Temperature-dependent thermal conductivities of one-dimensional nonlinear Klein-Gordon lattices with a soft on-site potential

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The temperature-dependent thermal conductivities of one-dimensional nonlinear Klein-Gordon lattices with soft on-site potential (soft-KG) are investigated systematically. Similarly to the previously studied hard-KG lattices, the existence of renormalized phonons is also confirmed in soft-KG lattices. In particular, the temperature dependence of the renormalized phonon frequency predicted by a classical field theory is verified by detailed numerical simulations. However, the thermal conductivities of soft-KG lattices exhibit the opposite trend in temperature dependence in comparison with those of hard-KG lattices. The interesting thing is that the temperature-dependent thermal conductivities of both soft- and hard-KG lattices can be interpreted in the same framework of effective phonon theory. According to the effective phonon theory, the exponents of the power-law dependence of the thermal conductivities as a function of temperature are only determined by the exponents of the soft or hard on-site potentials. These theoretical predictions are consistently verified very well by extensive numerical simulations.

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I. INTRODUCTION

Since the first discovery of anomalous heat conduction in one-dimensional (1D) Fermi-Pasta-Ulam β (FPU-β) lattices where thermal conductivity diverges with lattice size [1], enormous efforts have been applied to the study of heat transport in 1D nonintegrable lattices, trying to unravel the underlying physical mechanism [2–45]. The consensus reached in this community is that the total momentum conservation plays an important role in determining the system's heat conduction behavior. For momentum-nonconserving nonintegrable lattices with on-site potentials, there is no dispute that they should have normal heat conduction. However, for momentum-conserving nonintegrable lattices, the issue whether they should necessarily give rise to anomalous heat conduction is still under intense debate. The hydrodynamic theory has predicted that momentum conservation will naturally induce anomalous heat conduction in 1D nonintegrable lattices [18]. But this theory fails to explain the normal heat conduction numerically found for the rotor model, which is also a momentum-conserving lattice [46–48]. There are some arguments that the 1D rotor model should exhibit anomalous heat conduction in the thermodynamical limit where proof or disproof is very hard to obtain by numerical simulations due to the huge computation cost [49]. Most recently, normal or anomalous heat transport in asymmetrical momentum-conserving lattices has attracted much attention [50–52], but more studies of this new topic must be done before a final conclusion can be drawn. For a thorough explanation of the heat transport problems in low-dimensional systems, please refer to some excellent review articles for further reading [53–55].

Even though the study of normal/anomalous heat conduction or size-dependent thermal conductivities still causes much debate in this community, the exploration of the temperature dependence of thermal conductivities in 1D nonintegrable lattices turns out to be more successful. The difficulty of studying size dependence arises from the fact that numerical simulations on extremely long lattices need to be calculated in order to reach asymptotic behavior. In contrast, a very short lattice, usually in the hundreds or thousands of atoms, is enough to obtain stable temperature dependence of thermal conductivities [12,15,56–62]. The most important thing is that the diversity of the temperature dependence for various lattice models can provide a perfect testbed for any heat conduction theory, especially a phenomenological theory. According to numerical simulations, the thermal conductivities of the FPU-β lattice depend on the temperature as $\kappa(T) \propto 1/T$ in the low-temperature limit and $\kappa(T) \propto T^{1/4}$ in the high-temperature limit [15,56,61]. H_n models have a monotonically ascending temperature dependence for thermal conductivities as $\kappa(T) \propto T^{1/2-1/n}$ [61], while hard-KG lattices exhibit monotonically descending temperature dependence as $\kappa(T) \propto T^{-\frac{4(n-2)}{n+2}}$, where $n > 2$ is the exponent of the on-site potential [62]. Interesting enough, all these temperature dependences can be *quantitatively* and *consistently* interpreted by the same phenomenological effective phonon theory [56,61,62], which is based on renormalized phonons [4,63–69] occurring in nonlinear lattices.

