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Universality of thermal conduction in vibrating chains for a class of potentials

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We present calculations for the relaxation rates of phonons in one-dimensional chains in which atoms interact with a class of pairwise potentials which are anharmonic with odd powers. The calculations are based on a self-consistent procedure for second order processes and lead to integral equations for the wave-vector-dependent on-shell relaxation rate Γ_q for phonons. For the cubic anharmonicity, one finds that for small q, $\Gamma_q \propto q^{3/2}$. The self-consistent procedure is extended to potentials with higher odd powers and one finds that the leading order behavior is still $\Gamma_q \propto q^{3/2} + O(q^2)$. With the assumption that the transport relaxation rate has the same wave-vector dependence, this result implies that the thermal conductivity, κ diverges with the chain size, N, as $\kappa \propto N^{1/3}$ for this class of potentials. Thus, our calculations provide a microscopic basis for one class of universal behavior.

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I. INTRODUCTION

One-dimensional chains of vibrating atoms coupled by anharmonic potentials have evoked a lot of interest in recent times in the context of thermal conduction. The thermal conductivity, κ, of such chains diverges with the system size, N, as $\kappa \propto N^{\alpha}$. Much numerical and analytical effort has been expended to obtain the values of α for a number of interatomic potentials [1]. The transport behavior is intimately related to the dispersion and relaxation of normal modes in the system. Hence the value of α also reflects the manner in which the wave-vector-dependent transport or the current relaxation rate, $\Gamma_{tr}(q)$, depends on the wave-vector q especially for small q.

The numerical studies have been largely done on Fermi-Pasta-Ulam chains which have cubic (FPU-α chain) and quartic (FPU-β chain) anharmonicities [2,1]. Several earlier studies on FPU-β chains of few thousand atoms gave values of $\alpha \approx 0.4$, which also implies a nonanalytic form for $\Gamma_{tr}(q)$, $\Gamma_{tr}(q) \propto q^{\beta}$ with $\beta = (1-\alpha)^{-1} \approx 5/3$ [1,3]. A slightly larger value of 0.44 for α has been found for FPU-α chains [4], while a numerical study of diatomic Toda lattice finds α in a similar range [5]. A recent study on much longer on FPU-β chains, however, claims that $\alpha = 0.33$ [6], the earlier value being attributed to finite-size errors, though another study on the same size chain finds $\alpha \approx 0.4$, but at low energy density [7]. Curiously, a study which includes both longitudinal and transverse vibrations finds two kinds of behaviors: in one parameter range where the effect of transverse vibrations are negligible, $\alpha \approx 0.4$, whereas in other parameter regimes $\alpha \approx 0.33$ [8]. These results have naturally brought focus to questions of universality of conduction and mode relaxations in these chains and other one-dimensional systems. In a numerical study we explored the extent of universality by considering chains with longer range couplings, and found that for weak additional couplings α is still around 0.4, but seems to increase with the strength of additional couplings [9].

Analytical studies for classical FPU chains have employed two kinds of methods: The mode-coupling method and the kinetic theory method. The mode-coupling procedure basically calculates the mode-mode correlation function $G(q,t)$ or its frequency transform $G(q,z)$ for the mode of wave vector q. The first calculation, due to Lepri *et al.* [10] and Lepri [3], found that the associated relaxation function $\Gamma(q,z) \propto q^2/z^{1/3}$ for both cubic and quartic anharmonicities. The nonanalytic z dependence is rather generic to one dimension. Setting z equal to normal mode frequency, one obtains the mode relaxation rate $\Gamma(q) \propto q^{5/3}$. Wang and Lee [11] have carried out a similar calculation for a chain in which both longitudinal and transverse vibrations are permitted. They find that for their model the relaxation functions for the two kinds of modes have different frequency dependences, and consequently, $\alpha = 0.4$ when the transverse modes can be neglected, but $\alpha = 0.33$ when the transverse modes influence the conduction process. This is in accordance with their numerical results [8]. Recently, Delfini *et al.* [12,13] have refined the mode-coupling analysis and found that the results do depend on the nature of the nonlinearity of the interatomic potential. They found that for the cubic anharmonicity, $G(q,t) \propto e^{i\omega_q t} \exp(-bq^2 t^{4/3})$, while for quartic anharmonicity $G(q,t) \propto e^{i\omega_q t} \exp(-bq^2 t)$, where ω_q denotes the harmonic frequency of the mode. The former result corresponds to $\alpha = 1/3$, while the latter is the expectation from the standard hydrodynamic analysis corresponding to the mode relaxation rate $\Gamma(q) \propto q^2$ and $\alpha = 1/2$.

The kinetic theory treatment was first presented by Pereverzev who analyzed the problem for the quartic anharmonicity, using a classical version of the Boltzmann equation for the modes [14]. In this case modes relax only through umklapp scattering process and the collision integral is singular at small q leading to the relaxation rate for the energy in the mode to be proportional to $q^{5/3}$. This result has recently been put on a firmer mathematical footing by Lukkarinen and Spohn [15].

