Scaling and the thermal conductivity of the Frenkel-Kontorova model

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We have studied the dependence of the thermal conductivity κ on the strength of the interparticle potential λ and the strength of the external potential β in the Frenkel-Kontorova model. We found that the functional relation can be expressed in a scaling form, $\kappa \propto \frac{\lambda^{3/2}}{\beta^2}$. This result is first obtained by nonequilibrium molecular dynamics. It is then confirmed by two analytical methods, the self-consistent phonon theory and the self-consistent stochastic reservoirs method. The thermal conductivity κ is therefore a decreasing functon of β and an increasing function of λ.

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I. INTRODUCTION

The Frenkel-Kontorova (FK) model was originally proposed by Frenkel and Kontorova in 1938 to study surface phenomena [1,2]. Since then it has been applied to a variety of physical systems, such as adsorbed monolayers, Josephson junctions, charge density waves, magnetic spirals, tribology, and DNA denaturation. Because of its relation to elementary excitations, the FK model has attracted special attention in different branches of solid state physics. In the continuum-limit approximation, the FK model reduces to the exactly integrable sine-Gordon (SG) equation which describes simultaneously three different types of elementary excitations: phonons, kinks, and breathers. To date, discreteness of the FK model has provided deep physical insights into the dynamics of nonlinear excitations, despite the fact that the FK model is not exactly integrable.

The Hamiltonian of the FK model is

$$H=\sum_{i=1}^{N}\left[\frac{p_i^2}{2m}+\frac{\lambda}{2}(q_{i+1}-q_i-l_0)^2+\beta\left(1-\cos\frac{\pi}{a}q_i\right)\right], \quad (1)$$

where N is the number of particles, $m=1$ the mass of particles, p_i the momentum of the ith particle, q_i its displacement, $2a$ the periodicity of the external potential, $l_0=2.0$ the natural length of the spring, λ the strength of the interparticle potential, and β the strength of the external potential. l is the atomic mean distance and $\frac{l}{2a}$ is the winding number. If $\frac{l}{2a}$ is a rational number, the FK model is in the commensurate phase; else if $\frac{l}{2a}$ is an irrational number, the FK model is in the incommensurate phase. Despite its simplicity, the FK model exhibits very rich and complex behavior; a prominent example is its heat conduction behavior.

Scaling laws can describe a variety of physical phenomena, such as critical and transport phenomena. A well-known example is single-phase flow in a pipe, where the density ρ, the velocity ν, the pipe diameter D, and the viscosity μ are interrelated via the dimensionless Reynolds number $R_e=\frac{\rho\nu D}{\mu}$. In the FK model, there are four independent parameters λ, β, l_0, and a. An interesting question is whether there also exist scaling laws for nonequilibrium heat transport in the FK model, in addition to the known scaling laws for the equilibrium behavior of the FK model. For equilibrium studies of the FK model [1], one can employ the following rescaled Hamiltonian:

$$H'=\sum_{i=1}^{N}\left[\frac{p_i^2}{2m}+\frac{1}{2}(q_{i+1}-q_i-1)^2+\beta'\left(1-\cos\frac{\pi}{a'}q_i\right)\right], \quad (2)$$

where $\beta'=\frac{\beta}{\lambda l_0^2}$ and $a'=\frac{a}{l_0}$ are the only two independent scaling parameters.

Concerning the parameter dependence of heat conduction in the FK model, Savin and Gendelman studied the temperature dependence of the thermal conductivity [3]. Hu and Yang studied the dependence of the thermal conductivity on the system size N, the strength of the external potential β, and the periodicity $2a$ of this external potential [4,5]. In this paper, we report on a study of the dependence of the thermal conductivity on λ and β, as well as the scaling relation between these two quantities. The study of heat conduction is not purely of theoretical interest; it also has practical implications in heat control and management in nanoscale devices. Terraneo, Peyrard, and Casati pointed out the possibility of designing a thermal diode by coupling three nonlinear chains, where a lattice with a strong Morse on-site potential is sandwiched between two lattices each with a weak Morse on-site potential [6]. Li, Wang, and Casati proposed a higher-gain model that consists of two coupling FK lattices connected by a harmonic spring [7]. Hu, Yang, and Zhang pointed out the valid conditions for the operation of a forward thermal diode, and they found that the rectification can be reversed via a change in the properties of the interface and in the system size [8].

