Parameter-dependent thermal conductivity of one-dimensional ϕ^4 lattice

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We examine the thermal conductivity of a one-dimensional ϕ^4 lattice with strong on-site harmonic potential. The expression for the thermal conductivity in terms of different parameters is derived from the effective phonon theory. Numerical calculations using nonequilibrium molecular dynamics are compared with the predictions of the effective phonon theory and the theory of the Peierls-Boltzmann transport equation. It is found that the numerical results are consistent with the prediction of the effective phonon theory in the intermediate parameter range and approach the predictions of Peierls-Boltzmann transport theory in the strongly pinned limit.

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I. INTRODUCTION

Heat conduction in one dimensional (1D) nonlinear lattice models has been studied intensively in the last decade [1]. According to molecular dynamics simulations, it is commonly believed that for lattices without on-site potential, like the Fermi-Pasta-Ulam (FPU) lattice, the thermal conductivity diverges with increasing lattice length [2,3], namely, $\kappa \sim N^{\alpha}$, where N is the system size. For lattices with on-site potential, the thermal conductivity converges to a constant value in the thermodynamic limit $N \to \infty$, recovering the Fourier's heat conduction law [4]. To fully understand the physical mechanism of the anomalous heat conduction in 1D nonlinear lattices, many theoretical works have been done [5]. In particular, the debate has been focused on the value of the exponent α.

Compared with the system size dependence of thermal conductivity, much less is known about the dependence of thermal conductivity on temperature and/or other system parameters. Only recently has study been extended to the temperature dependence of thermal conductivity in general 1D nonlinear lattice models, using the effective phonon theory [6,7]. It is found that the nonlinearity plays an important role in determining the power law dependence of thermal conductivity as a function of temperature, $\kappa \sim T^{\delta}$.

In fact, the study of thermal conductivity as a function of temperature and/or other system parameters rather than the system size has its own experimental motivation. From an experimental point of view, the measurement of size-dependent thermal conductivity at the nanoscale is very difficult, since one needs to fabricate a sample of different size for each test. The recent experimental breakthrough in low-dimensional thermal devices also inspires further investigation of the thermal conductivity as a function of system parameters. Most remarkably, a solid state thermal rectifier has been realized experimentally with asymmetric nanotubes [8]; this is merely few years after the first theoretical work on thermal rectifiers [9]. Deeper understanding of thermal conductivity will definitely benefit the design of solid state thermal devices such as thermal diodes [9] and thermal transistors [10], etc.

However, the dependence of thermal conductivity on relevant system parameters in general 1D nonlinear lattices has not yet been studied systematically except for the work of Lefevere and Schenkel (LS) [11]. They have studied the 1D ϕ^4 model with strong harmonic on-site potential [11], and a formula for thermal conductivity as a function of all system parameters considered in the strongly pinned limit has been derived.

In this paper, we shall study this problem using the effective phonon theory. We consider a 1D ϕ^4 lattice model with strong on-site potential. The Hamiltonian of the system is

$$H = \sum_{i=1}^{N} \left(\frac{p_i^2}{2} + \omega^2 \mu^2 \frac{x_i^2}{2} + \frac{\lambda}{4} x_i^4 + \frac{\omega^2}{2} (x_{i+1} - x_i)^2 \right), \qquad (1)$$

where ω^2 is the coupling strength of the harmonic nearest-neighbor interaction, and $\omega^2\mu^2$ and λ are the strengths of the harmonic and anharmonic (nonlinear) parts of the on-site potential, respectively. x_i is the displacement of the ith particle from its equilibrium position. This model is the same as the one considered by LS in Ref. [11]. By applying the Peierls-Boltzmann equation for phonons, LS obtained an expression for the thermal conductivity in terms of system parameters in the strongly pinned limit ($\mu^2 \gg 1$):

$$\kappa \propto \frac{\omega^9 \mu^3}{\lambda^2 T^2}. \qquad (2)$$

The purpose of the current paper is twofold. First, we shall derive the thermal conductivity as a function of all system parameters from the effective phonon theory for the ϕ^4 model beyond the strongly pinned limit. Second, we shall calculate the thermal conductivity, using nonequilibrium molecular dynamics (NEMD), as a function of four parameters T, λ, μ, and ω, and compare the numerical results with the predictions of Eq. (2) and predictions from the effective phonon theory.

