Asymmetric heat conduction through a weak link

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We study the heat conduction of two nonlinear lattices joined by a weak harmonic link. When the system reaches a steady state, the heat conduction of the system is decided by the tunneling heat flow through the weak link. We present an analytical analysis by the combination of the self-consistent phonon theory and the heat tunneling transport formalism, and then the tunneling heat flow can be obtained. Moreover, the nonequilibrium molecular dynamics simulations are performed and the simulations results are consistent with the analytical predictions.

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The study of electric currents has led to the invention of electric rectifiers, diodes, and transistors. An interesting problem is the following: Can we design a thermal diode as we do for electric conductivity? A thermal diode refers to the general thermal tunneling transport formalism and the heat tunneling transport formalism, and then the tunneling heat flow can be obtained. Moreover, the nonequilibrium molecular dynamics simulations are performed and the simulations results are consistent with the analytical predictions.

In this paper, we consider a model of the thermal diode that consists of two different Morse on-site potential lattices coupled by a weak harmonic spring. Two heat baths respectively connect to two ends of the model. The two lattices will achieve two nearly equilibrium states of different temperatures, since the strength of the harmonic spring is weak. Then the self-consistent phonon (SCP) theory can take into consideration the nonlinearity of the lattices. The SCP theory has been applied to deal with the nonlinear Morse on-site potential for the DNA denaturation problem [6]. Thus we can use the general thermal tunneling transport formalism [7] to calculate the heat flux through the weak harmonic spring. When the system approaches the steady state, the heat flux in every site should be identical and the total heat flux can be obtained.

The Hamiltonian is

\[
H = H_L + \frac{k_3}{2}(q_1 - q_0)^2 + H_R,
\]

FIG. 1. Plot of \(J\) versus the dimensionless temperature difference \(\Delta\) at \(T_0 = 13.33\), \(k_3 = 0.05\). Here \(J\) is obtained on the thermodynamical limit and \(k_3 \to 0\).

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FIG. 2. (Color online) Plot of temperature profiles $T_i$; the inset shows the heat flux. Here, $N=64$, $T_s=26$, and $T_- =3$.

$$H_L = \sum_{i=-N/2+1}^{0} \left( \frac{p_i^2}{2m_i} + \frac{k_1}{2}(q_{i+1} - q_i)^2 + D_1(e^{-\alpha_1 q_i} - 1)^2 \right),$$

$$H_R = \sum_{i=1}^{N/2} \left( \frac{p_i^2}{2m_i} + \frac{k_2}{2}(q_{i+1} - q_i)^2 + D_2(e^{-\alpha_2 q_i} - 1)^2 \right),$$

(1)

where $N$ is the total number of the particles, $m_i = 1$ the mass of particles, $p_i$ the momentum of the $i$th particle, and $q_i$ its displacement from the equilibrium position. $k_1$, $k_2$, and $k_3$ are the strength of the interparticle harmonic potential, $k_1 = k_2 = 1$. For the left segment $D_1 = 30$, and $\alpha_1 = 0.316$; for the right segment $D_2 = 20$ and $\alpha_2 = 0.316$. When the heat bath $T_s$ connects with the $i$th $(i=-N/2+1)$ particle, $T_-$ connects with the $i$th $(i=N/2)$ particle, the heat flux $J_+$ goes through the system, and $J_+ = j \cdot N$ is the total heat flux. When the heat bath $T_-$ connects with the $i$th $(i=-N/2+1)$ particle, $T_s$ connects with the $i$th $(i=N/2)$ particle, the heat flux $J_-$ goes through the system, and $J_- = j \cdot N$ is the total heat flux.

$H_L$ and $H_R$ can be approximated [6] by the SCP theory as

$$H_L = \sum_{i=-N/2+1}^{0} \left( \frac{p_i^2}{2} + \frac{k_1}{2}(q_{i+1} - q_i)^2 + f_1(q_i) \right),$$

$$H_R = \sum_{i=1}^{N/2} \left( \frac{p_i^2}{2} + \frac{k_2}{2}(q_{i+1} - q_i)^2 + f_2(q_i) \right),$$

(2)

where the effective harmonic potential coefficient $f_l(T)$ $(l = 1, 2)$ is obtained from the self-consistent equation

$$\ln(2\alpha^2_l D_l f_l) = (\alpha^2_l k_R T/N) \sum_p [1 + f_l + 4k_l \sin^2(p \pi/N)].$$

