Different thermal conductance of the inter- and intrachain interactions in a double-stranded molecular structure

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A double-stranded system, modeled by a Frenkel-Kontorova lattice, is studied through nonequilibrium molecular dynamics simulations. We have investigated the thermal conductance influenced by the intrachain interaction as well as by the interchain interaction. It is found that the intrachain interaction always enhance the thermal conductance. The interchain interaction, however, has a positive effect on the thermal conductance in the case of strong nonlinear potential, and has a negative effect on the thermal conductance in the case of weak nonlinear potential. This phenomenon can be explained by the transition of thermal transport mode and the phonon band shift of the particles. It is suggested that the inter- and intrachain interactions present different thermal properties in double-stranded lattices.

I. INTRODUCTION

Deriving macroscopic physics laws from simple microscopic models is one of the tasks of nonequilibrium statistical mechanics [1]. So far single-chain lattices have attracted great interest and extensive studies in the recent decades for the simple reason that they are easier to study through simulations and through whatever analytical methods are available [2–5]. For one-dimensional single-chain systems, some of the most interesting results that have been obtained are as below: 1) The heat current J decreases with system size N as $J \sim 1/N^{\alpha}$, where $\alpha < 1$ [6–9]. 2) The thermal conductivity κ increases with the interparticle coupling λ as a scaling law $\kappa \sim \lambda^{\gamma}$, here $\gamma \sim 1.5$ [10]. In other words, the thermal conductivity is directly proportional to the interaction of the particles in single-chain systems.

In double-stranded and multistranded lattices, which are more common structures in nature such as DNA double helix [11], double- and multichain polymers [12], multistranded nanofibers [14] and nanotubes [13] [15], there are few detailed studies and it is fair to say that it is totally unclear as to whether they have the same properties as those the single-chain lattices have, and if not, then what they are different from. Liu and Li [16] have studied the interchain coupling in simple networks consisting of different one dimensional nonlinear chains. They reported that the coupling between chains has different functions in heat conduction comparing with that in electric current. However, the double chains they have studied, which are coupled together only with two particles, are far different from the true double-stranded structure. For two dimensions nonlinear systems, which are much similar to double-stranded and multistranded lattices, Lee and Dhar [17] have performed simulations to determine the system size (L) dependence of the heat current (J). Unfortunately, the inter- and intrachain interactions in their models have been still regarded as the same interactions.

Up to now lots of the studies about the low dimensional thermal conductance focus on the single-chain lattices and the couplings of the particles [1], which is called the intrachain interactions here. However, few researchers address on the influence of the inter-chain interactions on the thermal conductance. Moreover, in biological and chemical research areas, some previous investigations have shown that interchain interactions play an important role in the properties of materials. For instance, the inter-chain interactions can affect the denaturation of DNA [18–21], the luminescent properties of polymer [22] and the electronic properties of the dimer [23]. Therefore, it is highly necessary to study the thermal properties and relevant transport problems of the interchain interaction. Particularly, the difference between the intra- and interchain interaction is an important issue to be discussed.

In this paper, We consider heat conduction in a double-chains Frenkel-Kontorova (FK) system as shown in Fig. 1. We expect that the interchain interaction can lead to some interesting and rather surprising results in thermal conductance. In this model the interchain interaction means the interaction between A-chain and B-chain. The intrachain interaction, which is corresponding to the coupling of the particles in single chain system, refers to the coupling of the particles in A chain or in B-chain. It have been reported that strong intrachain interactions always raise the heat conductance in the single-chain FK lattice [1,10]. A similar calculation for the inter-chain interaction is so far not available in the double chains case, and we will address this specific question.