We have recently done a quantum calculation of the phonon relaxation and the thermal conductivity for FPU-β chain [16]. The phonon relaxation rate was obtained at low temperatures as $\Gamma_q \propto T^2 q^{5/3}$ for small q. Here, also, only the umklapp processes contributed to the phonon relaxation and the singular behavior again comes from the collision integral identical to the kinetic theory calculation. The calculation of thermal conductivity was done using the Kubo-Green formula and the transport relaxation rate was obtained taking into account the vertex corrections. The transport relaxation rate was found to have the same wave-vector dependence as above and we obtain $\alpha=2/5$. Motivated by our numerical results, we also examined the effect of increasing the range of interaction on phonon relaxation rate for FPU-β chain. We found that when the ratio of the second neighbor interaction to the first neighbor interaction is small, the relaxation rate $\Gamma_q \sim Aq^{5/3}+Bq^2$ [17]. This means that the asymptotic value of α is $2/5$, but there are crossover effects for finite chains due to the q^2 term, leading to a higher effective value for α for short chains.

The universality of anomalous conduction in one dimension has been explored further by considering transport in fluids. Narayan and Ramaswamy (NR) [18] obtained $\alpha=1/3$ from a renormalization group study of the hydrodynamic equations and argued that this result applies to any momentum-conserving system in which local thermal equilibrium is established. The value of $\alpha=1/3$ was supported by numerical studies on particles interacting with a hard sphere potential [19]. The hydrodynamic arguments have been further extended by Lee-Dadswell *et al.* [20]. Recognizing that the energy transport and momentum transport are coupled, they also studied the frequency dependent longitudinal viscosity $\zeta(\omega)$ and found that it has two different behaviors depending on whether $\gamma=c_p/c_v$ is equal to 1 or not. This leads to different behaviors of the frequency dependent conductivity $\kappa(\omega)$. For $\gamma=1$, $\zeta(\omega)\to\zeta_0$ leading to $\kappa(\omega)\propto\omega^{-1/2}$ whereas for $\gamma\neq 1$, $\zeta(\omega)\propto\omega^{-1/2}$ leading to $\kappa(\omega)\propto\omega^{-1/3}$. The mode-coupling results of Delfini *et al.* are consistent with this analysis as for the cubic anharmonicity $\gamma\neq 1$ while for the quartic case $\gamma=1$. It may be pointed out that for the quartic interaction there is a variance in the results of the mode-coupling analysis ($\alpha=2/5$ or $1/2$), and it does not take into account the umklapp scattering which is a key ingredient in the microscopic approach.

To summarize, calculations on chains with different potentials give rise to three values of α, namely 0.4, 0.33, and 0.5. The hydrodynamic and mode coupling theories suggest two universality classes of conduction behavior, corresponding to the latter two values of α. All the results are open to some doubt: Numerical due to finite-size effects and analytical due to inevitable approximations. In this paper we present a quantum study of the phonon relaxation for chains with potentials of odd anharmonicity, with a view to examine the question of universality from a microscopic point of view.

This paper is organized as follows. In the next section we present detailed calculations for FPU-α chain. The cubic anharmonicity has an important difference with the quartic anharmonicity studied earlier [16]. For the cubic case there are no microscopic processes that contribute to the relaxation rate of the phonons in second and third order in the coupling strength of the nonlinear term. This is because the mode dispersion ω_q being nonlinear in q, does not permit simultaneous energy and momentum conservation for these processes. So, we do a self-consistent study of the second order processes, in which the internal propagators are dressed and have a wave-vector-dependent width. The width of the internal lines relaxes the energy-momentum conservation and we are led to a self-consistent integral equation for the wave-vector-dependent width. The integral equation is singular in a way, which enables us to show that, $\Gamma(q)\propto T^{1/2}q^{3/2}$ for small q.

Since this is different from the quartic case, a natural course is to examine other potentials. So in Sec. III, we consider the fifth power interaction and again look at the second order diagrams. These bare diagrams do not contribute to the relaxation rate as again the momentum and energy conservation cannot be satisfied simultaneously. So we proceed with the self-consistent treatment. A set of these diagrams just lead to an effective third order interaction, while the others lead to an integral equation for $\Gamma(q)$. Analysis of the integral equation shows that the latter diagram gives analytical corrections like q^2, giving a leading order self-consistent answer $\Gamma(q)\propto q^{3/2}$. The analysis for higher power potentials is carried out using power counting arguments and gives the same dominant low q behavior as the cubic anharmonicity. We conclude the paper with a summary in Sec. IV.