The paper is organized as follows. In Sec. II, the thermal conductivity of the FK model as functions of the parameters λ and β is calculated via nonequilibrium molecular dynamics (NEMD) simulations. In Sec. III, the dependence of the ther-

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mal conductivity on λ and β is studied using the self-consistent phonon (SCP) theory. In Sec. IV, we use the self-consistent stochastic reservoirs method to study the thermal conductivity as functions of the parameters λ and β. In Sec. V, we give our discussions and conclusions.

II. NONEQUILIBRIUM MOLECULAR DYNAMICS

Using nonequilibrium molecular dynamics (NEMD) simulation, we calculate the thermal conductivity of the FK model as functions of the parameters λ and β. In the simulations we use fixed boundary conditions [assumed $q_0=0$, $q_{N+1}=(N+1)l_0$] and the chain is connected to two heat baths at temperatures T_+ and T_-, respectively. $T_+=1.05$ and $T_-=0.95$. In the attempt to provide a self-consistent description of out-of-equilibrium processes, various types of deterministic heat baths have been introduced [9]. This was also motivated by the need to overcome the difficulties of dealing with stochastic processes. The scheme that has received the largest support within the molecular-dynamics community is perhaps the so-called Nośe-Hoover heat baths [10,11]. So Nośe-Hoover heat baths are taken. The Nośe-Hoover heat baths act on the first and the last particle at temperature T_+ and T_-, respectively.

$$\ddot{q}_1 = -\xi_+\dot{q}_1 - \frac{\partial H}{\partial q_1}, \quad \dot{\xi}_+ = \frac{\dot{q}_1^2}{T_+} - 1,$$

$$\ddot{q}_i = -\frac{\partial H}{\partial q_i}, \quad i = 2, \ldots, N-1,$$

$$\ddot{q}_N = -\xi_-\dot{q}_N - \frac{\partial H}{\partial q_N}, \quad \dot{\xi}_- = \frac{\dot{q}_N^2}{T_-} - 1, \tag{3}$$

where H is the Hamiltonian of the FK model. $\xi_\pm$ are two auxiliary variables modeling the microscopic action of the heat baths. The action of the heat baths can be understood in the following terms. Whenever the (kinetic) temperature of the particles connected to heat baths is, say, larger than $T_\pm$, $\xi_\pm$ increases becoming eventually positive. Accordingly, the auxiliary variable acts as a dissipation in Eq. (3). Since the opposite occurs whenever the temperature falls below $T_\pm$, this represents altogether a stabilizing feedback around the prescribed temperature. The dynamical equations are invariant under time reversal $p_i \to -p_i$. This property represents the main reason for the success of this class of heat baths, since dissipation is not included as a priority, but it rather follows self-consistently from the dynamical evolution [12].

The equations of motion are integrated by using a fourth-order Runge-Kutta algorithm [13]. Double-precision floating point computer arithmetic is used and the time step is fixed as $h=0.01$. 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 chain. To obtain a steady state, the total integration is typically 10^9 units. We have checked that this is sufficient for the system to reach a steady state since the temperature profile in the central region is linear and the time-averaged heat flux j_i is independent of the site i, where j is the local heat flux. The local heat flux is defined as $j_i = l_0\lambda\langle \dot{q}_i(q_i - q_{i-1} - l_0)\rangle$ [12]. The local temperature is defined as $T=m\langle \dot{q}_i^2\rangle$. The system is connected to two heat baths with a temperature difference ΔT, the temperature difference $\Delta T = T_+ - T_-$. The thermal conductivity κ is defined as $\kappa = J/\Delta T = jN/\Delta T$, where $J=jN$ is the total heat flux. We should point out that we have performed computations using other types of heat baths, and no qualitative difference was found.

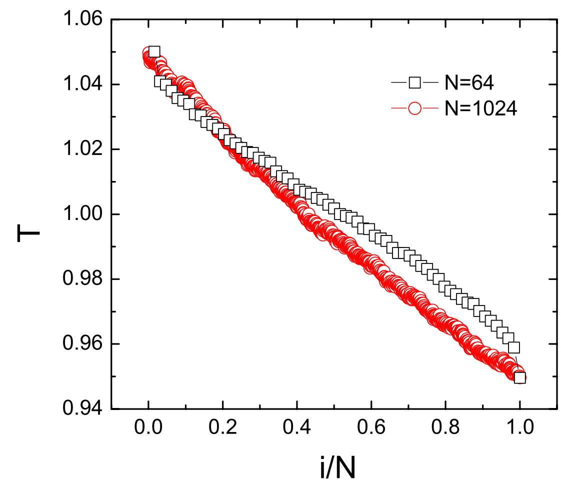

FIG. 1. (Color online) The two temperature profile for system size $N=64$ and 1024 with $\lambda=1$, $\beta=0.5$, $l_0=2$, $a=1$, $T_+=1.05$, and $T_-=0.95$.