The paper is organized as follows. In Sec. II we give the theoretical derivation of the thermal conductivity in terms of system parameters from the effective phonon theory. In Sec.

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III we show the numerical results. In Sec. IV we give a discussion and conclusions.

II. EFFECTIVE PHONON THEORY

The effective phonon theory is a mean field theory dealing with the heat conduction in 1D general nonlinear lattices [6], using which the temperature dependence of the thermal conductivity was systematically discussed in Ref. [7]. In this section, we shall derive an expression for the thermal conductivity of the ϕ^4 model in terms of the parameters T, λ, μ, and ω from the effective phonon theory.

For general 1D nonlinear lattices, the Hamiltonian can be written as

$$H = \sum_{i=1}^{N} \left(\frac{1}{2} p_i^2 + V(\delta x_{i,i+1}) + U(x_i) \right). \tag{3}$$

For convenience, we consider a periodic boundary condition $x_1 \equiv x_{N+1}$. $\delta x_{i,i+1} = x_i - x_{i+1}$. The interparticle potential $V(\delta x_{i,i+1})$ and the on-site potential $U(x_i)$ can be generally expressed as

$$V(\delta x_{i,i+1}) = \sum_{s=2}^{\infty} g_s \frac{(\delta x_{i,i+1})^s}{s}, \quad U(x_i) = \sum_{s=2}^{\infty} \sigma_s \frac{x_i^s}{s}, \tag{4}$$

respectively. According to the effective phonon theory [6], the spectrum of effective phonons $\hat{\omega}_k$ is

$$\hat{\omega}_k^2 = \alpha(\omega_k^2 + \gamma), \tag{5}$$

where $\omega_k = 2 \sin k/2$ is the spectrum of the harmonic lattice. The coefficients α and γ are

$$\alpha = \sum_{s=2}^{\infty} g_s \frac{\left\langle \sum_{i=1}^{N} (\delta x_{i,i+1})^s \right\rangle}{\left\langle \sum_{i=1}^{N} (\delta x_{i,i+1})^2 \right\rangle},$$

$$\gamma = \frac{1}{\alpha} \sum_{s=2}^{\infty} \sigma_s \frac{\left\langle \sum_{i=1}^{N} x_i^s \right\rangle}{\left\langle \sum_{i=1}^{N} x_i^2 \right\rangle}, \tag{6}$$

where $\langle \cdot \rangle$ means the canonical ensemble average. In principle, these two coefficients can be calculated from statistical mechanics.

For the ϕ^4 model with the Hamiltonian of Eq. (1), all the coefficients in the expansion (4) vanish except $g_2 = \omega^2$, $\sigma_2 = \omega^2 \mu^2$, and $\sigma_4 = \lambda$. by definition, the system coefficient $\alpha = \omega^2$ and the coefficient γ can be expressed as

$$\gamma = \frac{1}{\omega^2} \frac{\omega^2 \mu^2 \left\langle \sum_i x_i^2 \right\rangle + \lambda \left\langle \sum_i x_i^4 \right\rangle}{\left\langle \sum_i x_i^2 \right\rangle} = \mu^2 (1 + \beta), \tag{7}$$

where $\beta = (\lambda / \omega^2 \mu^2) \langle \Sigma_i x_i^4 \rangle / \langle \Sigma_i x_i^2 \rangle$.

The thermal conductivity can be evaluated by the modified Debye formula [7]

$$\kappa = \frac{c}{2\pi} \int_0^{2\pi} P(k) v(k) l(k) dk, \tag{8}$$

where c is the specific heat, $P(k)$ the normalized power spectrum of the total heat flux, $v(k) = \partial \hat{\omega}_k / \partial k$ the velocity of the effective phonons, and $l(k)$ the mean free path of the effective phonons. $l(k) = v(k) \tau(k)$, where $\tau(k)$ is the effective phonon relaxation time which is proportional to the quasiperiod of the effective phonons, $\tau(k) = (1/\epsilon) 2\pi / \hat{\omega}_k$, and the dimensionless ϵ is the strength of the nonlinearity defined in Ref. [7]. Dropping off constants, the thermal conductivity becomes