II. FPU-α CHAIN

The system consists of a chain of particles of mass m, arranged on a lattice, that interact with their nearest neighbors. The Hamiltonian of the system is given by

$$H=\sum_{l=1}^{N}\left[\frac{p_l^2}{2m}+V(x_l-x_{l+1})\right], \tag{1}$$

where x_l and p_l are respectively the position and the momentum of the particle whose equilibrium position is la, a being the lattice spacing. The interaction potential is $V(x)=\frac{1}{2}m\omega_0^2x^2+(g_3/3!)x^3$. For the quantum treatment, one writes the Hamiltonian in terms of phonon creation and annihilation operators $a_k^\dagger$ and a_k. In units defined by $\hbar=\omega_0=a=1$, the Hamiltonian takes the form,

$$H=\sum_k \omega_k\left(\frac{1}{2}+a_k^\dagger a_k\right)+\frac{\tilde{g}_3}{3!\sqrt{N}}\sum_{k,q,p}v(k,q,p)A_kA_qA_p, \tag{2}$$

where

$$\omega_k=2|\sin k/2|, \quad A_k=a_k+a_{-k}^\dagger,$$

$$v(k,q,p)=\frac{\gamma_k\gamma_q\gamma_p}{\sqrt{\omega_k\omega_q\omega_p}}\Delta(k+q+p), \quad \gamma_q=1-e^{-iq}. \tag{3}$$

The Δ function represents the momentum conservation in phonon collisions. $\Delta(k)=1$ when k is either zero, corresponding to normal processes, or a nonzero integer multiple of 2π, corresponding to umklapp processes; otherwise $\Delta(k)=0$. $\tilde{g}_3$ is the dimensionless coupling constant.

The thermal Green's function for phonons is defined in the standard manner

$$D(q,\tau)=-\langle T_\tau[A_q(\tau)A_{-q}(0)]\rangle=G(q,\tau)+G(-q,-\tau),$$

$$G(q,\tau)=-\langle T_\tau[a_q(\tau)a_q^\dagger(0)]\rangle. \tag{4}$$

Here T_τ is the usual time-ordering operator and $0\leq\tau\leq\beta$. One also defines the frequency transform as

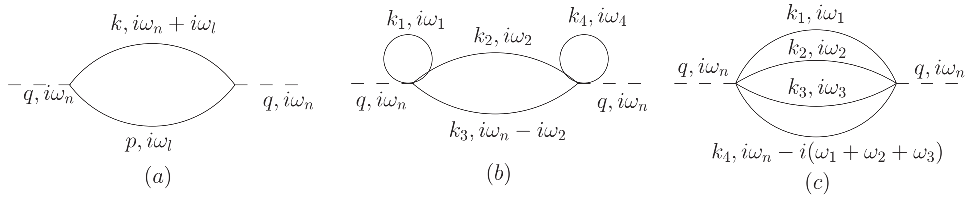

FIG. 1. Second order contribution to the self-energy $\Sigma(q, i\omega_n)$ (a) for the cubic interaction and (b) and (c) for the fifth power interaction. Solid lines represent bare phonon Green's functions D_0.

$$D(q,i\omega_n) = \int_0^\beta D(q,\tau) e^{i\omega_n \tau} d\tau, \tag{5}$$

where $\omega_n = 2\pi n T$ are the Matsubara frequencies where we set the Boltzmann constant $k_B = 1$. We now calculate the self-energy of the phonon perturbatively. The self-energy $\Sigma(q, i\omega_n)$ has the usual definition: $\Sigma(q, i\omega_n) = D_0^{-1}(q, i\omega_n) - D^{-1}(q, i\omega_n)$, where $D_0(q, i\omega_n)$ is the unperturbed propagator given by $-2\omega_q/(\omega_q^2 + \omega_n^2)$. The relaxation rate $\Gamma(q,\omega)$ is obtained from the following equation:

$$\Gamma(q,\omega) = -\operatorname{Im} \lim_{\delta \to 0} \Sigma(q, i\omega_n \to \omega + i\delta). \tag{6}$$

The lowest order contribution to the self-energy is from the second-order diagram given by Fig. 1(a). This contribution is

$$\Sigma^{(2)}(q,i\omega_n) = -\frac{\tilde{g}_3^2}{2N\beta} \sum_{p,k} \sum_l |v(-q,p,k)|^2 \times D_0(k, i\omega_n + i\omega_l) D_0(p, i\omega_l). \tag{7}$$

The corresponding on-shell relaxation rate is given as $\Gamma^{(2)}(q,\omega_q) = \Gamma_A^{(2)}(q,\omega_q) + \Gamma_B^{(2)}(q,\omega_q)$, with

$$\Gamma_A^{(2)}(q,\omega_q) = -\frac{\tilde{g}_3^2 \pi}{2N} \omega_q \sum_{p,k} \omega_p \omega_k (1 + n_k + n_p) \Delta(-q+p+k) \times [\delta(\omega_q + \omega_p + \omega_k) - \delta(\omega_q - \omega_p - \omega_k)],$$

$$\Gamma_B^{(2)}(q,\omega_q) = -\frac{\tilde{g}_3^2 \pi}{N} \omega_q \sum_{p,k} \omega_p \omega_k (n_k - n_p) \times \Delta(-q-p+k) \delta(\omega_q + \omega_p - \omega_k). \tag{8}$$

With the dispersion in Eq. (3) the energy and momentum conservation conditions represented by the delta functions cannot be satisfied, resulting in a zero contribution by both the normal and umklapp processes. Therefore, a self-consistent approach is required.