When the system size is finite, there is a boundary jump in the temperature profile. It is nontrivial that the conductivity is influenced by the boundary jump [14]. From Ref. [4], when system size increases, the boundary jump will decrease. Figure 1 shows the two temperature profile for system size $N=64$ and 1024 with $\lambda=1$, $\beta=0.5$, $l_0=2$, $a=1$, $T_+=1.05$, and $T_-=0.95$. From Fig. 1, when $N=64$, the boundary jump is obvious, and when $N=1024$, the boundary jump can be neglected. So in the simulations, the system size is taken as $N=1024$.

Figure 2(a) shows the dependence of the thermal conductivity κ on β for various λ with $N=1024$, $l_0=2$, $a=1$, $T_+=1.05$, and $T_-=0.95$. Figure 2(b) shows the rescaled thermal conductivity $\kappa/\lambda^{3/2}$ vs β for various λ. The slope of the dashed line is −2. The results show that the scaling form is

$$\kappa \propto \frac{\lambda^{3/2}}{\beta^2} \tag{4}$$

when β is in the interval [0.05, 0.5]. So, the parameters λ and β can be rescaled when β is in this interval.

III. SELF-CONSISTENT PHONON THEORY

The self-consistent phonon (SCP) theory can take into consideration the nonlinearity of the lattices. In this section, the dependence of the thermal conductivity on λ and β is studied by the SCP theory. The SCP theory has been applied to deal with the nonlinear on-site potential, such as the Morse on-site potential for the DNA denaturation problem [15] and the asymmetric heat transport in the two coupling nonlinear lattices through a weak link [16].

