Heat conduction of symmetric lattices

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Heat conduction of symmetric Frenkel-Kontorova (FK) lattices with a coupling displacement was investigated. Through simplifying the model, we derived analytical expression of thermal current of the system in the overdamped case. By means of numerical calculations, the results indicate that: (i) As the coupling displacement d equals to zero, temperature oscillations of the heat baths linked with the lattices can control magnitude and direction of the thermal current; (ii) Whether there is a temperature bias or not, the thermal current oscillates periodically with d, whose amplitudes become greater and greater; (iii) As d is not equal to zero, the thermal current monotonically both increases and decreases with temperature oscillation amplitude of the heat baths, dependent on values of d; (iv) The coupling displacement also induces nonmonotonic behaviors of the thermal current vs spring constant of the lattice and coupling strength of the lattices; (v) These dynamical behaviors come from interaction of the coupling displacement with periodic potential of the FK lattices. Our results have the implication that the coupling displacement plays a crucial role in the control of heat current.

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I. INTRODUCTION

Understanding heat conduction at a molecular level is of fundamental and practical importance [1]. In recent years, much attention has been paid to heat conduction of nonlinear lattice [2] for two reasons. One is that various thermal devices controlling heat flow, such as thermal diodes [3,4], thermal transistors [5], thermal logic gates [6], thermal memories [7], and so on, can be designed theoretically. The other is how these thermal devices may be realized experimentally. The first realization of solid-state thermal diode has been put forward with help of asymmetric nanotubes [8]. Single-photon heat conduction between two resistors coupled weakly to a single superconducting microwave cavity should be experimentally observable [9]. Phonons, as carriers of heat conduction, are by far more difficult to control than electrons and photons. Thus understanding further behavior of phonon and intrinsic mechanism of heat transfer at the molecular level is still an underlying challenge for mankind.

According to the thermodynamic second law, heat cannot spontaneously flow from a subsystem at lower temperature to another coupled subsystem at higher temperature. Thus, in order to get a steady heat flow against thermal bias, we must let the system operate away from thermal equilibrium by means of some effective measures. A typical situation is that rocking periodically temperature of one heat bath can direct a steady heat flux from cold bath to hot bath against a nonzero thermal bias in nonlinear lattice junctions [10]. Three necessary conditions for emergence and control of heat current are nonequilibrium source, symmetry breaking, and nonlinearity [11,12]. It is pronounced that thermal rectifying results from symmetry breaking of system. The authors of Ref. [13] studied heat conduction in anharmonic lattices with mass gradient, and found phenomena of negative differential thermal resistance (NDTR) [14] and thermal rectification [15–18]. In fact, a steady heat current against thermal bias also occurs in symmetric systems.

In this paper, we will investigate analytically the heat conduction via two segments of symmetric coupled Frenkel-Kontorova (FK) nonlinear lattices that are sandwiched between two heat baths, and consider effect of coupling displacement between them on heat current. It will be seen that the coupling displacement plays a crucial role in determining magnitude and direction of the heat current. The paper is constructed as follows: First, model and theoretical analysis of heat conduction of the symmetric system are presented. An analytical expression of heat current will be derived. Then results and discussions are provided. Finally conclusions are made.

II. MODEL AND THEORETICAL ANALYSIS

Here we study the heat conduction of two segments of coupled Frenkel-Kontorova lattices [19,20] with a coupling displacement, and their two ends contact with two heat baths, respectively. The nonlinear lattices' Hamiltonian reads

$$H = \sum_{i=1}^{N_1}\left[\frac{p_i^2}{2m} + \frac{1}{2}k_L(q_i - q_{i-1})^2 + \frac{V_L}{(2\pi)^2}\cos\left(\frac{2\pi q_i}{a}\right)\right] + \frac{k_{\text{int}}}{2}(q_{N_1+1} - q_{N_1} + d)^2 + \sum_{i=N_1+1}^{N}\left[\frac{p_i^2}{2m} + \frac{1}{2}k_R(q_{i+1} - q_i)^2 + \frac{V_R}{(2\pi)^2}\cos\left(\frac{2\pi q_i}{a}\right)\right], \quad (1)$$

where p_i is the momentum for the ith atom, m is the atom mass, the $q_i = x_i - ia$ denotes the displacement from the equilibrium position ia for the ith atom, a is the lattice period, k_L and k_R are the spring constants, V_L and V_R are the on-site potentials a of the FK lattices, k_{int} is the coupling strength between the two segments of FK Lattices, and d is the coupling displacement. The coupling displacement may be formed in the coupling process between the two segments of FK lattices. Depending on the sign of d, the system will tend to bend to left or right. Another physical motivation is based on design