In the self-consistent calculation the bare phonon lines in the diagram of Fig. 1(a) are replaced by the full phonon Green's functions. The contribution is as in Eq. (7), with D_0 being replaced by D. The next step uses the following spectral representation for G.

$$G(p,i\omega_l) = \int \frac{d\omega'}{2\pi} \frac{A(p,\omega')}{i\omega_l - \omega'}. \tag{9}$$

The spectral function $A(q,\omega)$ is given as

$$A(q,\omega) = -2 \operatorname{Im} \lim_{\delta \to 0} G(q, i\omega_n \to \omega + i\delta) = \frac{2\Gamma(q,\omega)}{[\omega - \omega_q - \Sigma_R(q,\omega)]^2 + \Gamma^2(q,\omega)}, \tag{10}$$

where Σ_R and Γ are obtained from $\lim_{\delta\to 0} \Sigma(q, i\omega_n \to \omega + i\delta) = \Sigma_R(q,\omega) - i\Gamma(q,\omega)$. We now substitute the spectral forms for G's in the equation for Σ and perform the frequency summation to obtain $\Gamma(q,\omega) = \Gamma_A(q,\omega) + \Gamma_B(q,\omega)$, with

$$\Gamma_A(q,\omega) = \frac{\tilde{g}_3^2 \pi}{2N} \omega_q (e^{\beta\omega} - 1) \sum_{p,k} \omega_p \omega_k \int \frac{d\omega'}{(2\pi)^2} A(p,\omega') n(\omega') \times [A(k,\omega - \omega') n(\omega - \omega') - A(k, -\omega - \omega') n(-\omega - \omega')] \Delta(q-p-k),$$

$$\Gamma_B(q,\omega) = \frac{\tilde{g}_3^2 \pi}{N} \omega_q (e^{\beta\omega} - 1) \sum_{p,k} \omega_p \omega_k \times \int \frac{d\omega'}{(2\pi)^2} A(p,\omega') [1 + n(\omega')] \times n(\omega + \omega') A(k, \omega + \omega') \Delta(q+p-k). \tag{11}$$

Our interest in this paper is to evaluate the on-shell relaxation rate $\Gamma(q,\omega_q)$ for small wave number phonons, and in this limit the above expressions can be considerably simplified. We first use the physical argument that for small q, $\Gamma_q \ll \omega_q$, and the spectral function is well approximated by a narrow peak at $\omega = \tilde{\omega}_q = \omega_q + \Sigma_R(q,\omega_q)$. This allows us to replace $A(p,\omega) f(\omega) \approx A(p,\omega) f(\tilde{\omega}_p)$, where $f(\omega)$ is any smooth function of ω, like the Bose factor $n(\omega)$. In the same spirit, we also take

$$A(p,\omega) \approx \frac{2\Gamma(p,\tilde{\omega}_p)}{(\omega - \tilde{\omega}_p)^2 + \Gamma^2(p,\tilde{\omega}_p)}. \tag{12}$$

Denoting the on-shell relaxation rate $\Gamma(p,\tilde{\omega}_p) = \Gamma_p$ we obtain, after performing the integral over ω', and using the above approximation for $A(p,\omega)$,

$$\Gamma_A(q,\tilde{\omega}_q) = \frac{\tilde{g}_3^2}{2N} \omega_q (e^{\beta\tilde{\omega}_q} - 1) \sum_{p,k} \omega_p \omega_k n(\tilde{\omega}_p) n(\tilde{\omega}_k) \times \Delta(-q+p+k) \left\{ \frac{\Gamma_k}{(\tilde{\omega}_q - \tilde{\omega}_p - \tilde{\omega}_k - i\Gamma_p)^2 + \Gamma_k^2} + \frac{\Gamma_p}{(\tilde{\omega}_q - \tilde{\omega}_p - \tilde{\omega}_k + i\Gamma_k)^2 + \Gamma_p^2} \right.$$

$$+\frac{\Gamma_k}{(\tilde{\omega}_q+\tilde{\omega}_p+\tilde{\omega}_k+i\Gamma_p)^2+\Gamma_k^2} + \left.\frac{\Gamma_p}{(\tilde{\omega}_q+\tilde{\omega}_p+\tilde{\omega}_k-i\Gamma_k)^2+\Gamma_p^2}\right\} \tag{13}$$

and

$$\Gamma_B(q,\tilde{\omega}_q)=\frac{\tilde{g}_3^2}{N}\omega_q(e^{\beta\tilde{\omega}_q}-1)\sum_{p,k}\omega_p\omega_k[1+n(\tilde{\omega}_p)]n(\tilde{\omega}_k) \times\Delta(-q-p+k)\left\{\frac{\Gamma_k}{(\tilde{\omega}_q+\tilde{\omega}_p-\tilde{\omega}_k+i\Gamma_p)^2+\Gamma_k^2} + \frac{\Gamma_p}{(\tilde{\omega}_q+\tilde{\omega}_p-\tilde{\omega}_k-i\Gamma_k)^2+\Gamma_p^2}\right\}. \tag{14}$$

From the form of the interaction, it is seen that $\tilde{\omega}_q \propto \omega_q$, the proportionality factor being a temperature-dependent constant for small q. This factor does not turn out to be important in further analysis, so in the following we replace $\tilde{\omega}_q = \omega_q$.