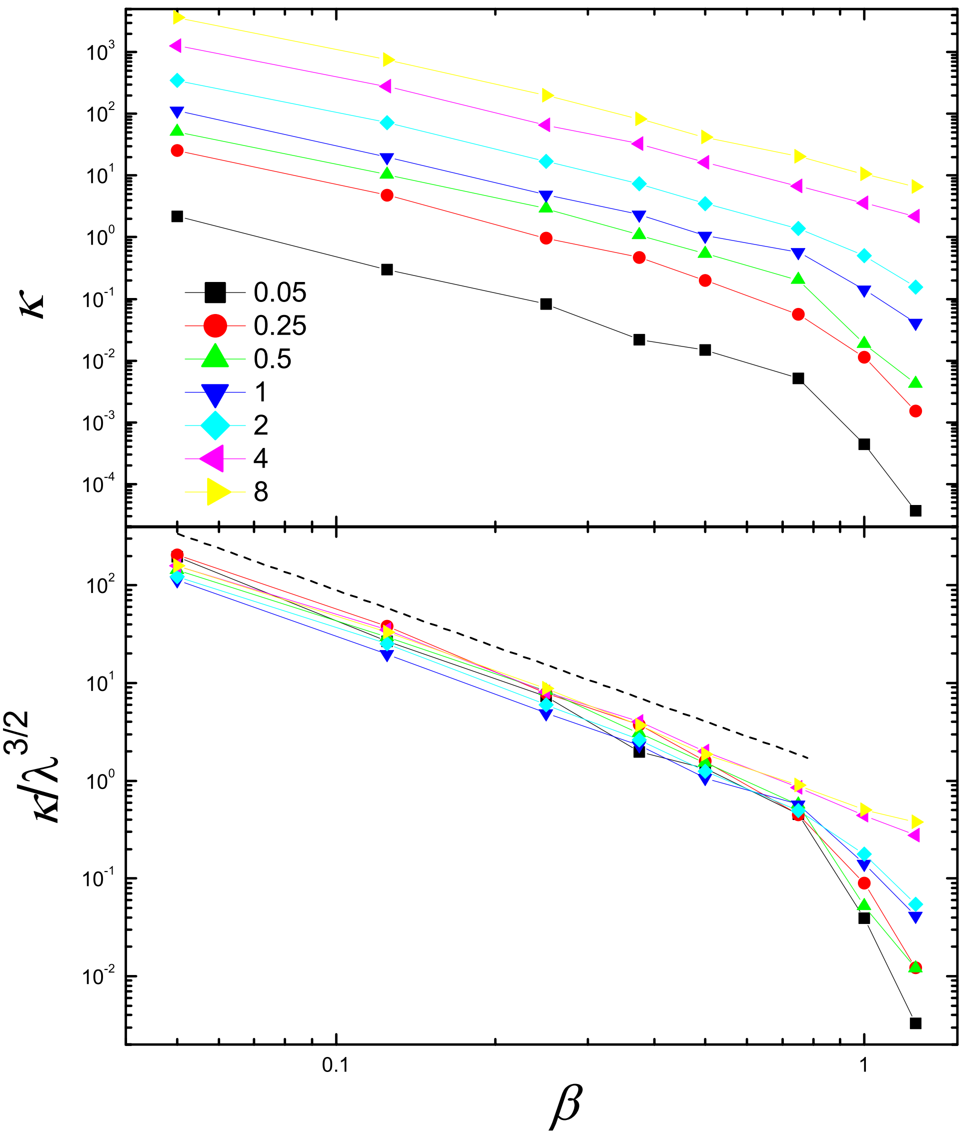

FIG. 2. (Color online) (a) Dependence of the thermal conductivity κ on β for various λ. $N=1024$, $l_0=2$, $a=1$, $T_+=1.05$, and $T_-=0.95$. (b) The rescaled thermal conductivity $\kappa/\lambda^{3/2}$ vs β for various λ. When β is in the interval [0.05, 0.5], the curve is linear. The slope of the dashed line is -2.

Using the SCP theory [15,17], the Hamiltonian of the above FK model can be approximated to an effective harmonic Hamiltonian as

$$H_{eff}=\sum_{i=1}^{N}\left[\frac{p_i^2}{2m}+\frac{\lambda}{2}(u_{i+1}-u_i)^2+\frac{f}{2}u_i^2\right], \tag{5}$$

where u_i is the displacement from the equilibrium position of the ith particle. λ is the strength of the interparticle potential, and f is the effective harmonic potential coefficient. According to the SCP theory, the first and second derivatives of the external potential $V(q_i)=\beta(1-\cos\frac{\pi}{a}q_i)$ are replaced by their thermal average with respect to the effective harmonic Hamiltonian H_{eff}.

Thus one can obtain

$$\left\langle\frac{\partial V}{\partial u_i}\right\rangle=0,$$

$$\left\langle\frac{\partial V}{\partial u_i^2}\right\rangle=f, \tag{6}$$

where the thermal average $\langle A\rangle$ is defined as

$$\langle A(\vec{u},\vec{p})\rangle=\frac{\int\cdots\int A\exp\left[-\frac{1}{k_BT}H_{eff}(\vec{u},\vec{p})\right]d\vec{u}d\vec{p}}{\int\cdots\int \exp\left[-\frac{1}{k_BT}H_{eff}(\vec{u},\vec{p})\right]d\vec{u}d\vec{p}}. \tag{7}$$

Then the effective harmonic potential coefficient f is obtained from the following self-consistent equation deduced from Eqs. (6) and (7) [18]:

$$f=\frac{\pi^2\beta}{a^2}\exp\left[-\frac{\pi^2k_BT}{2a^2\sqrt{f(4\lambda+f)}}\right]. \tag{8}$$

The effective dispersion relation is $\omega_k^2=f+4\lambda\sin^2\frac{k}{2}$. Figure 3 shows the effective dispersion relation ω_k as a function of k for various β with $\lambda=1$, $a=1$, and $k_BT=1$.

So the velocity of the effective phonon $v(k)$ is

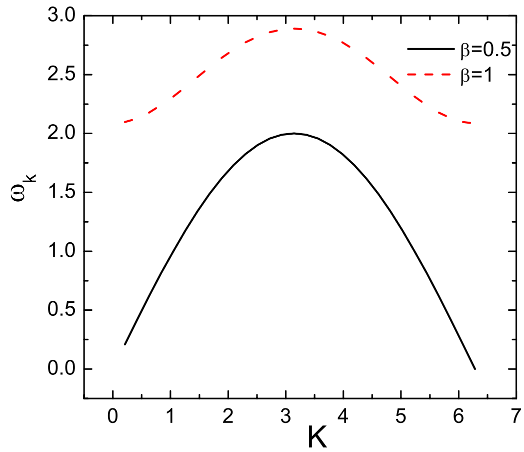

FIG. 3. (Color online) The effective dispersion relation ω_k as a function of k for various β with $\lambda=1$, $a=1$, and $k_BT=1$.

