, it is also observed that the heat flux flowing along the small external potential is different from that along the large external potential. As the value of V_a/V_b increases, the heat flux of the system

mostly flows more easily along the small external potential chain (B-chain) than along the large external potential chain (A-chain). When the asymmetric ratio V_a/V_b increases to 7, we can have $J_b \to J$ and $J_a \to 0$, which also indicates that the heat always tends to go along the chain with weak external potential.

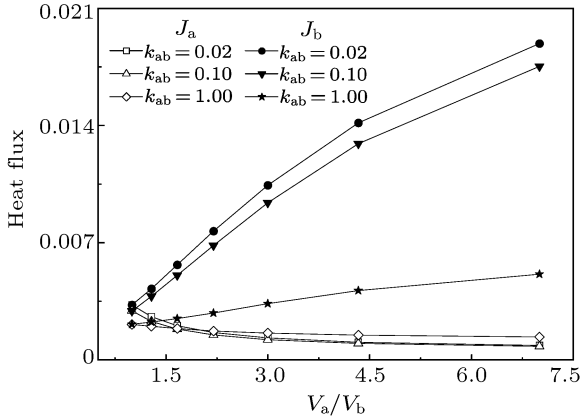


Fig. 5. Dependences of the intrachain heat fluxes J_a and J_b on the value of V_a/V_b. The remaining parameters are the same as those in Fig. 4.

3.3. Phonon spectral behaviour and finite-size effect

It is expected that the match of the phonon spectra can explain the different thermal conductivities between the asymmetrical and the symmetrical double chains. We choose three kinds of double-chain structures and acquire the phonon spectrum of the middle particle of each structure. As shown in Fig. 6(a), the system with greater conductivity has a smaller overlapping region. However, figures 6(b) and 6(c) show that the system with weaker conductivity has a greater overlapping region. This phenomenon is very different from the result for a single-chain system.[19,24,25] Therefore, phonon spectral overlapping of the two chains fails to explain the dependence of the thermal conductivity on the asymmetry of the double chains.

We also investigate the system finite-size effect of the asymmetric double-chain lattice. Figure 7 shows the dependence of thermal conductivity on system size for three kinds of double chains. The thermal transport mode exhibits a transition from ballistic transport to diffusion with increasing system size. It is shown that an asymmetric structure does not affect the system transport mode, which is similar to the result reported for single FK chain.[3]

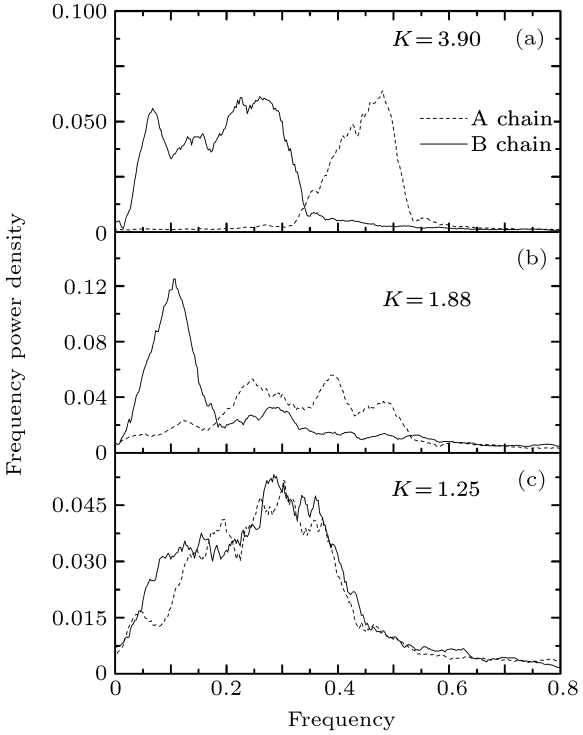


Fig. 6. Phonon spectra of the middle particle of each chain for different double-chain structures. (a) $k_a = k_b = 0.9$, $V_a = 7.0$, and $V_b = 1.0$; (b) $V_a = V_b = 4.0$, $k_a = 1.7$, and $k_b = 0.1$; (c) $k_a = k_b = 0.9$, and $V_a = V_b = 4.0$.