The on-shell relaxation rate Γ_q has to be obtained by self-consistently solving Eq. (13) and Eq. (14) using $\Gamma_q = \Gamma_A(q,\omega_q)+\Gamma_B(q,\omega_q)$. Further simplifications can be done for the Γ_A term. For narrow widths the last two terms in the expression for Γ_A are nonzero only if $\omega_q+\omega_p+\omega_k\approx 0$. Since this can be satisfied only for very small q's and p's, the contribution from these terms is of higher order in q compared to that from the other terms. Accordingly, we neglect these. Further, for small q we can approximate $\omega_q+\omega_p-\omega_{q+p}\approx q[1-\cos(p/2)]=q\chi_p$. Similarly, $\omega_q-\omega_p-\omega_{q-p}\approx q[1-\cos(p/2)]-2\omega_p=q\tilde{\chi}_p-2\omega_p$. Substituting these Eqs. (13) and (14) assume the form

$$\Gamma_A(q,\omega_q)=\frac{\tilde{g}_3^2}{2}\omega_q(e^{\beta\omega_q}-1)\int_0^{2\pi}\frac{dp}{2\pi}\omega_p\omega_{q-p}n(\omega_p)n(\omega_{q-p}) \times\frac{(\Gamma_{q-p}+\Gamma_p)[(q\tilde{\chi}_p-2\omega_p)^2+(\Gamma_p-\Gamma_{q-p})^2]}{[(q\tilde{\chi}_p-2\omega_p)^2+\Gamma_{q-p}^2+\Gamma_p^2]^2-4\Gamma_{q-p}^2\Gamma_p^2}, \tag{15}$$

$$\Gamma_B(q,\omega_q)=\tilde{g}_3^2\omega_q(e^{\beta\omega_q}-1)\int_0^{2\pi}\frac{dp}{2\pi}\omega_p\omega_{q+p}n(\omega_{q+p})[1+n(\omega_p)] \times\frac{(\Gamma_{q+p}+\Gamma_p)[q^2\chi_p^2+(\Gamma_{q+p}-\Gamma_p)^2]}{(q^2\chi_p^2+\Gamma_{q+p}^2+\Gamma_p^2)^2-4\Gamma_{q+p}^2\Gamma_p^2}. \tag{16}$$

These equations are rather complex, but the leading analytical behavior at small q can be obtained by assuming $\Gamma_q \propto q^x$ with $x>1$. With this assumption, which will be justified *a posteriori*, we note that at $q=0$, the integrands in above expressions for both Γ_A and Γ_B diverge due to singularity at $p=0$. The major contribution to the integrals comes from small p region and to examine the singularity we can safely take, $\omega_p n(\omega_p)=\omega_{q\pm p}(1+n(\omega_{q\pm p}))=1/\beta$. Now we note that the integrand in Eq. (15) behaves like $p^x/(p^2+p^{2x})\approx p^{x-2}$, since we expect $1<x<2$. This makes the integral finite. On the other hand, the integrand in Eq. (16) behaves like p^{-x} and the integral diverges. This means that when we consider this integral at nonzero q, it diverges as some inverse power of q and the leading power of Γ_q in q is less than 2. Therefore the leading order contribution to Γ_q comes from Γ_B. We first show that the leading order behavior of Γ_B gives a self-consistent exponent and then observe that, with this behavior for Γ_q, the contribution from Γ_A is of higher order.

Expanding in powers of q and keeping the first few terms, Eq. (16) becomes

$$\Gamma_B(q,\omega_q)=\Gamma_1(q,\omega_q)+\Gamma_2(q,\omega_q)+\Gamma_3(q,\omega_q),$$

$$\Gamma_1(q,\omega_q)\propto Tq^2\int_0^{2\pi}\frac{dp}{\Gamma_p+\Gamma_{q+p}}, \tag{17}$$

$$\Gamma_2(q,\omega_q)\propto -Tq^4\int_0^{2\pi}dp\frac{p^4(\Gamma_{q+p}^2+\Gamma_p^2)}{(\Gamma_{q+p}^2-\Gamma_p^2)(\Gamma_{q+p}+\Gamma_p)}, \tag{18}$$

$$\Gamma_3(q,\omega_q)\propto Tq^4\int_0^{2\pi}dp\frac{p^4}{(\Gamma_{q+p}^2-\Gamma_p^2)(\Gamma_{q+p}-\Gamma_p)}. \tag{19}$$