$$v(k)=\partial\omega_k/\partial k=\frac{\lambda\sin k}{\sqrt{f+4\lambda\sin^2\frac{k}{2}}}. \tag{9}$$

The thermal conductivity is given by the Debye formula,

$$\kappa=\frac{c}{2\pi}\int_0^{2\pi}v(k)l(k)dk, \tag{10}$$

where c is the specific heat, $v(k)$ the velocity of the effective phonon, and $l(k)$ the mean-free path of the effective phonon. $l(k)=v(k)\tau(k)$, where $\tau(k)$ is the effective phonon relaxation time which is proportional to the quasiperiod of the effective phonon [19], $\tau(k)\propto(\frac{1}{\epsilon})2\pi/\omega_k$. ϵ is the strength of the nonlinearity defined in Ref. [20], $\epsilon=\frac{|\langle E_n\rangle|}{\langle E_l+E_n\rangle}$, $0\leqslant\epsilon\leqslant1$. For a harmonic lattice with a small nonlinear perturbation, the average of the nonlinear potential energy $\langle E_n\rangle$ is negligible compared to the average of quadratic potential energy $\langle E_l\rangle$. Thus ϵ can be approximated by $\epsilon\approx\frac{|\langle E_n\rangle|}{\langle E_l\rangle}$, where the average of the quadratic potential energy $\langle E_l\rangle\propto\lambda Nk_BT/2\beta$.

ϵ can be expressed as

$$\epsilon\approx\frac{\left\langle\sum_i\beta\left(1-\cos\frac{\pi}{a}q_i\right)\right\rangle}{\left\langle\sum_i\frac{\lambda}{2}(q_{i+1}-q_i-l_0)^2\right\rangle}\propto\frac{N\beta}{\lambda Nk_BT/2\beta}=\frac{2\beta^2}{\lambda k_BT}. \tag{11}$$

So the thermal conductivity κ becomes

$$\kappa\propto\frac{c\lambda^{3/2}}{\beta^2}\int_0^{2\pi}\frac{\sin^2k}{\left(4\sin^2\frac{k}{2}+\frac{f}{\lambda}\right)^{3/2}}dk. \tag{12}$$

For simplicity, c is assumed to be a constant. From this equation, we can obtain κ as a function of β for various λ, as shown in Fig. 4. The inset shows the rescaled thermal conductivity $\kappa/\lambda^{3/2}$ as a function of β for various λ. The slope of the dashed line is -2. The results show that

$$\kappa\propto\frac{\lambda^{3/2}}{\beta^2} \tag{13}$$

when β is in the interval [0.05 0.27]. The calculation results agree with the rescaled form as shown in Fig. 2.