II. MODEL AND SIMULATION METHOD

We consider heat conductance in a double-stranded FK crystal described by a total Hamiltonian

$$H = H_A + H_B + H_{int}. \tag{1}$$

As shown in Fig. 1, we couple the ith particle of A-chain with the same order particle of B-chain via a harmonic spring, and the coupling Hamiltonian $H_{int} = \Sigma_{i=1}^{N}[k_0(x_{A,i} - x_{B,i})^2]$, where k_0 is the strength of the interchain coupling. The Hamiltonian of each chain can be written as
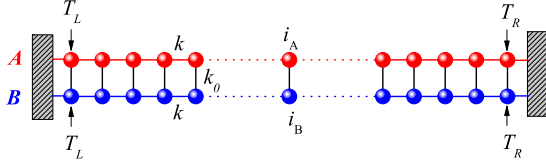
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FIG. 1. (Color online) Diagram of the double-stranded lattices. A-chain (red) and B-chain (blue) are coupled together via a harmonic spring k_0. k is the strength of intrachain interaction. T_L and T_R are the temperature of the heat baths connected to the first and the last particles of each chain.

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

with $x_{M,i}$ and $p_{M,i}$ denote the displacement from equilibrium position and the conjugate momentum of the ith particle in chain M, where M stands for A or B. N is the number of the particles in A or B chain. m is the mass of the particle. The parameters V and k are the strength of the nonlinear external potential and the intrachain interaction for the FK lattice, respectively. We set the masses of all the particles be unit and use fixed boundaries, $x_{M,N+1} = x_{M,0} = 0$. The first and the last particles of A chain and B chain are connected to heat baths. The temperature of the left and right heat baths is, respectively, $T_L = 0.25$ and $T_R = 0.10$. The temperature used here and in the following numerical computations is dimensionless. It is connected with the true temperature T_θ of the materials through the relation [24]: $T_\theta = (m\omega_\theta^2 \phi^2 T)/k_B$, here m is the mass of the particle and ϕ is the period of external potential. ω_θ is the oscillating frequency. k_B is the Boltzmann constant.

In our simulations we use Langevin thermostat and integrate the equations of motion by using the fourth-order Runge-Kutta algorithm [25]. We chose a step size of the simulation $\Delta t = 0.005$ and averaging over 2×10^9 time steps. We have checked that our results do not depend on the particular thermostat realization (for example, Nose-Hoover thermostat [26]). The local temperature is defined as $T_i = \langle p_i^2 \rangle$, $\langle \ \rangle$ means time average. The local heat flux in double chains is defined as $j_i = k\langle p_{A,i}(x_{A,i} - x_{A,i-1})\rangle + k\langle p_{B,i}(x_{B,i} - x_{B,i-1})\rangle + k_0\langle p_{A,i}(x_{A,i} - x_{B,i})\rangle + k_0\langle p_{B,i}(x_{B,i} - x_{A,i})\rangle$, which is derived from the equations of motion and the expression of thermal flux $\Sigma(F_{M,i} \cdot v_{M,i})$, where M stands for A and B [1]. 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 transport coefficient is an important quantity for characterizing the transport mode of a thermal transport process [27]. The thermal conductance evaluated as $K = Nj/\triangle T$ represents an effective transport coefficient that includes both boundary and bulk resistances [1].

III. RESULTS AND DISCUSSION

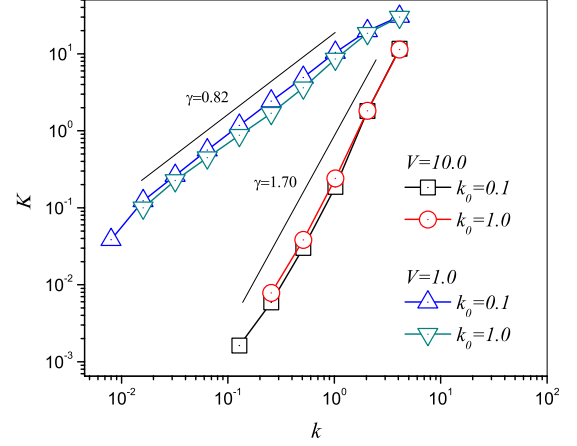The interchain interaction is compared to the intrachain interaction in the thermal conductance and the phonon spec-

FIG. 2. (Color online) Thermal conductance as a function of the intra-chain interaction for various values of V and $k0$ at a system size of $N=64$.

tra of the particles. Figure 2 shows the dependence of thermal conductance on the intrachain interaction for the system size $N=64$. For various nonlinear external potentials $V=1.0$ and 10.0 as well as two kinds of interchain couplings $k_0 = 0.1$ and 1.0, the thermal conductance monotonously increases with the intrachain interaction. This result is good agreement with that of the single-chain FK lattice, which is also clearly confirmed by the analytical calculations based on the self-consistent phonon theory [10].