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of devices similar to the structure ABA (e.g., the Josephson junction), and d is the thickness of layer B.

The first atom and the Nth atom are assumed to be put into contact with two Langevin heat baths possessing temperature T_L and T_R, respectively. The two heat baths are two Gaussian white noises, satisfying the following statistical properties:

$$\langle \xi_{L/R}(t)\rangle = 0, \quad \langle \xi_{L/R}(t)\xi_{L/R}(t')\rangle = 2k_B\eta T_{L/R}\delta(t-t'), \tag{2}$$

where k_B is the Boltzmann constant, and η denotes the coupling strength between system and heat bath. Let the temperatures of the two heat baths oscillate periodically at angular frequencies ω and ω_1 with driving strengths A and A_1, respectively. This yields

$$\begin{aligned} T_L(t) &= T_0[1+\Delta + A\sin(\omega t)], \\ T_R(t) &= T_0[1-\Delta + A_1\sin(\omega_1 t)], \end{aligned} \tag{3}$$

where $T_0 = \overline{[T_L(t)+T_R(t)]}/2$ is the temporally averaged environmental reference temperature, and $\Delta = \overline{[T_L(t)-T_R(t)]}/T_0$ represents the normalized temperature difference.

In order to open out analytically intrinsic mechanism of the heat conduction, we simplify the system, and think that it only consists of two atoms coupled by a spring. Thus, in the overdamped case and under fixed boundary conditions, the Langevin equations describing the system are given by

$$\dot{q}_1 = -k_L q_1 - k_{\text{int}}(q_1 - q_2 + d) + f(q_1) + \xi_L(t), \tag{4}$$

$$\dot{q}_2 = -k_R q_2 + k_{\text{int}}(q_1 - q_2 + d) + f(q_2) + \xi_R(t), \tag{5}$$

where the periodic force $f(q_i) = -\frac{V_0}{2\pi a}\sin(\frac{2\pi q_i}{a})$, (i = 1,2, $V_L = V_R = V_0$). As $k_L = k_R = k$, the system is symmetric.

Applying adiabatic approximation to Eqs. (4) and (5), the following Langevin equation with one variable can be obtained

$$\dot{x} = H(x) + g_1(x)\xi_L(t) + g_2(x)\xi_R(t), \tag{6}$$

where

$$\begin{aligned} x &= \frac{q_1+q_2}{2}, \quad H(x) = -kx + F(x) + \frac{\left[Q(x)+\frac{1}{2}kd\right]G(x)}{2k_{\text{int}}+k-R(x)}, \\ g_1(x) &= \frac{1}{2}\left[1+\frac{G(x)}{2k_{\text{int}}+k-R(x)}\right], \quad g_2(x) = \frac{1}{2}\left[1-\frac{G(x)}{2k_{\text{int}}+k-R(x)}\right], \end{aligned} \tag{7}$$

with

$$\begin{aligned} F(x) &= \frac{f(x-d/2)+f(x+d/2)}{2}, \quad G(x) = \frac{f'(x-d/2)-f'(x+d/2)}{2}, \\ Q(x) &= \frac{f(x-d/2)-f(x+d/2)}{2}, \quad R(x) = \frac{f'(x-d/2)+f'(x+d/2)}{2}. \end{aligned}$$

As the time scales of ω^{-1} and ω_1^{-1} of the temperature manipulation of the heat baths are assumed to vary much slower than the time scale to reach local thermal equilibrium, the Fokker-Planck equation corresponding to Eqs. (2) and (6) can be written into [21]

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\{[H(x)+g(x)g'(x)]P(x,t)\} + \frac{\partial^2}{\partial x^2}[g^2(x)P(x,t)], \tag{8}$$

where $g(x) = \sqrt{g_1^2(x)T_L(t)+g_2^2(x)T_R(t)}$, and dimensionless parameters are used, with $k_B = 1$, $\eta = 1$.