In this work, we would like to extend the analytical and numerical investigations of the temperature dependence of thermal conductivities to several soft-KG lattices with $1 < n < 2$. The spectra of renormalized phonons are numerically calculated in comparison to the predictions from classical field theory. The temperature-dependent thermal conductivities are systematically studied via nonequilibrium molecular dynamics. Consistent and quantitative comparisons

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between numerical simulations and theoretical predictions from effective phonon theory are performed. The paper is organized as follows: in Sec. II soft-KG lattice models are introduced and the properties of renormalized phonons are presented. Section III reports the results of temperature-dependent thermal conductivities and compares them with the theoretical predictions from effective phonon theory. We give conclusions and summarize in Sec. IV.

II. SOFT-KG LATTICES AND THEIR RENORMALIZED PHONONS

Symmetrical nonlinear KG lattices have the Hamiltonian

$$H = \sum_{i=1}^{N} \left[\frac{1}{2} p_i^2 + \frac{1}{2}(x_i - x_{i-1})^2 + \frac{1}{n}|x_i|^n \right], \qquad (1)$$

where x_i and p_i denote the dimensionless displacement and momentum for the ith atom and n is the exponent of the nonlinear on-site potential. For $n > 2$, the on-site potentials are hard types which are harder than the referenced quadratic potential with $n = 2$. The Hamiltonian, Eq. (1), with $1 < n < 2$ is then called soft-KG lattices. In contrast to hard-KG lattices, soft-KG lattices approach a harmonic system in the high-temperature limit. In order to gain a consistent understanding of the thermal properties of soft-KG lattices, three soft-KG lattices, with $n = 1.25$, 1.50, and 1.75, are investigated systematically. Dimensionless units have been applied. For simplicity, periodic boundary conditions with $x_i = x_{N+i}$ are used for theoretical analysis, while fixed boundary conditions with $x_0 = x_{N+1} = 0$ are used for molecular dynamics simulations. In principle, the different boundary conditions will not cause any difference in their thermal properties in the thermodynamical limit.

The dispersion relation of renormalized phonons for the Hamiltonian, Eq. (1), can be generally expressed as [62,65]

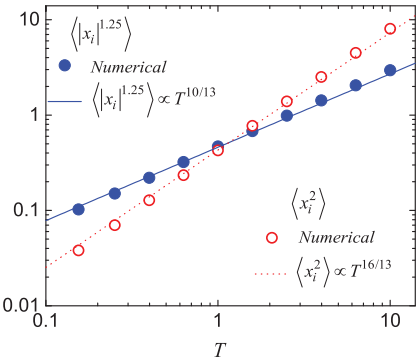
$$\hat{\omega}_k = \sqrt{\omega_k^2 + \gamma},\ \omega_k = 2\sin\frac{\pi k}{N},\quad \gamma = \frac{\sum_i \langle |x_i|^n \rangle}{\sum_i \langle x_i^2 \rangle}, \qquad (2)$$

where $k,i = 1,\ldots,N$ and $\langle\cdot\rangle$ denotes the ensemble average at thermal equilibrium. The renormalization coefficient γ contains the information on nonlinearity and depends on the temperature or the strength of the nonlinearity. It is very interesting that γ depends on the temperature with a power-law behavior which can be predicted by the classical field theory approach [62,65].

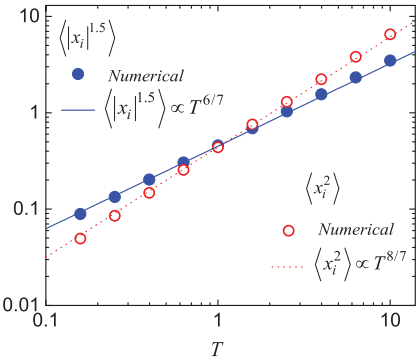
According to Ref. [62], the scaling of components $\langle x_i^2 \rangle$ and $\langle |x_i|^n \rangle$ of γ can be derived as a function of temperature as

$$\begin{aligned} \langle x_i^2 \rangle &\propto T^{\sigma_2},\quad \sigma_2 = \frac{4}{n+2}, \\ \langle |x_i|^n \rangle &\propto T^{\sigma_n},\quad \sigma_n = \frac{2n}{n+2}, \end{aligned} \qquad (3)$$

