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Anomalous thermal conduction in one dimension: A quantum calculation

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In this paper, we study the thermal conductivity of an anharmonically coupled chain of atoms. Numerical studies using classical dynamics have shown that the conductivity of a chain with nearest neighbor couplings diverges with chain length L as L^{α}; earlier studies found $\alpha \approx 0.4$ under a range of conditions, but a recent study on longer chains claims $\alpha = 1/3$. Analytically, this problem has been studied by calculating the relaxation rate Γ_q of the normal modes of vibration as a function of its wave vector q. Two theoretical studies of classical chains, one using the mode-coupling formulation and the other the Boltzmann equation method, led to $\Gamma_q \propto q^{5/3}$, which is consistent with $\alpha = 0.4$. Here we study the problem for a quantum anharmonic chain with quartic anisotropy. We develop a low-temperature expansion for Γ_q and find that, in the regime $\hbar\omega_q \ll k_B T$, $\Gamma_q \propto q^{5/3} T^2$, where ω_q is the frequency of the mode. In our analysis, the relaxation arises due to umklapp scattering processes. We further evaluate the thermal conductivity of the chain using the Kubo formula, which enables us to take into account the transport relaxation time through vertex corrections for the current-current correlator. This calculation also yields $\alpha = 0.4$.

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I. INTRODUCTION

Our understanding of heat conduction and other transport processes is based on phenomenological laws like the Fourier law. The basic assumption that underlies such laws is that of local thermal equilibrium (LTE), in which the noneqilibrium state of the system can be described in terms of slow spatiotemporal variations of the thermodynamic variables of the system. While these laws have provided a very useful description of a vast range of near-equilibrium phenomena, their microscopic basis is far from being understood [1–4].

In this context, much effort has been made to study one-dimensional systems, as they are amenable to farther analytical and numerical progress [5]. The first such effort was the celebrated work of Fermi, Pasta, and Ulam (FPU), who considered vibrations of a classical chain of anharmonically coupled atoms [6]. Their observations regarding the lack of energy sharing among long-wavelength modes in the system has led to a large body of work examining relationships of dynamical chaos with ergodicity, equipartition, energy diffusion among modes, stochasticity, etc. [7,8].

Another important early study examining heat flow under temperature gradient is due to Rieder, Lebowitz, and Lieb [9], who obtained an exact solution for a harmonically coupled chain. They showed that the thermal conductivity diverges linearly with the chain length, and the temperature profile departs from the expectations of the Fourier law. The lack of LTE could be attributed to ballistic transport in a harmonic system; however, the precise conditions on the dynamics needed to obtain LTE in the system remains a goal of the work being pursued currently. The transport behavior is intimately related to the dispersion and relaxation of normal modes in the system. The latter aspect, in turn, depends crucially on the dimensionality of the system. The role of dimensionality for the transport processes in general was brought out by hydrodynamic arguments [10], which typically give for a mode of wave vector q a relaxation rate of the form q^2. This implies a divergence of the transport coefficients in dimensions two and smaller, and for a finite chain the conductivity would diverge with chain length L as L^{α}, with $\alpha = 0.5$.

Recently, this problem has received a lot of attention through a number of numerical and analytical studies [5,11]. The first set of numerical studies on the FPU chain that obtained the divergence of conductivity found that $\alpha \approx 0.4$ for a range of anharmonicity parameters and temperatures [12,13]. Another system where the same exponent was seen is the diatomic Toda lattice [14]. But the value of the exponent and the extent of its universality have come under much scrutiny. In one set of studies, where the atoms are allowed both transverse and longitudinal motions, two sets of exponents were seen [15]. For a certain range of parameters, the exponent was seen to be 0.4, whereas in another range, where transverse motion seems to dominate, the exponent was found to be 1/3. In a study by us [16], two variations were made. One, next-nearest-neighbor couplings between atoms were introduced. Second, a two-ladder chain was used, in which atoms can vibrate both along and transverse to the ladder. In both cases, the divergence exponent was found to be 0.6, a significant change, as in our first variation the new couplings change only the dispersion of the modes. A very recent study on longer FPU chains, however, claims that the asymptotic exponent is 1/3, and it also shows the existence of LTE for such chains [17].