In the steady state, the stationary probability distribution function of the system is easily given by

$$p_{st}(x) = \aleph e^{-U(x)}, \tag{9}$$

where $\aleph$ is the normalization constant, and the generalized potential $U(x) = -\int^x \frac{H(x)-g(x)g'(x)}{g^2(x)}dx$.

In terms of Eq. (9), ensemble averages of some functions about the system's state variable x can be calculated. According to definition of thermal current and using Novikov's theorem [22,23], therefore, we can derive the analytical expression of thermal current of the system

$$\begin{aligned} J(t) &= k_{\text{int}}\langle \dot{q}_2(q_2-q_1+d)\rangle = k_{\text{int}}\left\{\left\langle H(x)\left[2d-\frac{2Q(x)+kd}{2k_{\text{int}}+k-R(x)}\right]\right\rangle + 2T_L(t)\left\langle g_1(x)\frac{\partial N_1(x)}{\partial x}\right\rangle\right. \\ &\left. + 2T_R(t)\left\langle g_2(x)\frac{\partial N_2(x)}{\partial x}\right\rangle + 4T_L^2(t)\left\langle g_1(x)\frac{\partial}{\partial x}\left[g_1(x)\frac{\partial N_3(x)}{\partial x}\right]\right\rangle + 4T_R^2(t)\left\langle g_2(x)\frac{\partial}{\partial x}\left[g_2(x)\frac{\partial N_4(x)}{\partial x}\right]\right\rangle\right\}, \end{aligned} \tag{10}$$

with

$$\begin{aligned} N_1(x) &= \left[2d-\frac{2Q(x)+kd}{2k_{\text{int}}+k-R(x)}\right]g_1(x) - \frac{H(x)}{2k_{\text{int}}+k-R(x)}, \\ N_2(x) &= \left[2d-\frac{2Q(x)+kd}{2k_{\text{int}}+k-R(x)}\right]g_2(x) + \frac{H(x)}{2k_{\text{int}}+k-R(x)}, \\ N_3(x) &= -\frac{g_1(x)}{2k_{\text{int}}+k-R(x)}, \quad N_4(x) = \frac{g_2(x)}{2k_{\text{int}}+k-R(x)}, \end{aligned}$$

where the sign $\langle\rangle$ represents the ensemble average.

After taking the average of Eq. (10) about t over one period of $2\pi/\omega$, we obtain the final analytical expression of the thermal current

$$J = \frac{\omega}{2\pi}\int_0^{\frac{2\pi}{\omega}} J(t)dt. \tag{11}$$

III. RESULTS AND DISCUSSIONS

From Eqs. (9)–(11), we can calculate numerically the thermal current as functions of the system's parameters, and the results were plotted in Figs. 1–7.

First, let us discuss the case of $d = 0$, i.e., without the coupling displacement between the two atoms. The system only possesses one kind of lattice. But modulating the temperature amplitudes A and/or A_1 of oscillations of the two heat baths can control magnitude and direction of the thermal current. The thermal current J as functions of A and A_1 at different values of normalized temperature differences were plotted in Figs. 1 and 2, respectively. Figure 1 indicates that the thermal current gradually decreases with A increasing as the other parameters are unchanged. In other words, the periodic oscillation of temperature of the heat bath with higher temperature will generate the impact that the heat goes from the lower-temperature heat bath to the higher-temperature heat bath through the lattices. The higher the temperature difference Δ and the greater the oscillation amplitude of the lower-temperature heat bath A_1, the greater the temperature oscillation amplitude of the higher-temperature heat bath that forms negative thermal currents. But with the increment of A_1, the thermal current gradually increases, see Fig. 2. This means that the temperature oscillation of the lower-temperature heat bath will induce heat to flow from the lower-temperature heat bath to the higher-temperature heat bath through the lattices. So it is deduced easily that as the temperature difference is equal to zero, the direction of the heat conduction is completely determined by the oscillation amplitudes of temperatures of the two heat baths, namely, $J < 0$ for $A > A_1$, while $J > 0$ for $A < A_1$. The ratchet