Thermal conductivity dependence on k and V can be explained by the self-consistent phonon (SCP) theory. The SCP theory has been applied to deal with the nonlinear Morse on-site potential for the DNA denaturation [28]. The SCP theory can be taken into consideration the asymmetric heat transport in the nonlinearity lattices [29].

Hamiltonian of FK model can be approximated an effective linear Hamiltonian by the SCP theory as [28]

$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + \frac{k}{2}(x_{i+1} - x_i)^2 + \frac{f}{2}x_i^2 \right], \tag{3}$$

where the effective harmonic potential coefficient f is obtained from the self-consistent equation,

$$f = \frac{\pi^2 V}{a^2} \exp\left[-\frac{\pi^2 k_B T}{2a^2 \sqrt{f(4k+f)}} \right]. \tag{4}$$

So, the spectrum of effective phonons is $\hat{\omega}_k^2 = f + 4k\sin^2\frac{k_i}{2}$.

As reported in Ref. [10], using Debye formula we can get the thermal conductivity as

$$K \propto \frac{ck^{3/2}}{V^2} \int_0^{2\pi} \frac{\sin^2 k_i}{\left(4\sin^2\frac{k_i}{2} + \frac{f}{k}\right)^{3/2}} dk_i, \tag{5}$$

where k_i is the wave vector. For the sake of simplicity, c is assumed a constant, from the equation, we can obtain the relationship of K vs V and k as below:
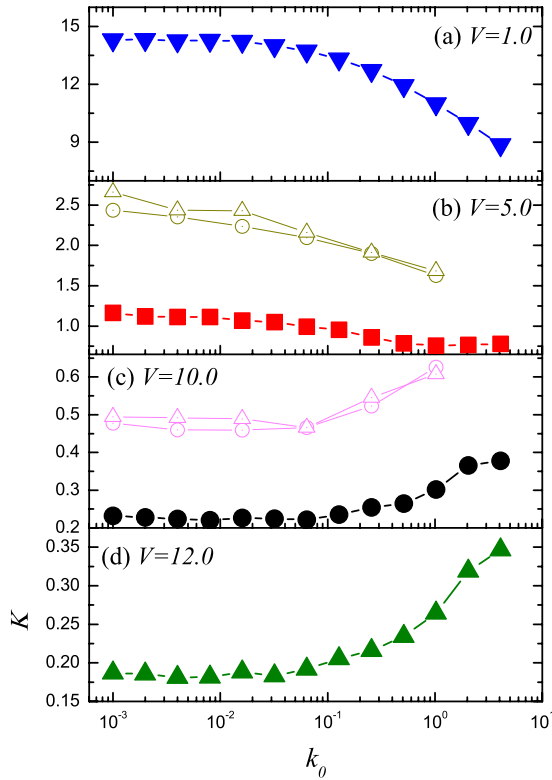
FIG. 3. (Color online) The dependence of thermal conductance on interchain interaction for various nonlinear external potential V =1.0, 5.0, 10.0 and 12.0. The system size is $N=64$ for full filled point [(a) blue, (b) red, (c) black and (d) green], 256 for circle and 512 for triangle [(b), (c)]. The remaining parameter is $k=1.0$.

$$K \propto \frac{k^{3/2}}{V^2}. \qquad (6)$$

Thus, it can be clearly seen that K increases with k as a scaling law $K \sim k^\gamma$, which is confirmed by numerical results as well as analytical results [10]. For single FK chain, the exponent γ is 3/2 and is independence of the on-site potential. However, for double FK chains, as shown in Fig. 2, γ changes with the on-site potential V obviously. When V increases, the exponent γ will decreases. It can be seen that the intrachain interaction performs a positive influence on thermal conductance not only for the single-chain lattice but also for the double-chain lattice.