$$\kappa \propto \int_0^{2\pi} P(k) v^2(k) \tau(k) dk, \tag{9}$$

where $v(k) = \omega \sin k / \sqrt{4 \sin^2 \frac{k}{2} + \mu^2 (1 + \beta)}$ and $\tau(k) = (1/\epsilon) 2\pi / \omega \sqrt{4 \sin^2 \frac{k}{2} + \mu^2 (1 + \beta)}$. From definition, the dimensionless strength of the nonlinearity ϵ is the ratio between the canonical ensemble average of the nonlinear potential energy and total potential energy, $\epsilon \approx \frac{1}{2} \beta$, where we have used the approximations $\frac{1}{4} \lambda \langle \Sigma_i x_i^4 \rangle \ll \frac{1}{2} \omega^2 \mu^2 \langle \Sigma_i x_i^2 \rangle$, $\langle \Sigma_i (x_i - x_{i-1})^2 \rangle \approx \langle \Sigma_i x_i^2 \rangle$, and $\mu^2 \gg 1$.

Substituting the explicit expressions of $v(k)$, $\tau(k)$ and ϵ into Eq. (9), we have

$$\kappa \propto \frac{1}{\beta} \int_0^{2\pi} P(k) \frac{\omega \sin^2 k}{\left[4 \sin^2 \frac{k}{2} + \mu^2 (1 + \beta) \right]^{3/2}} dk$$

$$= \frac{1}{\beta} \frac{\omega}{\mu^3} \mathcal{P} = \frac{\omega^3}{\lambda \mu} \frac{\left\langle \sum_i x_i^2 \right\rangle}{\left\langle \sum_i x_i^4 \right\rangle} \mathcal{P}, \tag{10}$$

where

$$\mathcal{P} = \int_0^{2\pi} P(k) \frac{\sin^2 k}{\left[4 \sin^2 \frac{k}{2} \Big/ \mu^2 + (1 + \beta) \right]^{3/2}} dk. \tag{11}$$

We see that the thermal conductivity consists of two items, one with the ensemble average and another with an integral over k, namely, $\mathcal{P}$. In the first item, we need to find the explicit expression of $\langle \Sigma_i x_i^2 \rangle / \langle \Sigma_i x_i^4 \rangle$. By analogy with Ref. [12], where $\langle \Sigma_i (\delta x_{i,i+1})^4 \rangle / N = A [\langle \Sigma_i (\delta x_{i,i+1})^2 \rangle / N]^2$ for the FPU-β model with constant A, we assume that in the ϕ^4 model $\langle \Sigma_i x_i^4 \rangle / \langle \Sigma_i x_i^2 \rangle = A \langle \Sigma_i x_i^2 \rangle / N$. The numerical simulations

confirm this relationship and give the constant $A \approx 2.7$. Actually, at the harmonic limit of $\mu^2 \gg 1$, $A=3$ can be derived analytically. From the general energy equipartition theorem [13], we have $T=\langle \Sigma_i x_i \partial H/\partial x_i \rangle /N \approx \omega^2 \mu^2 \langle \Sigma_i x_i^2 \rangle /N$, where the approximations $\beta \ll 1$ and $\mu^2 \gg 1$ have been used. Thus we have $\langle \Sigma_i x_i^4 \rangle / \langle \Sigma_i x_i^2 \rangle = A \langle \Sigma_i x_i^2 \rangle /N \approx AT/\omega^2 \mu^2$. Substituting this into Eq. (10), we obtain

$$\kappa \propto \frac{\omega^3}{\lambda \mu} \frac{\left\langle \sum_i x_i^2 \right\rangle}{\left\langle \sum_i x_i^4 \right\rangle} \mathcal{P} \propto \frac{\omega^5 \mu}{\lambda T} \mathcal{P}. \tag{12}$$

As far as the second item, $\mathcal{P}$, is concerned, as we have pointed out in Ref. [7] that, due to the lack of an explicit form of the power spectrum of the heat flux $P(k)$, the integral in $\mathcal{P}$ cannot be got rid of. However, the asymptotic behavior (increase or decrease) for different parameters in the expression of $\mathcal{P}$ can be determined. Substituting the expression for β into Eq. (13), we have

$$\mathcal{P} = \int_0^{2\pi} P(k) \frac{\sin^2 k}{\left[\left(4 \sin^2 \frac{k}{2} \right) \Big/ \mu^2 + (1 + A\lambda T/\omega^4 \mu^4) \right]^{3/2}} dk. \tag{13}$$

It is clear from this formula that $\mathcal{P}$ increases with increase of ω and μ, and decreases with increase of λ and T, despite the lack of information about $P(k)$.