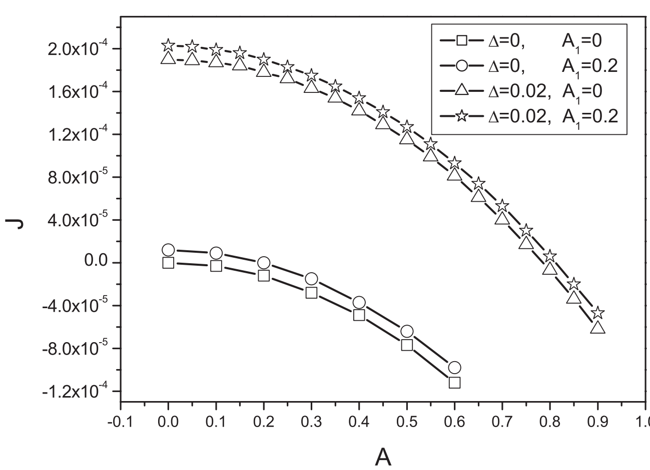

FIG. 1. The thermal current J vs higher temperature oscillation amplitude A for different normalized temperature differences: $\Delta = 0,0.02$ and different lower temperature amplitudes: $A_1 = 0,0.2$. The other parameters are $d = 0$, $k = 1$, $k_{\text{int}} = 0.2$, $a = 1$, $V_0 = 0.5$, $T_0 = 0.09$, $\omega = \omega_1 = 2\pi \times 0.001$.

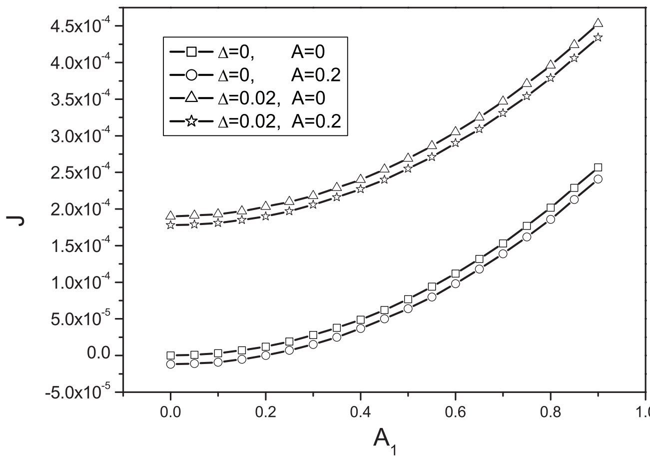

FIG. 2. J vs A_1 for different values of Δ and A. The other parameters are the same as in Fig. 1.

effects come from asymmetries of the rocking heat baths. In the process of numerical calculation, we also found that the magnitude and direction of the thermal current are independent of oscillation frequencies of temperature. This is due to the application of the adiabatic approximation to Eqs. (4) and (5), in which the modulation frequency is much slower than the system's oscillation frequency.

As the coupling displacement d is not equal to zero, we equally calculated the thermal current J as a function of d at different values of normalized temperature differences via Eqs. (9)–(11), and the results were displayed in Fig. 3. Figure 3 shows that as the coupling displacement is increased, the thermal current makes a periodic oscillation, whose amplitude also becomes greater and greater. This means that an optimal coupling displacement can make the thermal current maximal. The point is very similar to reflection-enhancing (or suppressing) coatings in optics. In addition, it tells us that as the temperature difference Δ is comparatively smaller, e.g., $\Delta = 0, 0.1$, the greater coupling displacement can induce negative thermal currents. It can be seen from the Langevin Eq. (6) that the periodically oscillatory behavior of the