The general heat flux formula across the weak harmonic spring is

$$J = \sum_{k>0} E_k v_k \alpha_k + \sum_{q<0} E_q v_q \alpha_q,$$

(3)

where $E_k$ and $E_q$ are the energy in the $k$th and $q$th mode, respectively, $v_k$ and $v_q$ the phonon group velocities on the left and right segments, and $\alpha_k$ and $\alpha_q$ the transmission coefficients. Here the reasonable mode-energy distributions of the classical system take $E = k_B T$. The effective phonon group velocities can be obtained from the effective Hamiltonian (2). For the transmission coefficients, we assume a wave incident from the left, which is reflected by the interface with amplitude $r$ and transmits across the interface with amplitude $t$ on the right:

$$q_i = e^{ik_1 a_i} + r e^{-ik_1 a_i}, \quad i \leq 0,$$

$$q_i = te^{ik_2 (i-1) a_2}, \quad i \geq 1,$$

(4)

where $I$ is the imaginary number unit. Through a tedious but straightforward algebraic manipulation, one obtains the transmission coefficient

$$\alpha = 2 \sin(k a_1) \sin(q a_2) k_3^2 \left[ 2 \cos(k a_1) \cos(q a_2) - \cos(k a_1) \cos(q a_2) - 1 \right] [k_1 k_2 - (k_1 + k_2) k_3] + 1 + \frac{k_1}{k_2} + \frac{k_2}{k_1}$$

$$+ \cos(k a_1 - q a_2) - \frac{k_1}{k_2} \cos(k a_1) - \frac{k_1 + k_2}{k_1} \cos(q a_2).$$

(5)

Thus the heat flux across the weak harmonic spring is obtained.

As $k_3 \rightarrow 0$, the transmission coefficient is

$$\alpha(\omega) = \frac{k_3^2}{k_1 k_2} \sqrt{\frac{(f_1 + 4k_1 - \omega^2) (f_2 + 4k_2 - \omega^2)}{(\omega^2 - k_1)(\omega^2 - k_2)}},$$

(6)

where $\omega^2 = f_1 + 4k_1 \sin^2(k a_1/2) = f_2 + 4k_2 \sin^2(q a_2/2)$. In the thermodynamical limit, we can use the integral by $\omega$ substituting the sum by $q$ in formula (3),

$$J = k_B(T_s - T_-) \int_{\omega_{\text{min}}}^{\omega_{\text{max}}} \alpha(\omega) d\omega.$$

(7)

Bringing the formula (6) into the formula (7), we obtain
...in this case and the inset shows the heat flux profiles at the same parameters. For the NEMD simulations results in Fig. 3, Fig. 4, and Fig. 6, the temperature profiles achieve nearly two equilibrium states on two heat baths’ temperature, respectively. For the NEMD simulations results in Fig. 3, Fig. 4, and Fig. 6, the temperature profiles are checked to ensure nearly equilibrium states.

The relation of \( J \) and \( \Delta \) is shown in Fig. 3; the line indicates only the line of sight. Here the solid circles show \( J \) by the analytical estimations with formula (3) at finite size \( N = 64 \). The solid squares show \( J \) by the NEMD simulations. The two curves exhibit similar behaviors; the difference between two sets of data is generally less than 10%. They both show a clear rectifying effect. We also investigate the relation of \( |J_r| \) and \( k_3 \) in Fig. 4. The NEMD simulations are consistent with the analytical estimations, and they both show the relation \( |J_r| \sim k_3^2 \) as \( k_3 < 0.1 \); the dotted lines show the functions \( |J_r| \sim k_3^2 \). The results show well the consistency of the NEMD simulations and the analytical estimations.

For the nonlinear on-site potential lattice, its thermal conductivity obeys Fourier’s law and its total heat flux is independent of the system size. However, the simulation results show that the total heat flux of the two segment diode models increase by the system size. In Fig. 3, the dependence of \( J \) for \( \Delta > 0 \) and \( \Delta \) is nearly zero for \( \Delta < 0 \). As \( \Delta < -0.9 \), \( J \) is exactly equal to zero and the gain \( r \rightarrow \infty \). The results are qualitatively the same as the NEMD simulations results of a similar model in Refs. [2,5].