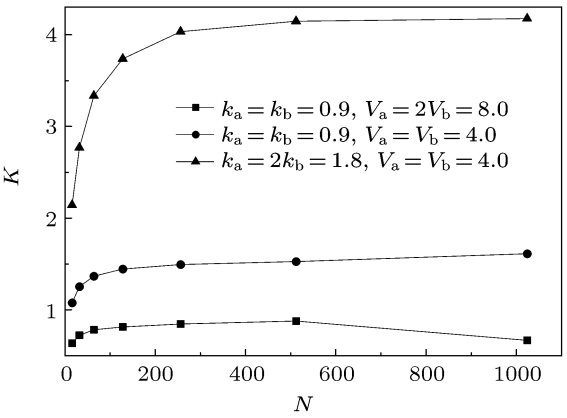


Fig. 7. Dependences of conductivity K on the system size for different double-chain structures. Here, interchain interaction $k_{ab} = 1.0$.

3.4. Intrachain and interchain heat flux channels

From Figs. 3 and 5, we have obtained the valuable conclusions that the A-chain has the same heat flux as the B-chain for a system of symmetrical structure and this balance is broken for an asymmetric double-chain structure. However, in order to give quantitative results, we introduce a double-heat flux channel to explain the enhanced effect of asymmetry on the

thermal conductivity of the double-stranded chain system. The double-heat flux channel refers to two kinds of heat flux, one along the chain (A-chain or B-chain) and the other between the chains. The former is relevant to the intrachain channel, and the latter to the interchain channel. The heat fluxes along the intrachain channel have been defined in Eqs. (5) and (6) respectively. Here we define the heat flux along the interchain channel (i.e., the heat current flows from the A-chain to the B-chain or from the B-chain tothe A-chain) as

$$j_{(i,\mathrm{a-b})} = k_{\mathrm{ab}}\langle p_{\mathrm{A},i}(x_{\mathrm{A},i} - x_{\mathrm{B},i})\rangle + k_{\mathrm{ab}}\langle p_{\mathrm{B},i}(x_{\mathrm{B},i} - x_{\mathrm{A},i})\rangle. \quad (7)$$

The total interchain heat flux is given by $J_{(\mathrm{a-b})} = \sum_{i=1}^{N} |j_{(i,\mathrm{a-b})}|$, where N is the number of interchain channels, which equals the system size.

As shown in Figs. 8 and 9, when the system has a symmetric structure, the heat flux flowing along the interchain channel is zero and the heat flux goes mainly along the intrachain channels. As the asymmetric ratio increases, the heat flowing along the interchain channel increases not only for asymmetric intrachain coupling but also for asymmetric external potential. When the asymmetric ratio $V_{\mathrm{a}}/V_{\mathrm{b}}$ is larger than 5.0 and $k_{\mathrm{a}}/k_{\mathrm{b}}$ is larger than 12.0, the value of the interchain flux will approach that of the intrachain flux. Correspondingly, the thermal conductivity increases with the increase of the asymmetric ratio. Therefore, it is reasonable to suggest that the interchain heat flux contributes to the improvement of the thermal conductivity.

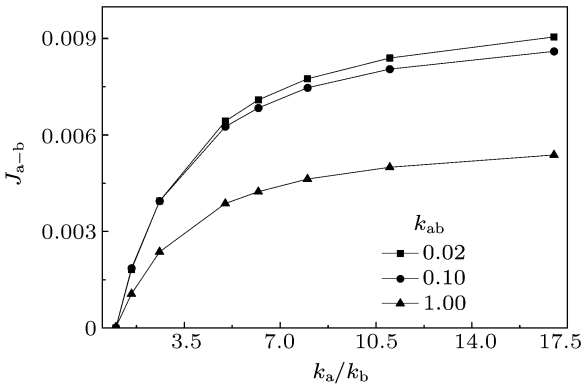


Fig. 8. Dependences of interchain heat flux on asymmetric intrachain interaction for different values of the interchain interactions. The remaining parameters are the same as those in Fig. 2.

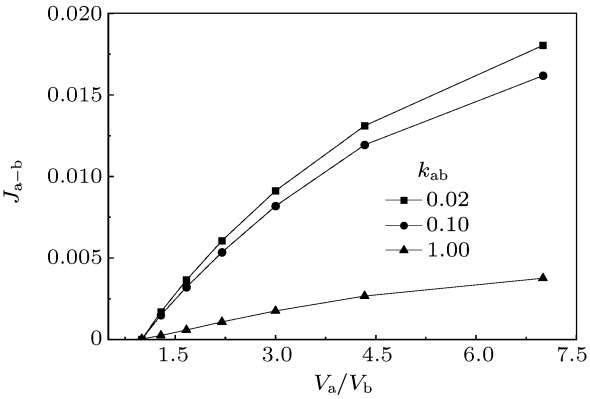


Fig. 9. Dependences of interchain heat flux on asymmetric external potential for different values of the interchain interactions. The remaining parameters are the same as those in Fig. 4.