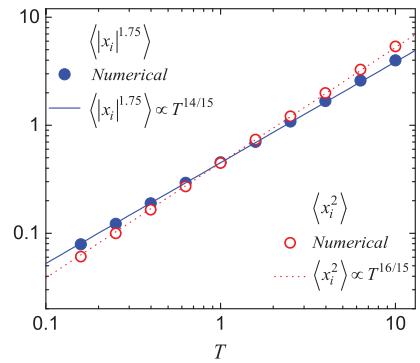
where $\langle x_i^2 \rangle$ and $\langle |x_i|^n \rangle$ are independent of the atom index i. For a soft-KG lattice with $n = 1.25$, the power-law dependence can be expressed as $\langle x_i^2 \rangle \propto T^{16/13}$ and $\langle |x_i|^n \rangle \propto T^{10/13}$. Similarly, the expressions are $\langle x_i^2 \rangle \propto T^{8/7}$ and $\langle |x_i|^n \rangle \propto T^{6/7}$ for $n = 1.5$ and $\langle x_i^2 \rangle \propto T^{16/15}$ and $\langle |x_i|^n \rangle \propto T^{14/15}$ for $n = 1.75$. To verify these theoretical predictions from classical field theory,



(a) Soft-KG lattice with $n = 1.25$



(b) Soft-KG lattice with $n = 1.50$



(c) Soft-KG lattice with $n = 1.75$

FIG. 1. (Color online) Time averages of $\langle x_i^2 \rangle$ and $\langle |x_i|^n \rangle$ as a function of temperature T for three soft-KG lattices with (a) $n = 1.25$, (b) $n = 1.5$, and (c) $n = 1.75$. Lines are predictions from Eq. (3), while their prefactors are chosen so as to fit the numerical data. All numerical simulations were performed at thermal equilibrium for a lattice with $N = 200$, where the two ends were coupled to the Langevin heat baths. The averages of $\langle x_i^2 \rangle$ and $\langle |x_i|^n \rangle$ are independent of the atom index i.

we have numerically calculated the time average of $\langle x_i^2 \rangle$ and $\langle |x_i|^n \rangle$ as a function of temperature for three soft-KG lattices with exponents $n = 1.25$, 1.5, and 1.75 as plotted in Fig. 1. It can be seen clearly that all the $\langle x_i^2 \rangle$ and $\langle |x_i|^n \rangle$ follow the predicted power-law dependence as a function of temperature over two order of magnitudes. In Fig. 2, the fitting exponents σ_2 and σ_n extracted from Fig. 1 are plotted compared with the

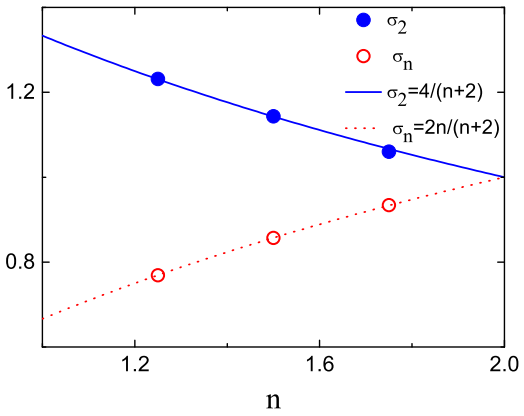


FIG. 2. (Color online) Exponents σ_2 and σ_n as a function of n. Symbols are numerical data and lines are predictions of Eq. (3).

theoretical predictions of Eq. (3). The good agreement between numerical simulations and theoretical predictions can be easily seen.