Thus from Eq. (12) of the effective phonon theory, it can be inferred that the thermal conductivity increases faster than $\kappa \propto \omega^5 \mu$ and decreases faster than $\kappa \propto 1/\lambda T$. In this way, the expression

$$\kappa \propto \frac{\omega^5 \mu}{\lambda T} \tag{14}$$

can be viewed as a lower limit for the parameter dependence of the thermal conductivity. The theoretical prediction of Eq. (2) from Ref. [11] is consistent with this result derived from the effective phonon theory.

III. NUMERICAL RESULTS

To verify the parameter-dependent thermal conductivities of the ϕ^4 model, we directly calculate the thermal conductivity using NEMD. The fourth-order Runge-Kutta method is used to integrate the equations of motion. The Langevin thermostat is used to simulate the heat bath. In all the following calculations, fixed boundary conditions are used.

A. T dependence

Temperature is the most convenient parameter that can be easily adjusted in real experiments. Understanding the temperature behavior of the thermal conductivity is very important for the application of thermal devices. In numerical simulations, the temperature dependence of the thermal conductivity is the most studied behavior after the size dependence. The temperature dependence of the thermal conductivity in the ϕ^4 model has been calculated for the parameter $\mu=0$ in Ref. [3], giving $\kappa \propto T^{-1.35}$. The ϕ^4 model exhibits normal heat conduction for any value of parameter μ. Here we calculate the thermal conductivity κ vs T for two different values of the parameter $\mu=0.5$ and 3. The other two parameters are set as $\lambda=0.2$ and $\omega=1$.

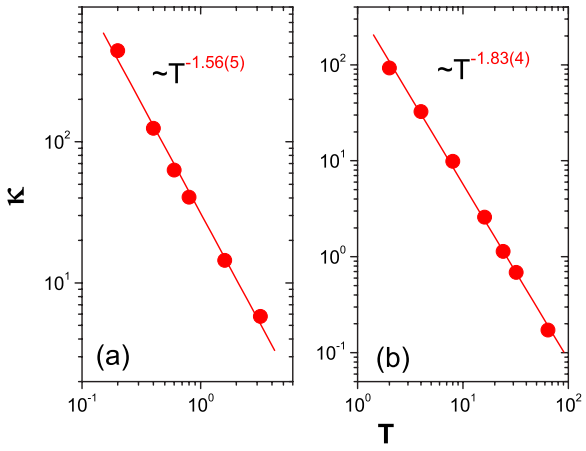

FIG. 1. (Color online) Thermal conductivity κ vs T for different values of parameter μ=(a) 0.5 and (b) 3. In both cases, $\lambda=0.2$, $\omega=1$, and the lattice length is $N=512$.

In Fig. 1(a), κ vs T is plotted for the parameter setting $\lambda=0.2$, $\mu=0.5$, and $\omega=1$. The best fitting gives rise to a power law dependence of thermal conductivity with temperature as $\kappa \propto T^{-1.56\pm0.05}$. Figure 1(b) is for the parameter setting $\lambda=0.2$, $\mu=3$, and $\omega=1$. At this setting, $\mu^2=9 \gg 1$ is closer to the strongly pinned limit described in Ref. [11]. The best fitting gives rise to $\kappa \propto T^{-1.83\pm0.04}$. The exponent is decreased from -1.56 to -1.83 when μ is increased from 0.5 to 3. The latter value, -1.83, is close to the limiting value of -2 predicted by Eq. (2) for very large μ. We point out that the problem of ergodicity for larger values of μ prevents us from calculating the thermal conductivity for much larger μ. But, for the present data, it is clear that the exponent is smaller than -1 and larger than -2, lying between the two predictions of Refs. [7,11].