3.5. Comparisons between single- and double-chain systems

Here, we should point out that we build the asymmetric double chains through a simple method by keeping the sum of the intrachain coupling and the external potential constant, and changing their ratio. When considering the mass asymmetry, which may be more reasonable than fixing the sum of the mass, we also obtain a mass asymmetric system and maintain the same values for other parameters. Figure 10 shows that the thermal conductivity increases with the mass asymmetry, which also contributes to the increase of the interchain flux. Therefore, the method used to build asymmetric double chains is valid not only for the intrachain coupling and the external potential, but also for the mass. Our result indicates that the asymmetric Frenkel–Kontorova double-chain is a homogeneous and additive system.

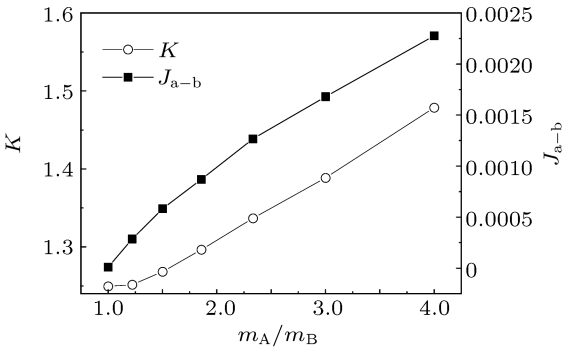


Fig. 10. Dependences of thermal conductivity and interchain heat flux on the mass asymmetric ratio $m_{\mathrm{A}}/m_{\mathrm{B}}$, where m_{A} and m_{B} are respectively the particle masses in the A-chain and B-chain. The remaining parameters are $k_{\mathrm{a}} = k_{\mathrm{b}} = 0.9$, and $V_{\mathrm{a}} = V_{\mathrm{b}} = 4.0$.

As shown in Figs. 2 and 4, we compare single-chains with double-chains without changing the sum of intrachain interaction and external potential. We

show the thermal conductivities of the chain with strong intrachain coupling and with weak external potential increasing with the variation of the asymmetry of intrachain interaction and external potential. The thermal conductivity of the other chain decreases with increasing asymmetry. As also displayed in Fig. 11, when considering the influence of particle mass on thermal conductivity, one can easily find that the chain (A-chain) with light mass has a better thermal conductivity while that of the chain with heavy mass (B-chain) is worse.

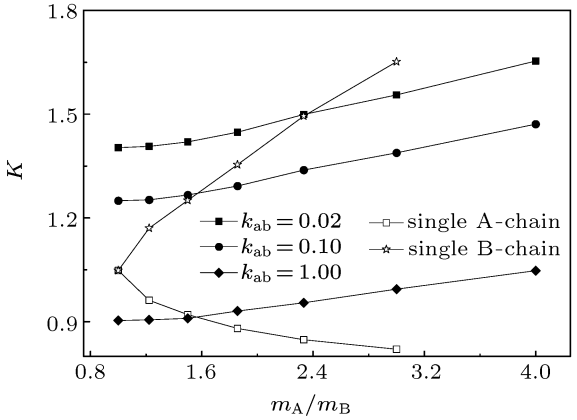


Fig. 11. Dependences of conductivity K on the asymmetric paticle-mass-ratio m_A/m_B for various values of the interchain interactions $k_{ab} = 0.02$, 0.1, 1.0, the external potential $V_a = V_b = 4.0$ and intrachain interaction $k_a = k_b = 0.9$.

Therefore, it must be emphatically pointed out that as the asymmetry of the double-chain increases, the thermal conductivity increases for one chain and decreases for the other. However, when coupling the two chains, we find that the total thermal conductivity increases with increasing asymmetry. This indicates that the increase of thermal conductivity in one chain exceeds the decrease in the other, which may contribute to the interchain interaction.

4. Conclusions

We build an asymmetric double-stranded chain system by adjusting the ratio of the intrachain interaction, external potential, and the mass in the A- and B-chains, respectively. We show that an asymmetric double-stranded chain structure enhances the thermal conductivity of the system. It is found that thermal conductivity increases significantly with the increase of the asymmetric ratio of the intrachain interaction and the external potentials in the A- and B-chains. For an asymmetric system, heat flux flows more easily from the small external potential chain and the strong intrachain interaction chain. It is also reported that phonon spectral behaviour cannot explain the enhancement of the thermal conductivity. We first define the double-heat flux channel: intrachain and interchain channels. We show that only the intrachain channel works for a symmetric structure. However, in an asymmetric structure, both channels are conducive to the thermal conductivity. Our results provide direct evidence that interchain channel flux enhances the thermal conductivity of an asymmetric double-chain system.

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