In order to confirm the existence of renormalized phonons predicted by Eq. (2), we should investigate the power spectrum of atom vibrations in different soft-KG lattices at different temperatures. From the above discussion of Eqs. (2) and (3), we know that the renormalization coefficient γ can be expressed as

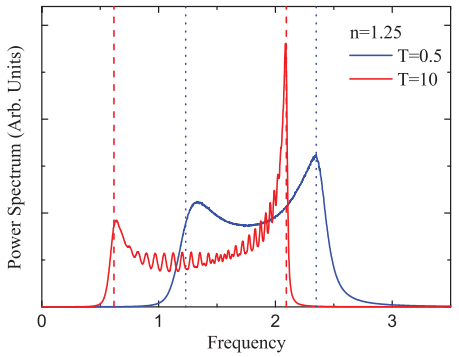
$$\gamma = \xi \cdot T^{\sigma_n - \sigma_2}, \tag{4}$$

where the prefactor ξ is a temperature-independent constant. In the absence of theoretical predictions, the prefactor ξ should be obtained from numerical simulations for each soft-KG lattice. For $n = 1.25$, 1.5, and 1.75, the numerical values of ξ have been calculated as 1.102,1.045, and 1.014, respectively. According to Eq. (2), the renormalized phonon spectra are bounded as

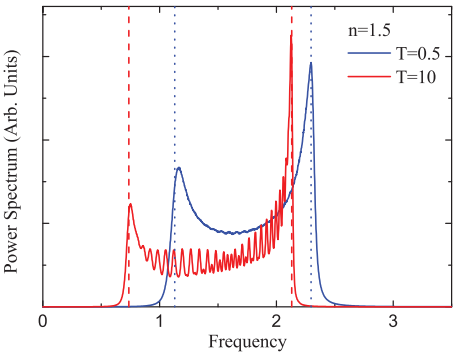
$$\hat{\omega}_k \in [\sqrt{\xi \cdot T^{\sigma_n - \sigma_2}}, \sqrt{4 + \xi \cdot T^{\sigma_n - \sigma_2}}], \tag{5}$$

where the upper and lower boundaries are both temperature dependent. The spectra of predicted renormalized phonons are therefore located within [1.232,2.349] at $T = 0.5$ and [0.617,2.093] at $T = 10$ for a lattice with $n = 1.25$. For $n = 1.5$, the predicted region is [1.129,2.297] at $T = 0.5$ and [0.736,2.131] at $T = 10$. For $n = 1.75$, the region should be [1.055,2.261] and [0.864,2.179] for $T = 0.5$ and $T = 10$, respectively.

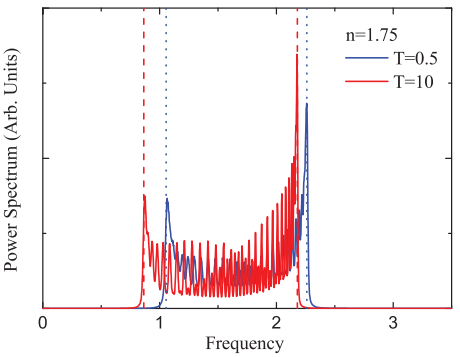
The phonon spectra can be obtained by calculating the power spectra of the atom velocity $\dot{x}_i(t)$ for each soft-KG lattice at a specified temperature [70]. In Fig. 3, the power spectra for soft-KG lattices at different temperatures are plotted. Vertical lines are the predictions from Eq. (5), which exactly match the numerical boundaries. The good agreement between numerical results and theoretical predictions confirms the existence of renormalized phonons in these nonlinear soft-KG lattices.