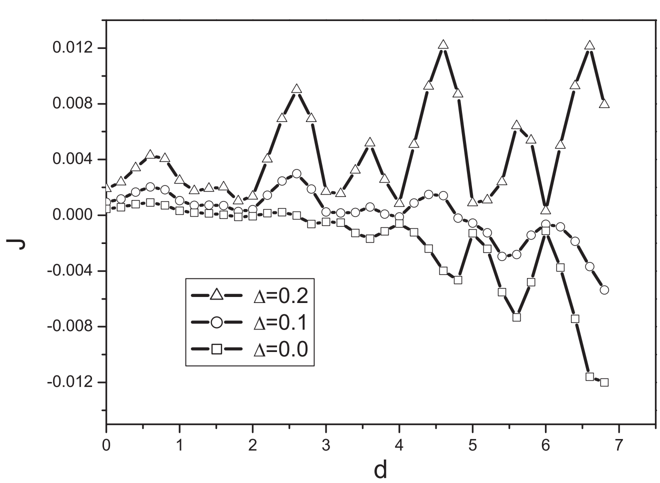

FIG. 3. The dependence of J on the coupling displacement d for different values of Δ, with $A = 0.2$, $A_1 = 0$. The other parameters are the same as in Fig. 1.

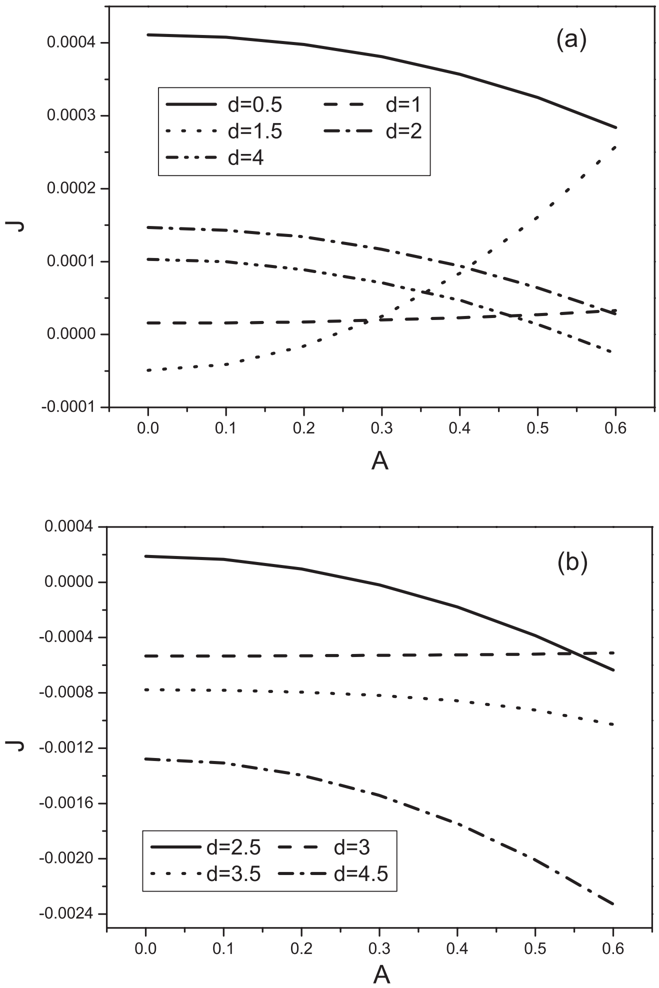

FIG. 4. J vs A at different values of d, (a) for $d = 0.5,1,1.5,2,4$; (b) for $d = 2.5,3,3.5,4.5$. The other parameters are $A_1 = 0$, $\Delta = 0.02$, $k = 1$, $k_{\text{int}} = 0.2$, $a = 1$, $V_0 = 0.5$, $T_0 = 0.09$, $\omega = \omega_1 = 2\pi \times 0.001$.