When we go to the double-stranded lattice and consider the interchain interaction, we will find some interesting and surprising results. As shown in Fig. 3, in the case of a weak nonlinear external potential $V=1.0$ or 5.0, the thermal conductance decreases with the increasing of the interchain interaction. On the contrary, when the nonlinear external potential goes to a higher value 10.0 or 12.0, the thermal conductance monotonously increase with the interchain interaction just as with the intrachain interaction. Due to the universe finite size effect in low-dimensional systems, we consider more system size $N=256$ and 512, as shown in Figs. 3(b) and 3(c), the thermal conductance as a function of the inter-chain interaction mentioned above is still invariant. This indicates that this kind of anomalous heat conduction
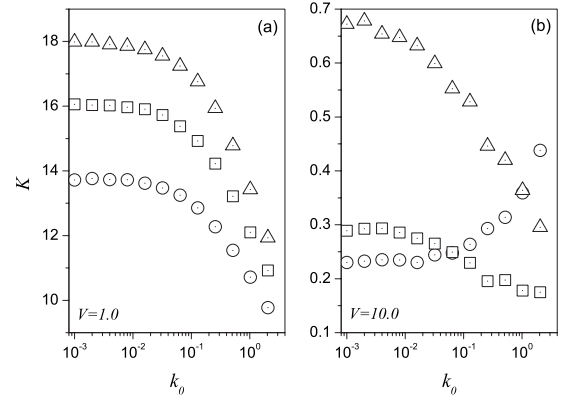

FIG. 4. Thermal conductance changes with the interchain interaction for various temperatures $T_0=0.35$ (triangle), 0.25 (square), 0.15 (circle).

induced by the interchain interaction is independent of the system size.

We also like to discuss the temperature dependence of the thermal conductance. Here we set the temperature of the system as T_0. The heat baths are respectively $T_L=T_0+dT$ and $T_R=T_0-dT$, where dT is 0.05. In the case of weak on-site potential, as shown in Fig. 4(a), the thermal conductance decreases with the increasing of inter-chain interaction, which is independence of the temperature. In the case of strong on-site potential, however, the relationship between the thermal conductance and the interchain interaction depends on the temperature of the system. As shown in Fig. 4(b), the thermal conductance increases with the increasing of inter-chain coupling at low temperature ($T_0=0.15$); On the contrary, the thermal conductance decreases with the increasing of interchain coupling at high temperature ($T_0=0.25$ and 0.35).

First, we apply the transition of the thermal transport mode to interpret the different thermal transport properties between intra and inter-chain interaction. For the intra-chain coupling, Figs. 5(a) and 5(b) show the temperature profile at different intra-chain couplings. As also shown in the inset of Figs. 5(c) and 5(d), the thermal conductivity is finite in the diffusive region and infinite in the ballistic region. Diffusive and ballistic regions are, respectively, corresponding to large and small temperature differences. When the intrachain coupling increases, the temperature different in the chain decreases, which indicate the thermal transport mode exhibits a transition from the diffusive to the ballistic transport. Ballistic transport means less collision of phonon and then the thermal current will increase. Therefore, it is easily understand why the intrachain coupling always enhances the thermal current in the chain. For the inter-chain coupling, as shown in Fig. 5(c), the interchain coupling cannot change the temperature profile of the chain in the case of weak nonlinear potential. However, Fig. 5(d) displays the thermal transport mode exhibits a transition from the diffusive to the ballistic transport when interchain coupling increases in the case of strong nonlinear potential. The strong interchain interaction refers to strong on-site potential or large effective mass of the particle, which performs negative effects on the heat current. The competitive effects of strong on-site potential
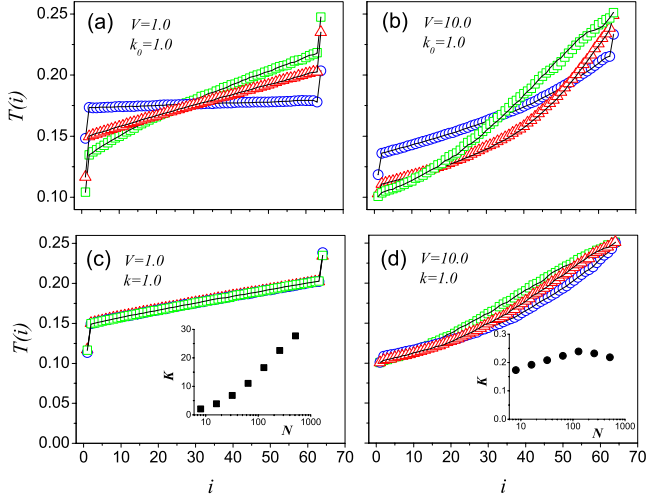
FIG. 5. (Color online) Temperature profiles along A chain (point) and B chain (line) at various intra- and interchain interactions. In (a) and (b), the parameter $k=0.1$ (Green square), 0.5 (Red triangle), 2.0 (Blue circle); In (c) and (d) the parameter $k_0=0.01$ (Green square), 0.1 (Red triangle), and 1.0 (Blue circle). Inset: the thermal conductivity changes with the system size for $k=1.0$ and $k_0=1.0$.