Here, Γ_1 is the leading order term in Γ_q and we first try to solve Eq. (17) self-consistently by taking $\Gamma_q\approx\Gamma_1(q,\omega_q)$. The solution is found by making a guess that $\Gamma_q\propto T^{1/2}q^{3/2}$. Then Eq. (17) becomes

$$\Gamma_1(q,\omega_q)\propto T^{1/2}q^2\int_0^{2\pi}dp\frac{1}{(q+p)^{3/2}+p^{3/2}}. \tag{20}$$

The integral diverges for $q=0$ and the singularity is extracted by substituting $p=zq$. This yields

$$\Gamma_1(q,\omega_q)\propto T^{1/2}q^{3/2}\int_0^{2\pi/q}dz\frac{1}{(1+z)^{3/2}+z^{3/2}}. \tag{21}$$

Setting $q=0$ in the integral results in a finite value for the integral and we get $\Gamma_1(q,\omega_q)\propto T^{1/2}q^{3/2}$. Substituting this form for Γ_p, it is directly seen that $\Gamma_2(q,\omega_q)\propto q^3$ and $\Gamma_3(q,\omega_q)\propto q^2$ and are thus of higher order.

Having obtained the leading order contribution of Γ_B to be proportional to $q^{3/2}$, we turn our attention to Γ_A. So, in Eq. (15), we set $\Gamma_p\propto p^{3/2}$ and make a small q expansion. It is easily established that the integrand has a singularity at $p=0$ like $p^{-1/2}$. Therefore, the integral is finite and we get $\Gamma_A(q,\omega_q)\propto q^2$. Thus the leading order contribution to Γ_q comes from Γ_1 [Eq. (17)], and the self-consistent solution is, $\Gamma_q\propto T^{1/2}q^{3/2}+O(q^2)$.

The conductivity can be obtained by using the standard kinetic theory formula. This, however, requires the knowledge of the transport or current relaxation rate, which, in principle, is different from the mode relaxation rate obtained above. As mentioned earlier, for the quartic interaction we have obtained the transport relaxation rate by including the vertex corrections in the Kubo-Green formula and found that the wave-vector dependence is the same as the mode relaxation. Assuming the same to hold here, as vertex corrections seem to be of higher order here, we have for the conductivity of a finite chain

$$\kappa = \int_0^{t_0} dt \int dq\, C_q v_q^2 \exp(-\Gamma_q t), \tag{22}$$

where C_q is the mode specific heat, v_q is the mode group velocity, and t_0 is of the order of the average time taken by the modes to traverse the chain and is proportional to N. The approximate evaluation of this formula for large N yields

$$\kappa \propto N^{1/3} T^{-1/3}. \tag{23}$$

Though our result for cubic anisotropy matches with that of mode-coupling analysis, it is interesting to contrast the nature of the two sets of arguments. The mode-coupling analysis basically finds that the time/frequency behavior of the correlator for the displacement mode is nonanalytic ($\sim \omega^{-1/3}$ for cubic anharmonicity), whereas our analysis, being a quantum calculation, sets up a self-consistent integral equation for the on-shell relaxation rate of the phonons. In this situation, the nonanalytic behavior arises from the wave-number dependence of the rate.

In view of the result that for the quartic potential $\Gamma_q \propto q^{5/3}$, one wonders if other potentials lead to still other exponents or there are few universality classes. We examine the higher order odd potentials in the next section.

III. ANALYSIS OF HIGHER ORDER POTENTIALS

We begin the analysis by considering the fifth power potential, given as

$$V_5 = \frac{g_5}{5\,!\,N^3} \sum_{\{k_i\}} v(k_1,k_2,k_3,k_4,k_5) A_{k_1} A_{k_2} A_{k_3} A_{k_4} A_{k_5},$$

$$v(k_1,k_2,k_3,k_4,k_5) = \left(\Pi_{i=1}^{5} \frac{\gamma_{k_i}}{\sqrt{\omega_{k_i}}} \right) \Delta(k_1 + k_2 + k_3 + k_4 + k_5). \tag{24}$$

The diagrams for the second order self energy are shown in Figs. 1(b) and 1(c). The diagram of Fig. 1(b) is like that of cubic anisotropy with an effective coupling $g_{\text{eff}} = (g_5/2N) \Sigma_k \omega_k (2n_k + 1)$ and simply renormalizes g_3. Considering this diagram alone would yield $\Gamma_q \propto q^{3/2}$, but for this to be the leading power we need to check if the diagram of Fig. 1(c) leads to a lower power. The bare diagram 1(c) fails to contribute to the relaxation rate as due to nonlinear dispersion of modes the momentum and energy conservation cannot be satisfied simultaneously. So, we proceed with the self-consistent treatment by using full propagators for the internal lines. Following the procedure described in the previous section, one find the following self-consistent equation for the on-shell relaxation rate:

$$\Gamma_q = \frac{\pi g_5^2}{4!} \omega_q (1 - e^{-\beta \omega_q}) \frac{1}{N^3} \sum_{\{s_i = \pm\}} \sum_{\{k_i\}} \omega_1 \omega_2 \omega_3 \omega_4 \times n_{s_1}(\omega_1) n_{s_2}(\omega_2) n_{s_3}(\omega_3) n_{s_4}(\omega_4) \times \Delta\left(q - \sum_i s_i k_i \right) J(q, \{k_i\}, \{s_i\}). \tag{25}$$