(a) Soft-KG lattice with $n = 1.25$



(b) Soft-KG lattice with $n = 1.50$



(c) Soft-KG lattice with $n = 1.75$

FIG. 3. (Color online) Power spectra of the atom velocity $\dot{x}_i(t)$ at two temperatures, $T = 0.5$ and $T = 10$, for three soft-KG lattices with (a) $n = 1.25$, (b) $n = 1.5$, and (c) $n = 1.75$. Predicted boundaries of power spectra are shown by vertical dotted (blue) lines for $T = 0.5$ and dashed (red) lines for $T = 10$, respectively. All numerical simulations were performed at thermal equilibrium for a lattice with $N = 60$.

III. TEMPERATURE-DEPENDENT THERMAL CONDUCTIVITIES AND EFFECTIVE PHONON THEORY

In dealing with temperature-dependent thermal conductivities, the effective phonon theory [56,61,62,67] has proven to be very successful. In the framework of renormalized phonons, the effective phonon theory is able to predict the temperature dependence of thermal conductivities. The derivation of the thermal conductivities for 1D soft-KG lattices is the same

as that for 1D hard-KG lattices. In particular, the thermal conductivities of 1D soft-KG can be expressed as [62]

$$\kappa(T) \propto \frac{1}{\epsilon\gamma^{3/2}}, \tag{6}$$

where γ is the renormalization coefficient and the nonlinearity strength ϵ is defined as the ratio of the nonlinear potential energy to the total potential energy, $\epsilon = \langle E_n\rangle/\langle E_t\rangle$, with E_n and E_t denoting the nonlinear and total potential energy, respectively.

The temperature dependence of γ has been derived in Eq. (4). Next we briefly introduce the derivation of the temperature dependence of the nonlinearity strength ϵ. By definition, the nonlinearity strength ϵ can be expressed as

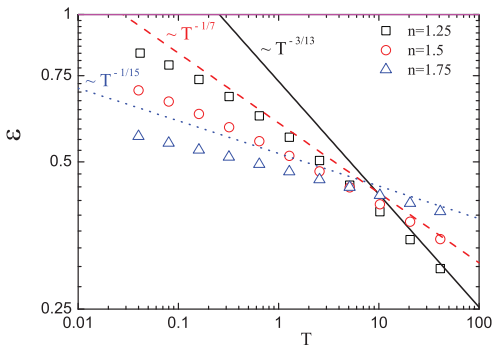
$$\epsilon = \frac{\sum_i \langle |x_i|^n\rangle/n}{\sum_i \langle (x_i - x_{i-1})^2\rangle/2 + \sum_i \langle |x_i|^n\rangle/n} \approx \frac{\sum_i \langle |x_i|^n\rangle/n}{\sum_i \langle (x_i - x_{i-1})^2\rangle/2} \propto T^{\sigma_n - 1}. \tag{7}$$

Since we only consider the high-temperature region where the quadratic interaction potential $\sum_i \langle (x_i - x_{i-1})^2\rangle$ dominates, the on-site potential term $\sum_i \langle |x_i|^n\rangle$ in the denominator can be ignored. From Eq. (3) we know that $\langle |x_i|^n\rangle \propto T^{\sigma_n}$. And the property of $\langle (x_i - x_{i-1})^2\rangle \propto T$ can be obtained due to equipartition theorem [62] in the high-temperature limit. This explains the $\epsilon \propto T^{\sigma_n - 1}$ behavior in the high-temperature region. On the other hand, the quadratic term can be ignored in the low-temperature region, which gives rise to the $\epsilon \approx 1$ behavior. In Fig. 4(a), the nonlinear strength ϵ is plotted as a function of the temperature for each soft-KG lattice. The intersection points between the line of $\epsilon = 1$ and the asymptotic line $\epsilon \propto T^{\sigma_n - 1}$ approximately describe the crossover points between the low- and the high-temperature region. For $n = 1.25$, it can be seen the crossover point is at about $T = 0.25$. The temperature at the crossover points for $n = 1.5$ and 1.75 is even lower. Therefore a temperature higher than $T = 0.25$ can be approximately viewed as a high temperature for soft-KG lattices with $n \geqslant 1.25$. However, for hard-KG lattices, the nonlinear strength ϵ approaches 1 in the high-temperature limit and $\epsilon \propto T^{\sigma_n - 1}$ in the low-temperature limit. As shown in Fig. 4(b), the temperature at the crossover point for $n = 4$ is about $T = 30$. A temperature lower than this value can be approximately viewed as a low temperature for hard-KG lattices with $n \leqslant 4$.