thermal current comes from the periodic part of the potential of the FK lattices. So the dynamical behavior only occurs in the lattice system with a periodic potential. Of course, oscillatory period of the thermal current with respect to d depends on the potential's period. The increment of the thermal current's amplitude with d is due to the interaction between the coupling displacement and the periodic potential of the FK lattices, which can be incarnated through the term $\frac{1}{2}kdG(x)/[2k_{\text{int}} + k - R(x)]$ of Eq. (7). Noting that its amplitude is modulated by d, and $G(x)$ and $R(x)$ are two periodic functions concerned with d, so the term can take both positive and negative values. As the term is smaller than zero, the potential corresponding to this force is greater than zero. This is equivalent to the case that another potential is added to the system to enhance the interaction between the two atoms, and make the thermal current magnified. Contrariwise, the thermal current is reduced. Essentially, the ratchet effect in Fig. 3 also comes from symmetry breaking caused by the coupling displacement. From Eq. (1), it can be easily seen that the nonzero d destroys the reflection symmetry between the two segments of FK lattices. For $d = 0$, the atoms of lattice have the same zero equilibrium displacement with $q_i = 0$.

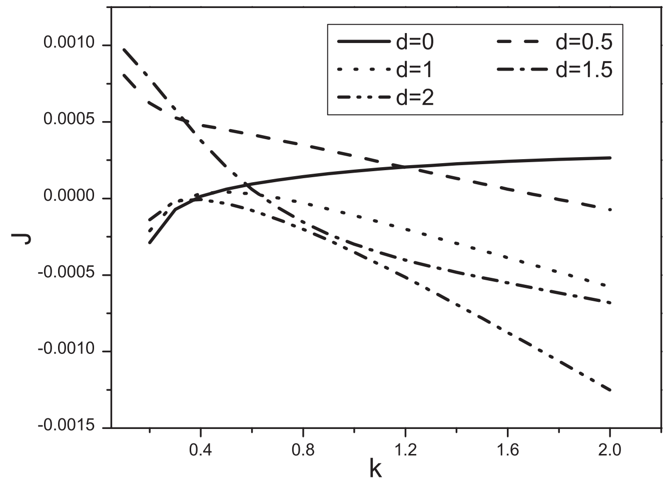

FIG. 5. J vs the spring constant k at different values of d: 0,0.5,1,1.5 and 2, with $A = 0.2$, $A_1 = 0$. The other parameters are the same as in Fig. 4.

But for nonzero d, the equilibrium displacement for q_i will deviate from zero, depending on the sign of d. If the bracket of the term $\frac{k_{\text{int}}}{2}(q_{N_1+1} - q_{N_1} + d)^2$ in Eq. (1) is open, we will obtain a standard interaction $\frac{k_{\text{int}}}{2}(q_{N_1+1} - q_{N_1})^2$ and a linear term $k_{\text{int}}(q_{N_1+1} - q_{N_1})d$. The linear term means that a force $k_{\text{int}}d$ exerts on the system, and makes the system's symmetry broken. The two atoms along the link spring bend the most and induce strong asymmetry. But the asymmetry effect will decrease as more and more atoms are considered.

Now let us discuss the effect of temperature manipulation on the thermal current in the case of $d \neq 0$. As the normalized temperature difference remains at a lower level of $\Delta = 0.02$, modulating the temperature oscillation amplitude of one end can cause some interesting dynamical behaviors. Figure 4 is the dependence of the thermal current on A at different values of d for $A_1 = 0$. It can be seen from Fig. 4 that: (i) As $A = 0$, the coupling displacement d can induce certain thermal current, even negative current for some values of d (e.g., $d = 1.5,3,4.5$). The emergence of the negative thermal

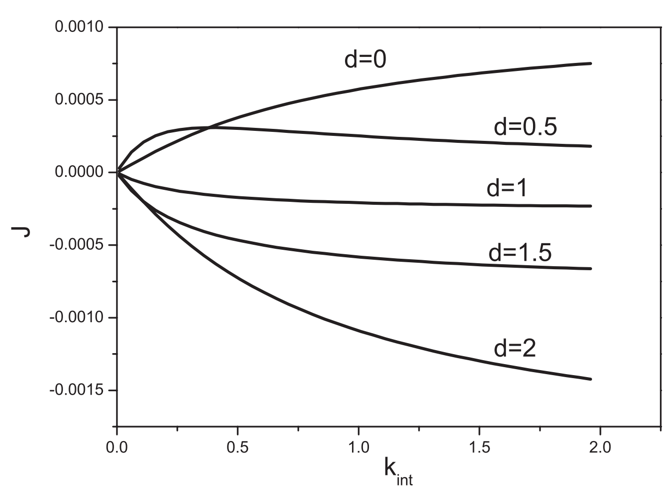

FIG. 6. J vs the coupling strength k_{int} at different values of d: 0,0.5,1,1.5 and 2, with $k = 1$. The other parameters are the same as in Fig. 5.