(negative effect) and the ballistic transport (positive effect) determine the influence of interchain coupling on thermal conductance. In the case of weak nonlinear potential, the transport mode is fixed and then the thermal conductance decreases with the interchain interaction increases. In the case of strong nonlinear potential, the on-site potential is strong enough; therefore, the transition from diffusive to ballistic transport will increase the heat current.

Second, we give another interpretation from the view of the phonon spectra. As shown in Fig. 6(a), when the intrachain interaction increases, the band width, namely the frequency range of the midparticle of A chain, expands. The phonon spectra of one particle can easily match the other, therefore the heat current increases. We have investigated many particles along the chain and observed similar results for other particles. However, as illustrated in Fig. 6(b), when the interchain interaction increases, the phonon spectra split into two branches when spreading. Obviously, interchain interaction can induce another branch of oscillation mode, which is of high-oscillating frequency. The phonon is a Boson whose energy is proportion to the frequency from equation $E=\hbar\omega$. And then the phonon with high frequency can easily overcome the on-site potential to transmit along the chain. On the other hand, the phonon with high frequency has more opportunities to collide with each other, which means the thermal conductance decreasing. The competitive effects as mentioned above are also observed in the change of phonon spectra induced by the interchain interaction.
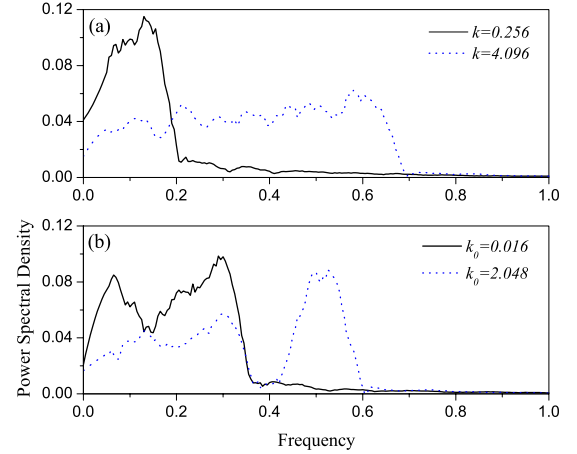

FIG. 6. (Color online) Power spectral density of the particle at the middle of A chain for different intra and interchain interaction with the parameter values $N=64$, $V=1.0$, and (a) $k_0=0.1$, (b) $k=1.0$.

IV. CONCLUSIONS

In summary, we have performed extensive numerical simulations of thermal conduction in a double-stranded FK lattice. It is reported that the interactions of the intra and interchain exhibit different thermal transport properties. In any case, the intrachain interaction always upgrades the thermal conductance. The interchain interaction, however, has both positive and negative effects on the thermal conductance: the positive effect at the strong nonlinear potential and the negative effect at the weak nonlinear potential. Moreover, the changes of the phonon spectra of the particles, which are induced by intrachain interaction, are quite different from those induced by interchain interaction. It is suggested that a simple coupling between the particles, which is a common point for both intrachain and interchain interaction, can develop various thermal transport phenomena under different situations. Although our model based on one dimensional lattice is insufficient to give a realistic description of real DNA and polymer systems, our result will provide a new physical view of DNA, polymer, nanomaterials and others structure, which are similar to double-stranded lattice.