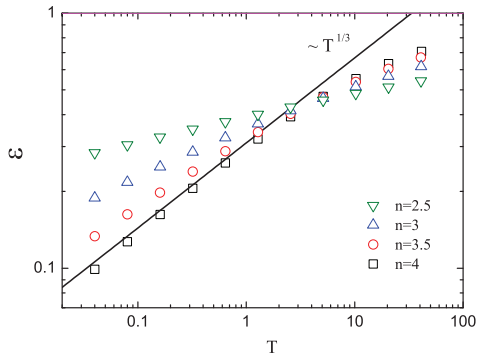
Therefore, from Eqs. (4), (6), and (7), the thermal conductivities for 1D soft-KG lattices can be derived as

$$\kappa(T) \propto T^{r_n}, \quad r_n = \frac{4(2-n)}{n+2}. \tag{8}$$

This power-law dependence is exactly the same as that for hard-KG lattices [62]. In both soft- and hard-KG lattices, the considered temperature regions are all close to the harmonic limit. One should note that this region refers to the low-temperature region for hard-KG lattices and the high-temperature region for soft-KG lattices. Our theory predicts that the thermal conductivities increase monotonically with temperature as $r_n > 0$ for soft-KG lattices with $n < 2$, which is totally different from hard-KG lattices, where $r_n < 0$ for $n > 2$. To verify these predictions, intensive numerical simulations of temperature-dependent thermal conductivities for soft-KG lattices need to be performed.



(a) Soft-KG lattices with $n = 1.25, 1.5$ and 1.75



(b) Hard-KG lattices with $n = 2.5, 3, 3.5$ and 4

FIG. 4. (Color online) Nonlinear strength ϵ as a function of temperature for (a) soft-KG and (b) hard-KG lattices. Intersection points between the line of $\epsilon = 1$ and the asymptotic lines of $\epsilon \propto T^{\sigma_n - 1}$ approximately separate the low-temperature region from the high-temperature region for each lattice model. All numerical simulations were performed at thermal equilibrium for a lattice with $N = 50$.

In Fig. 5, we numerically calculated the thermal conductivities as a function of temperature for soft-KG lattices with $n = 1.25$, 1.5, and 1.75 from nonequilibrium molecular dynamics simulations. For each thermal conductivity at a specific temperature, we have eliminated the size effect by using long enough lattices that the saturation of thermal conductivity has been confirmed. The power-law dependence of thermal conductivities as a function of temperature is clearly shown by the straight lines in the log-log scaled plot. Contrary to hard-KG lattices, the thermal conductivities of all soft-KG lattices increase monotonically with temperature. These are consistent with the prediction of effective phonon theory where $n = 2$ in Eq. (8) is the crossover point, $r_2 = 0$. The thermal conductivities of harmonic KG lattices with $n = 2$ must be independent of temperature as we would expect.