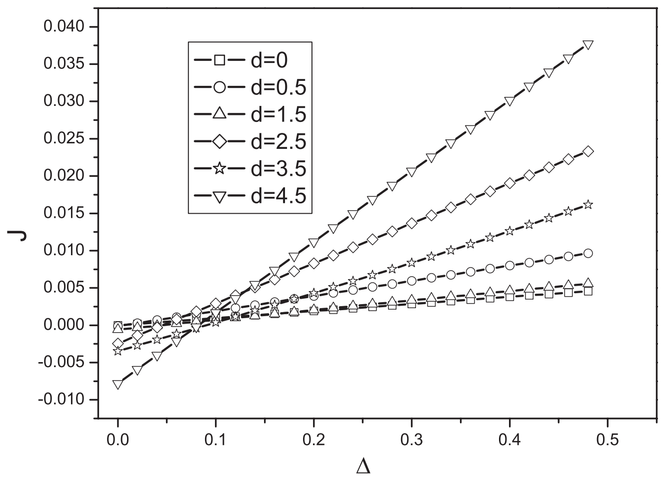

FIG. 7. J vs Δ at different values of d: 0,0.5,1.5,2.5,3.5,4.5, with $A = A_1 = 0$. The other parameters are the same as in Fig. 4.

current in the positive temperature bias is also brought about by the interaction between the coupling displacement and the periodic potential of the FK lattices. (ii) The thermal current can both increase and decrease monotonically with A increasing, dependent on d. As appropriate values of d are taken, modulating the temperature oscillation amplitude A can induce reversal of the thermal current. Of course, the change of the thermal current with A_1 also relies on d.

Figures 5 and 6 reflect the changes of the thermal current with the spring constant k of lattice and the coupling strength k_{int} between the two kinds of lattices at various values of d, respectively. Figure 5 indicates that the trend of the thermal current with k also depends on d. As $d = 0$, the thermal current first increases with k increasing then gradually approaches to saturation, which is due to that the increment of k means enhancement of the spring potential of lattice in a finite coupling strength k_{int}. But as $d \neq 0$, the thermal current as a function of k exhibits either monotonically decreasing behavior (e.g., $d = 0.5,1.5$) or nonmonotonic behavior (e.g., a peak for $d = 1,2$). Additionally, the coupling displacement d also affects the change of the thermal current J with k_{int}, see Fig. 6. As $d = 0$, the thermal current monotonically goes up with k_{int}. With the increment of d (e.g., $d = 0.5$), the monotonic behavior gradually vanishes, and a peak appears. As d is further increased, the system displays monotonically decreasing behavior of J vs k_{int}.

The dependence of the thermal current J on the normalized temperature difference Δ at various values of d is drawn in Fig. 7 as $A = A_1 = 0$. From Fig. 7, we can see that the thermal current is directly proportional to the temperature difference, and slopes of these lines are affected by the coupling displacement d. As $d = 0$, the change of J vs Δ is a line through the origin. But for $d \neq 0$, intercepts of the lines are not equal to zero. Their slopes make periodic oscillations with d. This means that heat conductivity of the system exhibits oscillatory behavior with d because the slopes reflect magnitudes of heat conductivity to some degree. Because the heat conduction we considered here takes place in the system of symmetric FK lattices, some phenomena (e.g., thermal rectification and NDTR) can not be observed.