According to the effective phonon theory, one can obtain the full T behavior of the thermal conductivity by integrating Eq. (13) when the expression for the normalized power spectrum $P(k)$ in Eq. (13) is given. If the system dynamics are strongly chaotic, where μ^2 is not too large, we can roughly approximate $P(k)$ as k independent. Thus Eq. (13) can be easily integrated for fixed temperature, since all other parameters are already known. The calculated integral of $\mathcal{P}$ versus T is plotted in Fig. 2 by using the same parameter settings as in Fig. 1(a). The best fitting gives rise to $\mathcal{P} \propto T^{-0.52}$ for small T and $\mathcal{P} \propto T^{-1.01}$ for large T, respectively. By using Eq. (12), the effective phonon theory gives the estimation of the full T dependence of the thermal conductivity between $\kappa \propto T^{-1.52}$ and $\kappa \propto T^{-2.01}$ for the parameters $\lambda=0.2$, $\mu=0.5$, and $\omega=1$. The estimation for a small value of the temperature is quite close to the result from NEMD, $\kappa \propto T^{-1.56\pm0.05}$.

B. λ dependence

The parameter λ is the coupling strength of the nonlinear part of the on-site potential. In the strongly pinned limit, this

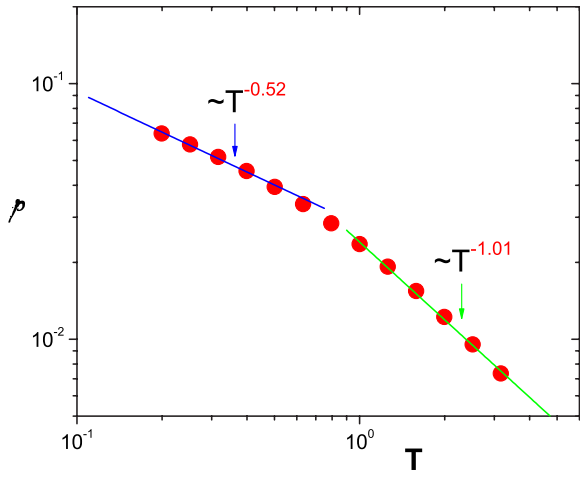

FIG. 2. (Color online) $\mathcal{P}$ vs T. The definition of $\mathcal{P}$ is given in Eq. (13). Parameter settings are the same as in Fig. 1(a).

nonlinear part is required to be much smaller than the harmonic part of the on-site potential, $\frac{1}{4}\lambda\langle\Sigma_i x_i^4\rangle \ll \frac{1}{2}\omega^2\mu^2\langle\Sigma_i x_i^2\rangle$. Here we calculate the λ dependence of the thermal conductivity for two different values of $\mu=1$ and 3. The other two parameters $T=1$ and $\omega=1$ are the same for both cases.

In Fig. 3(a), κ vs λ is plotted for $\mu=1$. The best fitting gives rise to $\kappa \propto \lambda^{-1.48\pm0.02}$. In Fig. 3(b), the parameter μ is changed from 1 to 3, and the power law dependence of the thermal conductivity with λ is now $\kappa \propto \lambda^{-1.79\pm0.03}$. The exponent of the power law is changed from -1.48 to -1.79. Once again, this exponent is smaller than -1 of Eq. (14) and larger than -2 of Eq. (2) and the trend to -2 when μ is increased is obvious.

Using the same analysis given in the last section, we assume that $P(k)$ is k independent for small μ^2. The calculated $\mathcal{P}$ is plotted in Fig. 4. $\mathcal{P}$ exhibits λ dependence as $\mathcal{P} \sim \lambda^{-0.25}$ for small λ and $\mathcal{P} \sim \lambda^{-0.73}$ for large λ. Thus the full λ dependence from Eq. (12) can be estimated as between $\kappa \propto \lambda^{-1.25}$ and $\kappa \propto \lambda^{-1.73}$, which is consistent with the result of numerical simulation, $\kappa \propto \lambda^{-1.48}$, for the case of $\mu=1$ in Fig. 3(a).