Lepri [18] has considered this question from two other points of view. First, the power law decay of the autocorrelation function of current was numerically computed, and found to decay asymptotically as $\langle J(t)J(0)\rangle \propto t^{-\beta}$, where $J(t)$ denotes the heat current. The exponent β, determined by studying the noise spectrum of the current in the low-frequency range, is found to be 0.63 [18]. Second, the wave-vector dependence of the decay rate Γ_q of the normal modes has been examined numerically [18], and here a power law dependence of the form $q^{1.64}$ has been seen for small q. Both these values are consistent with the the value $\alpha \approx 0.4$, however the question whether the asymptotic regime is reached remains.

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The one-dimensional conductivity problem has been explored in two other classes of systems. One class is that of fluidlike systems [19–22], where particles interact with a hard sphere potential, and the other class is that of coupled rotors [23,24]. For the fluid models, the conductivity diverges, and the exponent α obtained from the largest studies is $1/3$ [21]. For the rotor models, the conductivity is found to be finite.

A good perspective on the above results is obtained by considerations introduced by Prosen and Campbell, who argued that, in systems with momentum conservation, the conductivity would diverge on general grounds [25]. Narayan and Ramaswamy [26] (NR) pointed out a flaw in their argument, by showing that Prosen and Campbell wrongly included a convective term in their definition of thermal current, which makes the current-current correlator $\langle J(t)J(0)\rangle$ assume a nonzero value in the large-time limit, and is thus responsible for the divergence of the conductivity. NR [26] made a renormalization group study of the hydrodynamic equations of heat transport in a liquid, and argued that for any momentum-conserving one-dimensional system, in which local equilibrium is established, the exponent α is $1/3$. While their result is supported by numerical studies on fluids and studies on vibrational chains in which local potentials are added to violate the momentum conservation [27], the results for FPU chains and rotors show a curious contrast. Both these systems have translational invariance and the consequent Goldstone mode, but in the vibrational system the conductivity diverges, while in case of rotors, it does not [28]. Some further progress in the hydrodynamical arguments has been made by Lee-Dadswell *et al.* [29]. Since the mode-coupling formalism couples heat transport modes to momentum transport modes, these authors have also examined the frequency-dependent longitudinal viscosity $\zeta(\omega)$. They find, using simple hydrodynamic relations, that $\zeta(\omega)$ has distinct behaviors depending on whether $\gamma=c_p/c_v$ is 1 or greater than 1. For $\gamma=1$, $\zeta(\omega)\rightarrow\zeta_0$, whereas for $\gamma\neq 1$, $\zeta(\omega)\propto\omega^{-1/2}$. This in turn leads to different forms for the frequency-dependent thermal conductivity $\kappa(\omega)$. For $\gamma=1$, $\kappa(\omega)\propto\omega^{-1/2}$, while for $\gamma\neq 1$, $\kappa(\omega)\propto\omega^{-1/3}$. The NR argument is based on the latter behavior for $\zeta(\omega)$ and does not apply to the FPU chain with quartic interactions, as $\gamma=1$ for this system. Lee-Dadswell *et al.* have numerically examined the behavior for $\kappa(\omega)$ and $\zeta(\omega)$ for quartic oscillators, and find that, in the low-frequency limit, $\zeta(\omega)$ indeed tends to a constant, but $\kappa(\omega)$ does not show a single power law, though over a large frequency range it is $\propto\omega^{-0.38}$, which is consistent with $\alpha\approx 0.4$.