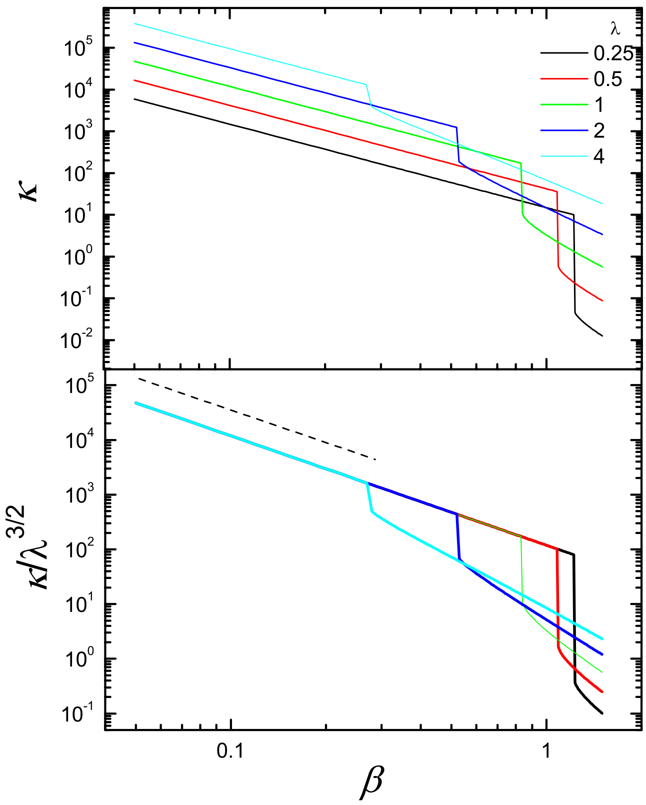

FIG. 4. (Color online) (a) Dependence of the thermal conductivity κ on β for various λ from self-consistent phonon theory ($a=1$). (b) The rescaled thermal conductivity $\kappa/\lambda^{3/2}$ vs β for various λ. When β is in the interval [0.05 0.27], the curve is linear. The slope of the dashed line is -2.

IV. SELF-CONSISTENT STOCHASTIC RESERVOIRS METHOD

An anharmonic model with self-consistent reservoirs has been studied via an analytical approach. Using perturbative calculations for a weak coupling between the sites and a weak anharmonic potential, Pereira and Falcao [21] have described an analytical approach and obtained an integral formalism suitable for the study of the correlation function. The perturbative calculation, which agrees with the exact solution of the harmonic model, has been applied to the rotator model [22] and the Frenkel-Kontorova model [23]. However, they calculated only the first-order approximation. In this section, we extend this calculation to second order to study the dependence of the thermal conductivity on the parameters λ and β. The results agree very well with that from NEMD and the self-consistent phonon theory.

When the external potential is weak and the system temperature is small, we can approximate the external potential of the FK model by

$$\beta\left(1-\cos\frac{\pi}{a}q_i\right)\approx\beta\left(\frac{\left(\frac{\pi}{a}q_i\right)^2}{2}-\frac{\left(\frac{\pi}{a}q_i\right)^4}{4!}\right). \tag{14}$$

The Hamiltonian becomes $(a=1)$

$$H=\sum_{i=1}^{N}\left[\frac{p_i^2}{2m}+\frac{\lambda}{2}(q_{i+1}-q_i-l_0)^2+\beta\left(\frac{(\pi q_i)^2}{2}-\frac{(\pi q_i)^4}{4!}\right)\right]. \tag{15}$$

We consider the stochastic Langevin dynamics of an anharmonic system with self-consistent stochastic reservoirs:

$$dq_i=p_i dt,$$

$$dp_i=-\frac{\partial H}{\partial q_i}dt-\xi_i p_i dt+\sqrt{2\xi_i T_i}dB_i, \tag{16}$$

where B_i is an independent Wiener process—i.e., dB_i/dt is an independent white noise, ξ_i the ith heat bath coupling constant, and T_i the temperature of the ith heat bath.

To analyze this anharmonic model, we use the fixed boundary condition $q_0=q_{N+1}=0$ and make use of the Girsanov theorem in the theory of stochastic differential equations [24,25]. If the steady distribution for the harmonic system with $\lambda=0$ is ρ_0, the new steady distribution is $\rho_0 Z(t)$, in which

$$Z(t)=\exp\left(\int_0^t u dB-\frac{1}{2}\int_0^t u^2 ds\right), \tag{17}$$

where $u_i=(-\lambda q_{i+1}+\frac{\beta\pi^4 q_i^3}{6})/\sqrt{2\xi_i T_i}$.

Using Wick's theorem and performing the Gaussian integral, we analyze the two-point correlation function. The average over the stationary distributions is

$$\lim_{t\to\infty}\langle q_u(t)p_v(t)\rangle=\langle q_u p_v Z(t)\rangle_0, \tag{18}$$

where $\langle\,\rangle_0$ means a time average of the harmonic oscillators in the equilibrium state.

Considering the second-order approximation in λ and β, we have

$$\lim_{t\to\infty}\langle q_u(t)p_v(t)\rangle=\frac{\lambda^2\left[(T_v-T_u)+\frac{3\beta\pi^4}{8(\beta\pi^2+\lambda)^2}(T_v^2-T_u^2)\right]}{(\beta\pi^2+\lambda)(\xi_u+\xi_v)}. \tag{19}$$

After some mathematical manipulations [21], we obtain an expression for the heat flux between nearest neighbors:

$$F_{i\to i+1}=\frac{\lambda^2\left[(T_{i+1}-T_i)+\frac{3\beta\pi^4}{8(\beta\pi^2+\lambda)^2}(T_{i+1}^2-T_i^2)\right]}{(\beta\pi^2+\lambda)(\xi_i+\xi_{i+1})}. \tag{20}$$