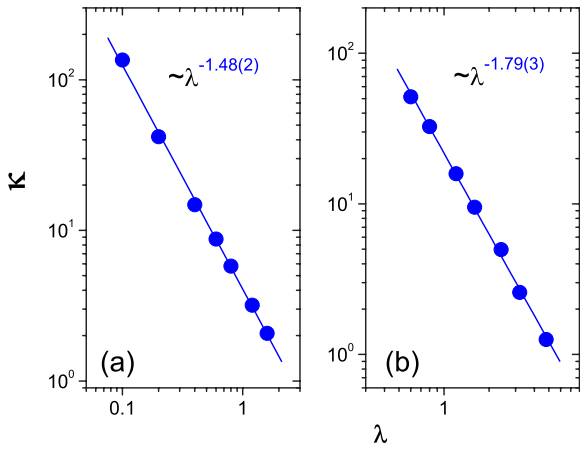

FIG. 3. (Color online) Thermal conductivity κ vs λ for different parameters μ with $T=1$, $\omega=1$, and length $N=512$. μ=(a) 1 and (b) 3.

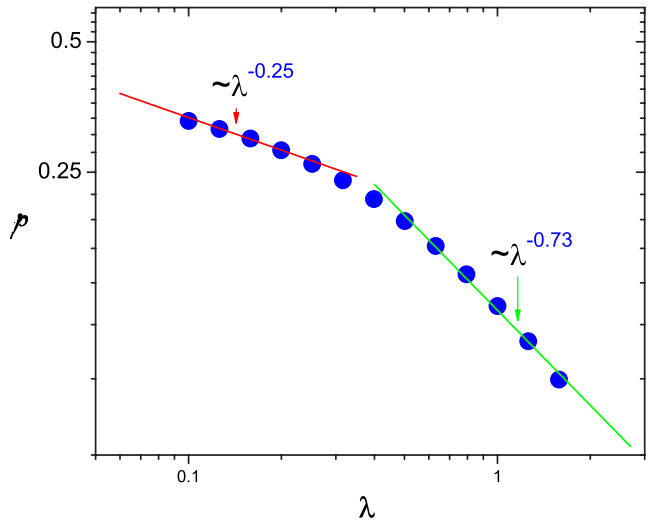

FIG. 4. (Color online) $\mathcal{P}$ vs λ. Same parameter settings are in Fig. 3(a).

C. μ dependence

The parameter $\omega^2\mu^2$ is the coupling strength of the harmonic part of the on-site potential. Since ω^2 is the coupling strength of the harmonic interparticle potential, μ^2 can be regarded as the ratio between the harmonic part of the on-site potential and the harmonic interparticle potential. Here we calculate the μ dependence of the thermal conductivity for the parameter settings $T=1$, $\lambda=1$, and $\omega=1$.

In Fig. 5, the best fitting gives us the power law dependence of thermal conductivity with μ as $\kappa \propto \mu^{2.34\pm0.06}$. The exponent lies between 1 of Eq. (14) and 3 of Eq. (2) and is closer to the prediction of Eq. (2) for the strongly pinned limit.

D. ω dependence

The parameter ω shows up in the harmonic interparticle potential as well as the harmonic part of the on-site potential. In the simulations, the other parameters are set as $T=1$, $\lambda=1$, and $\mu=1$. The reason why we set the parameter $\mu=1$ is

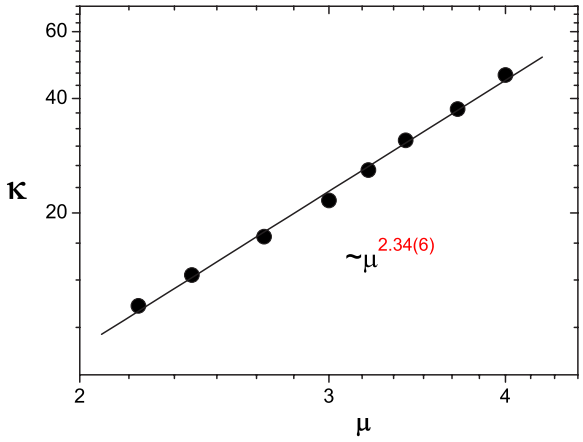

FIG. 5. (Color online) Thermal conductivity κ vs μ for the ϕ^4 model with $N=512$. The parameters are $T=1$, $\lambda=1$, and $\omega=1$.