Here, the variable s_i takes the value ± and we use the notations: $\omega_1 = \omega_{k_1}$, $n_+(\omega) = 1 + n(\omega)$ and $n_-(\omega) = n(\omega)$. This enables us to write all the contributions of Fig. 1(c) in a compact manner. The function J is a sum of eight terms, $J = \Sigma_1^8 J_n$, which have the typical form

$$J_1 = \frac{1}{\pi} \frac{\Gamma_{k_1}}{[\Delta_q(\{s_i\}) - i s_1 \Gamma_{k_4} + i s_2 \Gamma_{k_2} + i s_3 \Gamma_{k_3}]^2 + \Gamma_{k_1}^2}, \tag{26}$$

where $\Delta_q(\{s_i\}) = \Sigma_j^4 s_j \omega_j - \omega_q$. The other terms are some permutations among k_1, k_2, k_3 and are given in the Appendix. To analyse these equations for small q, we again assume $\Gamma_k \approx k^x$ with $1 < x \leq 2$ and check if the integrals involved diverge. Again one finds that for all the terms the integrand diverges when k_1, k_2, $k_3 \to 0$, and since this region contributes to the integral dominantly one may write the contribution from J_1 to leading order in q as

$$\Gamma_q^{(1)} \propto q^2 T^3 \int \int \int dk_1 dk_2 dk_3 \frac{\Gamma_{k_1}}{\Gamma_{k_1}^2 - (\Gamma_{q+k_1-k_2-k_3} + \Gamma_{k_2} - \Gamma_{k_3})^2}. \tag{27}$$

This is the analog of Eq. (17) and the other $J_n's$ contribute similar terms. We first analyze this equation independently by taking $\Gamma_k \sim \Gamma_k^{(1)}$. The solution of this equation is again obtained by trial. We take $\Gamma_k \propto k^2$ which makes the integrand most singular. With this the numerator of the integrand has five powers of momenta while the denominator has four, which implies that the integral does not diverge from the small-k singularity of the integrand. We have examined the integrals using polar representation and find that they are well behaved and yield constant values. A typical evaluation is presented in the Appendix. This means that the solution of Eq. (27) is, $\Gamma_q^{(1)} \propto q^2$. Now let us consider the contributions from both the diagrams together. If we set $\Gamma_q \sim q^{3/2} + O(q^2)$, the terms corresponding to Fig. 1(b) [which are similar to Eq. (17)] will yield $q^{3/2}$ while those corresponding to Fig. 1(c) will yield q^2 [as the integral in Eq. (27) is finite for $\Gamma_q \propto q^x$, $x \leq 2$]. Thus $\Gamma_q \propto q^{3/2} + O(q^2)$ is a self-consistent solution for the fifth power potential.

The analysis of potentials with higher odd powers follows a similar pattern. A set of second order diagrams renormalize the lower order couplings and the new contribution comes from analogs of Fig. 1(c). These diagrams lead to integral equations similar to Eq. (27), but with each higher order there are two additional integrals over momenta due to increase of two internal lines, whereas the denominator always contains squares of $\Gamma_k's$. The power counting argument shows that these integrals are well behaved and constants when we take $\Gamma_k \propto k^x$ with $x < 2$. This again yields $\Gamma_k \propto k^2$ for the contributions coming from analogs of diagrams of Fig. 1(c) for all higher odd power interactions. Since all these interactions also renormalize the cubic coupling, they yield the result, $\Gamma_q \propto q^{3/2} + O(q^2)$.

We should emphasize that our analysis applies only to odd potentials of polynomial type. The analysis is perturbative and is valid only at low temperatures where the vibration amplitudes are small compared to lattice constant. One may consider an odd potential, $V(x)=A-\cos(x)+b\sin(2x)$, which has been investigated by Giardina *et al.* [21]. For such potentials, which apply to a chain of coupled rotors, one obtains finite conductivity, presumably due to jumps between potential wells. Clearly our peturbative analysis does not apply to these situations.