The NEMD simulations are performed on the model. The heat baths are implemented as Nose-Hoover [8] baths in the simulations. The particles from \( i = -N/2 + 2 \) to \( i = N/2 - 1 \) follow the Hamiltonian equations of motion, while \( \dot{q}_{-N/2+1} = -\xi_5 \dot{q}_{-N/2+1} - \partial H/\partial q_{-N/2+1}, \dot{q}_{N/2} = -\xi_5 \dot{q}_{N/2} - \partial H/\partial q_{N/2}, \) and \( \xi_5 = q_{-N/2+1}/T_x - 1, \xi_5 = q_{N/2}/T_x - 1. \) The heat flux \( j \) takes the general expression of the heat flux [9]. Richardson’s method is used on the integration [10]. The total integration time is typically \( 10^8 \) to \( 10^9 \) units.

Figure 2 shows typical temperature profiles of the system and the inset shows the heat flux profiles at the same parameters, in this case \( |J_r| > |J_\perp| \) and \( r \sim 6 \). The left and right segments achieve nearly two equilibrium states on two heat baths’ temperature, respectively. For the NEMD simulations results in Fig. 3, Fig. 4, and Fig. 6, the temperature profiles are checked to ensure nearly equilibrium states.

The relation of \( J \) and \( \Delta \) is shown in Fig. 3; the line indicates only the line of sight. Here the solid circles show \( J \) by the analytical estimations with formula (3) at finite size \( N = 64 \). The solid squares show \( J \) by the NEMD simulations. The two curves exhibit similar behaviors; the difference between two sets of data is generally less than 10%. They both show a clear rectifying effect. We also investigate the relation of \( |J_r| \) and \( k_3 \) in Fig. 4. The NEMD simulations are consistent with the analytical estimations, and they both show the relation \( |J_r| \sim k_3^2 \) as \( k_3 < 0.1 \); the dotted lines show the functions \( |J_r| \sim k_3^2 \). The results show well the consistency of the NEMD simulations and the analytical estimations.

For the nonlinear on-site potential lattice, its thermal conductivity obeys Fourier’s law and its total heat flux is independent of the system size. However, the simulation results show that the total heat flux of the two segment diode models increase by the system size \( N \), where each segment is a FK lattice. For the model (1), the dependence of \( J \) on \( N \) for each segment is shown in Fig. 5. As the system size changes from \( N = 128 \) to \( 1024 \), the total heat fluxes \( J \) of \( H_L \) or \( H_R \) approach a constant as expected. In Fig. 6, the dotted lines show the functions \( |J_r| \sim N \); for the model (1) the NEMD simulation results and the analytical estimations of the total

FIG. 4. (Color online) Plot of \( J \) versus \( k_3 \). Here \( T_0 = 13.33 \) and \( \Delta = 0.5 \).

FIG. 5. (Color online) Plot of \( J \) versus \( N \) for pure Morse on-site potential models \( H_L (D = 30) \) and \( H_R (D = 20) \).

FIG. 6. (Color online) Plot of \( J \) versus \( N \); here \( T_0 = 13.33, \Delta = 0.5 \), and \( k_3 = 0.05 \).
heat flux $J(N)$ are shown. They nearly overlap and $|J_s|$ is in direct ratio to the system size $N$.

Here we need to clarify that the analytical estimation holds true only as the coupling between two segments is weak enough. Figure 7 shows the NEMD simulation results for different $k_3$ as the system size $N$ increases. For $k_3=0.25$, the NEMD simulation results leave the analytical estimations ($|J_s| \propto N$) at the separate point $N_0 \approx 100$. For $k_3=0.1$, the separate point $N_0$ increases as $k_3$ decreases. This means that the NEMD simulations will separate from the analytical estimations as the coupling $k_3$ is strong enough for a fixed system size $N$. When we check the temperature profiles, the two segments are no longer nearly in equilibrium states. The analytical analysis is not reliable on these cases.

In summary, we consider a model consisting of two different Morse on-site potential lattices coupled by a weak harmonic spring. Using the SCP theory and the general thermal tunneling transport formalism, the heat flux through the system can be estimated. The NEMD simulations are also performed. As $k_3$ is small enough for a fixed $N$, one can predict the NEMD simulation results by the analytical estimations quite well.

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