More specific analytical studies in this regard are those of Lepri *et al.* [13] and Lepri [18]. They used the mode-coupling formalism to analyze the wave-vector dependence of the vibrational modes in the FPU problem and found the behavior $\Gamma_q\propto q^{5/3}$ for small q. Pereverzev [30] has tackled the FPU problem with quartic nonlinearity, by looking at the classical version of the Peierls equation, which is essentially the Boltzmann equation for phonons. He has obtained the decay rate for the energy of a mode and finds its wave-vector dependence to be $q^{5/3}$. However, there is an essential difference between the last two set of arguments. In the Boltzmann equation approach, the decay rate of a mode comes from processes involving umklapp scattering, whereas, in the mode-coupling approach, the anomalous behavior arises from a singular frequency dependence of the memory kernel, a rather generic feature of the mode-coupling approach in one dimension. Thus, though the two approaches give the same answer, the basic mechanisms leading to the answer seem different. NR [26] have pointed out an inconsistency in the mode-coupling argument, which transfers the singular frequency behavior to singular wave-vector behavior. A recent mode-coupling study specific to cubic anharmonicity [31] yields the decay rate of $q^{3/2}$.

In view of the above, we have undertaken to calculate the thermal conductivity of the chain obeying quantum dynamics directly by using the Kubo formula. We expect that a quantum calculation will give further insights into the microscopic dynamics, and the hydrodynamic behavior which seems to underlie the anomalous transport. Particularly through energy-momentum conservation in the mode-mode scattering, the calculation of transport coefficients is sensitive to dispersion of harmonic modes, in common with Pereverzev's approach [30]. In addition, the quantum treatment offers several technical advantages over classical treatment, as it allows a systematic perturbation treatment for the calculation of current-current correlators. We can go beyond the Boltzmann equation approach and develop a low-temperature expansion for the phonon decay rate, as well as include the vertex corrections for the current-current correlator, which are of crucial importance for transport coefficients. The earlier studies on vibrating chains do not calculate the conductivity directly.

II. FORMULATION

We consider here a coupled chain of atoms each of mass m, with the Hamiltonian

$$H=\sum_{l=1}^{N}\left(\frac{1}{2m}p_l^2+\frac{1}{2}m\omega_0^2(x_l-x_{l+1})^2+\frac{g}{4!}(x_l-x_{l+1})^4\right), \quad (1)$$

where x_l and p_l denote, respectively, the displacement and momentum of the atom whose equilibrium position is la along the chain. With periodic boundary conditions, the quadratic part of the Hamiltonian is diagonalized by the normal mode coordinates given by

$$Q_k=\frac{1}{\sqrt{N}}\sum_{l=1}^{N}\exp(ikl)x_l,$$

$$P_k=\frac{1}{\sqrt{N}}\sum_{l=1}^{N}\exp(ikl)p_l, \quad (2)$$

where the wave vector k is given by $k=2\pi j/N$, and j is an integer chosen so that k lies in the Brillouin zone $(-\pi,\pi)$. For quantum calculations, one works with the annihilation and creation operators a_k and $a_k^{\dagger}$, with a_k defined as

$$a_k = \sqrt{\frac{m\Omega_k}{2\hbar}}\left(Q_k + \frac{iP_k}{m\Omega_k}\right), \tag{3}$$

where Ω_k are the normal mode frequencies given by

$$\Omega_k = 2\omega_0 |\sin k/2| = \omega_0 \omega_k. \tag{4}$$

The Hamiltonian in units of $\hbar\omega_0$, can now be written as

$$H = \sum_k \omega_k\left(\frac{1}{2} + a_k^\dagger a_k\right) + \frac{\tilde{g}}{4!N}\sum_{k,q,p,s} v(k,q,p,s) A_k^\dagger A_q^\dagger A_p A_s, \tag{5}$$

where

$$A_k = a_k + a_{-k}^\dagger, \tag{6}$$

$$v(k,q,p,s) = \frac{\gamma_k^* \gamma_q^* \gamma_p \gamma_s}{\sqrt{\omega_k \omega_q \omega_p \omega_s}} \Delta(k+q-p-s) \tag{7}$$

with

$$\gamma_q = 1 - e^{-iq}. \tag{8}$$

Further, $\tilde{g}$ denotes the dimensionless coupling constant

$$\tilde{g} = \frac{g\hbar}{4m^2\omega_0^3}, \tag{9}$$

and the function $\Delta(k)$ is zero, unless the argument k is zero or a multiple of 2π. $\Delta(0)=\Delta(2n\pi)=1$, the latter corresponding to the umklapp processes.