IV. CONCLUSION

Until now, we have investigated the heat conduction of the symmetric FK lattices with the coupling displacement. Applying adiabatic approximation to the system, the analytical expression of the thermal current were obtained. Although the system was simplified in order to get analytical solution of the thermal current, we can open out explicitly intrinsic mechanism of the heat conduction. The Langevin Eq. (6) shows clearly that the mass center of the two FK atoms is acted on by two kinds of potentials (i.e., spring and periodic potentials) and driven by two multiplicative noises. The interaction of the coupling displacement with the periodic potential makes the system display some interesting dynamical behavior. Whether there is a temperature difference between the two heat baths or not, the thermal current and the thermal conductivity oscillate periodically with d. The coupling displacement can induce a certain thermal current, even a negative current for a lower normalized temperature difference. The coupling displacement also can cause both increment and decrement of the thermal current with temperature oscillation amplitude, even for the appropriate values of d, modulating the temperature oscillation amplitude can induce reversal of the thermal current. In addition, the coupling displacement can induce nonmonotonic behaviors of the thermal current as functions of the spring constant of lattice and the coupling strength.

From the above findings, we can further understand the role that the coupling displacement plays in the process of heat conduction. And it is concluded that as long as systems of coupled lattices possess ingredients of periodic potential, the coupling displacement must act with the periodic potential and make dynamical properties of the systems more complex, especially for the systems with asymmetric lattices. Because dynamical behavior of heat conduction depends on potential and dimension of lattices to some degree [24,25], devotion of d to heat conduction of asymmetric lattices without periodic potential will be also an important research topic.

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[1] V. P. Carey *et al.*, Nanoscale Microscale Thermophys. Eng. **12**, 1 (2008).

[2] S. Lepria, R. Livib, and A. Politib, Phys. Rep. **377**, 1 (2003).

[3] B. Li, L. Wang, and G. Casati, Phys. Rev. Lett. **93**, 184301 (2004).

[4] T. S. Komatsu and N. Ito, Phys. Rev. E **81**, 010103(R) (2010).

[5] B. Li, L. Wang, and G. Casati, Appl. Phys. Lett. **88**, 143501 (2006).
[6] L. Wang and B. Li, Phys. Rev. Lett. **99**, 177208 (2007).
[7] L. Wang and B. Li, Phys. Rev. Lett. **101**, 267203 (2008).
[8] C. W. Chang, D. Okawa, A. Majumdar, and A. Zettl, Science **314**, 1121 (2006).
[9] P. J. Jones, J. A. M. Huhtamäki, K. Y. Tan, and M. Möttönen, Phys. Rev. B **85**, 075413 (2012).
[10] N. Li, P. Hänggi, and B. Li, Europhys. Lett. **84**, 40009 (2008).
[11] J. Ren and B. Li, Phys. Rev. E **81**, 021111 (2010).
[12] N. Li, F. Zhan, P. Hänggi, and B. Li, Phys. Rev. E **80**, 011125 (2009).
[13] N. Yang, N. Li, L. Wang, and B. Li, Phys. Rev. B **76**, 020301(R) (2007).
[14] J. P. Wu, L. Wang, and B. Li, Phys. Rev. E **85**, 061112 (2012).
[15] B. Hu, L. Yang, and Y. Zhang, Phys. Rev. Lett. **97**, 124302 (2006).
[16] M. Peyrard, Europhys. Lett. **76**, 49 (2006).
[17] D. Segal and A. Nitzan, Phys. Rev. Lett. **94**, 034301 (2005).
[18] M. Terraneo, M. Peyrard, and G. Casati, Phys. Rev. Lett. **88**, 094302 (2002).
[19] O. M. Braun and Y. S. Kivshar, Phys. Rep. **306**, 1 (1998).
[20] B. Hu, B. Li, and H. Zhao, Phys. Rev. E **57**, 2992 (1998).
[21] H. Risken, *The Fokker-Planck Equation* (Springer-Verlag, Berlin, 1984).
[22] V. V. Konotop and L. Vazquez, *Nonlinear Random Waves* (World Scientific, Singapore, 1994).
[23] N. Goldenfeld, *Lecture on Phase Transitions and the Renormalization Group* (Addison-Wesley, New York, 1992).
[24] L. Wang, D. He, and B. Hu, Phys. Rev. Lett. **105**, 160601 (2010).
[25] D. Roy, Phys. Rev. E **86**, 041102 (2012).