IV. SUMMARY

To summarize, we have shown by a self-consistent analysis of the second order process that the phonon relaxation rate for an FPU-α chain goes as $\Gamma_q \propto q^{3/2}+O(q^2)$. We further show that a similar analysis for interactions of higher odd powers also yield the same result, thereby establishing a universal behavior for the phonon relaxation. With the further assumption that the transport relaxation rate has the same wave-vector dependence, it is argued that for this whole class of potentials the thermal conductivity diverges with chain length as $\kappa \propto N^{1/3}$. For the cubic potential we have an additional result regarding temperature dependence, $\kappa \propto T^{-1/3}N^{1/3}$. Our result matches partially the results obtained from hydrodynamic considerations by providing support for one class of universal behavior. Moreover, the hydrodynamic criterion that distinguishes the two universal behaviors in terms of the value of $\gamma=c_p/c_v$ also holds here as $\gamma \neq 1$ for odd power potentials, which implies $\alpha=1/3$. Our results are dependent on the assumption that the self-consistent analysis of the second order diagram captures the essential physics of the phonon relaxation. From a microscopic point of view it would be tempting to obtain a universal result for even powered potentials, but for such potentials the relaxation occurs due to umklapp scattering and the analysis of such collision integrals for higher power interactions is quite tedious.

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APPENDIX

The function $J(q,\{k_i\},\{s_i\})$ in Eq. (25) is given by

$$J_q = \frac{1}{\pi}\left\{ \frac{\Gamma_1}{(\Delta_q - is_1\Gamma_4 + is_2\Gamma_2 + is_3\Gamma_3)^2 + \Gamma_1^2} + \frac{\Gamma_2}{(\Delta_q - is_1\Gamma_4 - is_2\Gamma_1 + is_3\Gamma_3)^2 + \Gamma_2^2} + \frac{\Gamma_2}{(\Delta_q + is_1\Gamma_1 - is_2\Gamma_4 + is_3\Gamma_3)^2 + \Gamma_2^2} \right.$$

$$\left. + \frac{\Gamma_3}{(\Delta_q - is_1\Gamma_4 - is_2\Gamma_1 - is_3\Gamma_2)^2 + \Gamma_3^2} + \frac{\Gamma_3}{(\Delta_q - is_1\Gamma_4 + is_2\Gamma_2 - is_3\Gamma_1)^2 + \Gamma_3^2} + \frac{\Gamma_3}{(\Delta_q + is_1\Gamma_1 - is_2\Gamma_4 - is_3\Gamma_2)^2 + \Gamma_3^2} + \frac{\Gamma_3}{(\Delta_q + is_1\Gamma_1 + is_2\Gamma_2 - is_3\Gamma_4)^2 + \Gamma_3^2} + \frac{\Gamma_4}{(\Delta_q + is_1\Gamma_1 + is_2\Gamma_2 + is_3\Gamma_3)^2 + \Gamma_4^2} \right\} \tag{A1}$$

where we have simplified the notation in the following way: $J_q=J(q,\{k_i\},\{s_i\})$, $\Delta_q=\Delta_q(\{s_i\})$ which is defined after Eq. (26) and $\Gamma_i=\Gamma_{k_i}$.

Now we evaluate a typical term in Eq. (25) corresponding to the first term in Eq. (A1) with $\{s_i\}=\{-,+,+,+\}$. This leads to Eq. (27) which can be written as $\Gamma_q^{(1)} \propto q^2T^3I(q)$. The integrand of $I(q)$ has singularity due to small-k behavior of Γ_k's. We now show if we assume $\Gamma_k \propto k^2$ the integral is finite and should be so for $\Gamma_q \sim q^x$ for $1<x<2$ as well. Noting that the major contribution comes from the small k behavior of Γ_k's, we get

$$I(q) \propto \int\int\int dk_1 dk_2 dk_3 \times \frac{k_1^2}{k_1^4 - (k_1^2 + 2k_2^2 + 2k_3^2 - 2k_1(k_2+k_3) + 2k_2k_3)^2}. \tag{A2}$$

Using the polar coordinates $k_1=K\cos\theta$, $k_2=K\sin\theta\cos\phi$ and $k_3=K\sin\theta\sin\phi$,

$$I(q) \propto -\int_0^{\pi} d\theta \int_0^{2\pi} d\phi \frac{\cos^2\theta\sin\theta}{\cos^2\theta S(\theta,\phi) + S^2(\theta,\phi)}, \tag{A3}$$

$$S(\theta,\phi) = \sin^2\theta(1+\sin\phi\cos\phi) - \cos\theta\sin\theta(\cos\phi+\sin\phi). \tag{A4}$$

The transformation $x=\cos\theta$ simplify this expression as

$$I(q) \propto \int_{-1}^{1} dx \int_0^{2\pi} d\phi \frac{x^2}{x^2\tilde{S}(x,\phi) + \tilde{S}^2(x,\phi)},$$

where $\tilde{S}(x,\phi)=(1-x^2)(1+\sin\phi\cos\phi)-x(1-x^2)^{1/2}(\cos\phi+\sin\phi)$. The integrand is singular at $x=\pm 1$ where it is like $(1-x^2)^{-1/2}(\cos\phi+\sin\phi)^{-1}$ and is integrable. We, therefore, conclude that the contribution from this term is of $O(q^2)$ even when we use $\Gamma_k \propto k^{3/2}$.

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