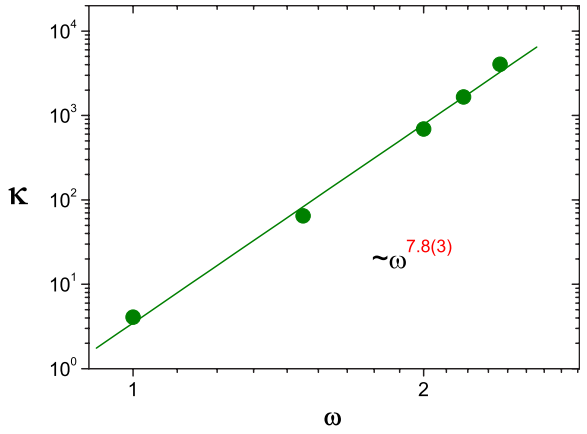

FIG. 6. (Color online) Thermal conductivity κ vs ω for the ϕ^4 model with $N=512$. The parameters are set as $T=1$, $\lambda=1$, and $\mu=1$.

that, when we increase the value of ω from 1, the product of $\omega\mu$ also increases, so that the requirement $\frac{1}{4}\lambda\langle\Sigma_i x_i^4\rangle \ll \frac{1}{2}\omega^2\mu^2\langle\Sigma_i x_i^2\rangle$ is satisfied.

In Fig. 6, the best fitting gives the power law dependence of thermal conductivity with ω as $\kappa \propto \omega^{7.8\pm0.3}$. The exponent is 7.8. This numerical value is larger than 5 of Eq. (14) and close to 9 of Eq. (2). Once again, the exponent lies between the predictions of effective phonon theory and the theory of Ref. [11].

IV. CONCLUSIONS AND DISCUSSIONS

In this paper, we first estimated the dependence of the thermal conductivity κ of the 1D ϕ^4 model on the system parameters temperature T, nonlinear coupling strength λ, harmonic interparticle coupling strength ω, and harmonic strength of the on-site potential μ, from the effective phonon theory. The result is given in Eq. (12). Then we numerically calculated the thermal conductivity and compared it with our theoretical prediction as well as the one from Ref. [11].

It is found that the exponents for these four parameters are consistent with the predictions of Eq. (12) from the effective phonon theory. For all the parameters we investigated, the numerical exponents lie between the lower limit of prediction from the effective phonon theory ($\kappa \propto \omega^5\mu/\lambda T$) and the prediction of Ref. [11] ($\kappa \propto \omega^9\mu^3/\lambda^2T^2$).

The prediction of Ref. [11] comes from the linearization of the Peierls-Boltzmann transport equation. The linearization requires a small perturbation of the nonlinear potential, which is $(\lambda/4)\Sigma_i x_i^4$ in the ϕ^4 model. By imposing another requirement, $\mu^2 \gg 1$, which is the strongly pinned limit, LS figured out the expression for the thermal conductivity, Eq. (2). Theoretically, the expression $\kappa \propto \omega^9\mu^3/\lambda^2T^2$ holds only at the two limits $\lambda \ll 1$ and $\mu^2 \gg 1$. However, in numerical simulations, which deal with finite systems in limited computer time, these two requirements are not rigorously satisfied since the two limits cannot be reached. The limit $\lambda \ll 1$ causes ergodic problems for finite systems. The exponentially increasing computer time prevents us from investigating the transport behavior for very small λ. Moreover, the computer simulation cannot be done for very large values of μ, because $\mu^2 \gg 1$ is the so-called anticontinuous limit [14]. In this limit, the system becomes an array of disconnected oscillators that cannot transport any energy. The numerical values deviate from the prediction of Eq. (2) because the parameters used in simulations do not satisfy the rigorous conditions used in derivation of this formula. From the numerical results, we notice that the exponents for all the parameters are approaching the predictions of Eq. (2) when the value of μ is increased. These results suggest that Eq. (2) might be exact for the strongly pinned limit considered in Ref. [11].

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