[1] S. Lepri, R. Livi, and A. Politi, Phys. Rep. **377**, 1 (2003).
[2] A. F. Neto, Humberto C. F. Lemos, and E. Pereira, J. Phys. A **39**, 9399 (2006).
[3] F. Bonetto, J. L. Lebowitz, and J. Lukkarinen, J. Stat. Phys. **116**, 783 (2004).
[4] B. Hu, B. Li, and H. Zhao, Phys. Rev. E **57**, 2992 (1998); B. Li, H. Zhao, and Bambi Hu, Phys. Rev. Lett. **86**, 63 (2001); B. Li and J. Wang, *ibid.* **91**, 044301 (2003).
[5] W. R. Zhong, P. Yang, B. Q. Ai, Z. G. Shao, and B. Hu, Phys. Rev. E **79**, 050103(R) (2009).
[6] A. Dhar, Phys. Rev. Lett. **86**, 3554 (2001).
[7] O. Narayan and S. Ramaswamy, Phys. Rev. Lett. **89**, 200601 (2002).
[8] S. Lepri, R. Livi, and A. Politi, EPL **43**, 271 (1998).
[9] P. Grassberger, W. Nadler and L. Yang, Phys. Rev. Lett. **89**, 180601 (2002).
[10] Z. G. Shao, L. Yang, W. R. Zhong, D. H. He, and Bambi Hu, Phys. Rev. E **78**, 061130 (2008).
[11] S. Wolfram, *Principles of Nucleic Acid Structure* (Springer-Verlag, New York, 1984).
[12] J. Brandrup, E. H. Immergut, and E. A. Grulke, *Polymer Handbook, 2 Volumes Set*, 4th ed. (Wiley, New York, 2003).
[13] M. J. O'Connell, *Carbon Nanotubes: Properties and Applications* (Taylor & Francis Group, Boca Raton, 2006).
[14] S. Maheshwari and H. C. Chang, Adv. Mater. **21**, 349 (2009).
[15] J. Diao, D. Srivastava, and M. Menon, J. Chem. Phys. **128**, 164708 (2008).
[16] Z. Liu and B. Li, Phys. Rev. E **76**, 051118 (2007).
[17] L. W. Lee and A. Dhar, Phys. Rev. Lett. **95**, 094302 (2005).
[18] Kerson Huang, *Lectures on Statistical Physics and Protein Folding* (World Scientific, Singapore, 2006).
[19] David R. Nelson, *Statistical Physics of Unzipping DNA* (Springer-Verlag, Netherlands, 2004).
[20] K. Drukker, G. Wu, and G. C. Schatz, J. Chem. Phys. **114**, 579 (2001).
[21] X. Yu and D. M. Leitnera, J. Chem. Phys. **122**, 054902 (2005).
[22] M. W. Wu and E. M. Conwell, Phys. Rev. B **56**, R10060 (1997).
[23] M. Ottonelli, G. Musso, D. Comoretto, and G. Dellepiane, J. Phys. Chem. B **109**, 5485 (2005).
[24] J. Lan and B. Li, Phys. Rev. B **74**, 214305 (2006).
[25] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes* (Cambridge University Press, Cambridge, England, 1992).
[26] S. Nosé, J. Chem. Phys. **81**, 511 (1984); W. G. Hoover, Phys. Rev. A **31**, 1695 (1985).
[27] J. S. Wang, Phys. Rev. Lett. **99**, 160601 (2007).
[28] T. Dauxois, M. Peyrard, and A. R. Bishop, Phys. Rev. E **47**, 684 (1993).
[29] B. Hu, D. He, L. Yang, and Y. Zhang, Phys. Rev. E **74**, 060101(R) (2006).