Soft-KG and hard-KG lattices display opposite temperature dependences of their thermal conductivities. The physical interpretation behind this scenario is that nonlinear lattices should possess higher thermal conductivities when they approach the harmonic limit. For hard-KG lattices, the harmonic limit is approached for the low-temperature limit. Therefore

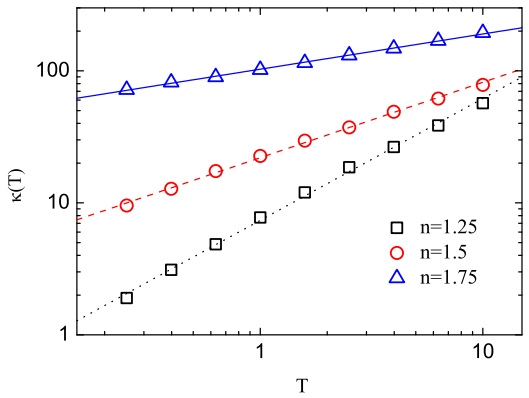


FIG. 5. (Color online) Thermal conductivities $\kappa(T)$ as a function of temperature T for different nonlinear KG lattices with $n = 1.25$, 1.5, and 1.75. Dotted, dashed, and solid lines are numerical fittings of the form $\kappa = A_n T^{r_n}$, where A_n and r_n are the fitting parameters. The system size to obtain the thermal conductivities is usually taken as $N = 800$. But for high-temperature cases, the longer system size of $N = 3200$ is usually chosen to avoid a finite-size effect.

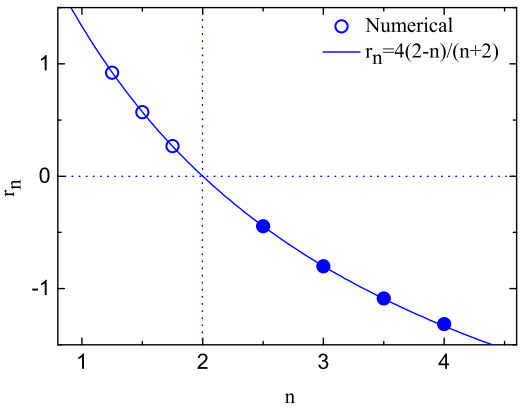


FIG. 6. (Color online) Exponents r_n as a function of n for $n = 1.25$, 1.5, and 1.75 for soft-KG lattices and $n = 2.5$, 3, 3.5, and 4 for hard-KG lattices. Open circles are numerical data of r_n extracted from Fig. 5 within the temperature range [0.15,10]. Filled circles are numerical data referenced from [62]. The dotted line is the theoretical prediction of Eq. (8) from effective phonon theory.

hard-KG lattices have higher thermal conductivities in the low-temperature region. However, soft-KG lattices approach the harmonic limit in the high-temperature region. Their thermal conductivities thus have higher values in the high-temperature region.

For each soft-KG lattice, the numerical value of the exponent r_n can be extracted with a standard fitting procedure. The resulting exponents r_n are plotted in Fig. 6 in comparison with the theoretical prediction of Eq. (8). It can be seen that the numerical data are in full agreement with the prediction of effective phonon theory. Therefore the effective phonon theory, developed from the assumption of renormalized phonons, can also explain *quantitatively* and *consistently* the temperature dependence of the thermal conductivities for soft-KG lattices.

IV. DISCUSSION

In summary, we have systematically studied the thermal properties of soft-KG lattices with nonlinear exponent $n < 2$. Renormalized phonons have been confirmed for these soft-KG lattices, as the temperature dependence of renormalization coefficients can be well explained by a classical field theory approach. The thermal conductivities have been calculated numerically and a power-law dependence as a function of temperature has been found. In contrary to hard-KG lattices, all the thermal conductivities of soft-KG lattices increase monotonically with temperature. All these numerical results are in good agreement with the prediction of effective phonon theory. In particular, the exponents of the temperature dependence of thermal conductivities have been found to be quantitatively consistent with the theoretical predictions of effective phonon theory.

There are other collective excitations in nonlinear lattices such as solitons [71–75] and breathers [76,77]. For a Toda lattice, the only excitations are solitons and the heat can only be conducted by solitons. It is also believed that solitons and breathers can influence the transport of phonons in some nonlinear lattices [7,38,42,49]. This kind of influence might depend on different lattice models, and further investigations are needed to obtain a full and clear picture of this issue.

ACKNOWLEDGMENTS

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