In the steady state, we have

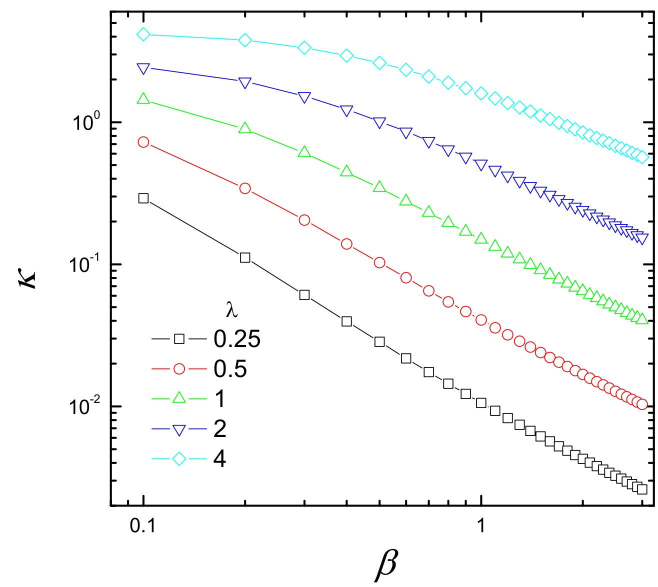

FIG. 5. (Color online) Dependence of the thermal conductivity κ on β for various λ from the self-consistent stochastic reservoirs method. $T_1=T_+=1.05$, $T_N=T_-=0.95$.

$$F_{\to}=F_{1\to 2}=F_{2\to 3}=\cdots=F_{N-1\to N}. \tag{21}$$

If we assume that the coupling constant between the inner baths is smaller than those between the left and right baths, the coupling constant with the inner bath is

$$\xi_2=\xi_3=\cdots=\xi_{N-1}\approx\frac{\xi_1}{\theta}=\frac{\xi_N}{\theta}. \tag{22}$$

Then we will get an approximation to the situation that the chain is only connected to the left and right baths (1 and N). From Eqs. (20)–(22), we get the heat flux as

$$F_{\to}=\frac{\lambda^2\left[1+\frac{3\beta\pi^4}{8(\beta\pi^2+\lambda)^2}(T_1+T_N)\right]}{(\beta\pi^2+\lambda)\xi_1}\times\frac{\theta}{2(\theta-1)+2(N-1)}(T_N-T_1). \tag{23}$$

When N is fixed and $\theta\to\infty$, the thermal conductivity is

$$\kappa\propto\frac{\lambda^2\left[1+\frac{3\beta\pi^4}{8(\beta\pi^2+\lambda)^2}(T_1+T_N)\right]}{(\beta\pi^2+\lambda)}. \tag{24}$$

In Fig. 5, we plot dependence of the thermal conductivity κ on β for various λ from Eq. (24) when $T_1=T_+=1.05$, $T_N=T_-=0.95$. The results show that the thermal conductivity κ is a decreasing function of β and an increasing function of λ. The result agrees with those from NEMD and the self-consistent phonon theory qualitatively.

V. CONCLUSION AND DISCUSSION

In this paper, the dependence of the thermal conductivity κ on the strength of the interparticle potential λ and the strength of the external potential β in the Frenkel-Kontorova model is studied. First, we use nonequilibrium molecular dynamics (NEMD) to calculate the thermal conductivity of the FK model as functions of the parameters λ and β. We obtain a scaling form $\kappa \propto \frac{\lambda^{3/2}}{\beta^2}$, when β, the strength of the external potential, is in the middle region. Then, using the self-consistent phonon (SCP) theory, we confirm the scaling form. Finally, using the self-consistent stochastic reservoirs method to study the approximated Hamiltonian of the FK model, the thermal conductivity dependence on λ and β is studied. The thermal conductivity κ is an increasing function of λ and a decreasing function of β, which agrees with those from NEMD and the self-consistent phonon theory. The scaling form depends on the temperature, and the scaling form would have some deviation when the temperature is too small or too large. The dependence of the thermal conductivity κ on the λ and β and the scaling relationship between them can not only shed light on the nonlinear dynamics and the heat transport of the FK model, but also help us to choose better parameters to design thermal devices in practice, such as thermal diode, thermal transistor, etc.

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