The calculation of thermal conductivity requires evaluation of the following thermal Green's function of the heat current operator J:

$$W(\tau) = -\langle T_\tau J(\tau) J(0)\rangle, \tag{10}$$

where the angular brackets denote the thermal average, T_τ is the usual time ordering operator, and $J(\tau) = \exp(\tau H) J \exp(-\tau H)$. Here, τ lies in the range $(-\beta, \beta)$, where $\beta = \hbar\omega_0 / k_B T$ is proportional to the inverse temperature, T. The thermal conductivity κ is now given by [32]

$$\kappa = -\frac{1}{T}\lim_{\omega\to 0}\frac{\mathrm{Im}\, W(i\omega_n \to \omega + i\delta)}{\omega}, \tag{11}$$

where

$$W(i\omega_n) = \int_0^\beta W(\tau) e^{i\omega_n \tau} d\tau, \tag{12}$$

and $\omega_n = 2\pi n/\beta$ are the Matsubara frequencies.

For the above Hamiltonian, the classical expression for the current is

$$J = (am)\mathrm{Im}\sum_k v_k \Omega_k \dot{Q}_k Q_{-k} + \frac{ga}{3!N}\sum_{k,q,p,s}\gamma_k\gamma_q\gamma_p^*(1+e^{is}) \times \Delta(k+q-p-s) Q_k Q_q Q_{-p}\dot{Q}_{-s}, \tag{13}$$

where $v_k = \omega_0 \partial\omega_k / \partial k$, is the group velocity of the mode, and $\dot{Q}_k$ denotes the time derivative. Henceforth, we choose units in which $\omega_0 = a = \hbar = k_B = 1$. In most of the traditional analysis, only the first term of this operator is analyzed, as the physically significant results come from this term, while the second term provides largely higher-order quantitative corrections. Neglecting the second term, one obtains for the current

$$J = \sum_k v_k \omega_k a_k^\dagger a_k. \tag{14}$$

Thus, for calculation of conductivity, we need to evaluate the following Green's function:

$$W(\tau) = -\frac{1}{N}\sum_{k,p} j_k \langle T_\tau [a_k^\dagger(\tau) a_k(\tau) a_p^\dagger(0) a_p(0)]\rangle j_p, \tag{15}$$

where $j_p = v_p \omega_p$. In the next section, we present the necessary formalism of the diagrammatic perturbation theory to calculate W and the conductivity.

III. PERTURBATION THEORY FORMALISM FOR CONDUCTIVITY

We follow the standard perturbation treatment, but note that in one dimension a special care needs to be taken. We include in the unperturbed Hamiltonian H_0 the diagonal part of the nonlinear interaction. Denoting the number operator $a_q^\dagger a_q$ by $\hat{n}_q$, we write

$$H_0 = \sum_q \omega_q \hat{n}_q + \frac{\tilde{g}}{12N}\sum_{k,q} v(k,q,k,q)(\hat{n}_k + \hat{n}_{-k} + 1)(\hat{n}_q + \hat{n}_{-q} + 1). \tag{16}$$

The diagonal terms in the perturbation Hamiltonian need to be projected out in the perturbation series, as they cause vanishing energy denominators. In higher dimensions, this need not be done explicitly, as the associated phase space is vanishingly small; however, this is not so in one dimension, causing spurious divergences. Due to separability of the interaction term, the thermal and dynamical properties of H_0 are easily obtained. We use the Hartree-Fock approximation for unperturbed energies and occupation numbers,

$$\epsilon_q = \omega_q + \frac{\tilde{g}}{3N}\sum_k v(k,q,k,q) n_k, \tag{17}$$

$$n_q = n(\epsilon_q) = \frac{1}{\exp(\beta\epsilon_q) - 1}. \tag{18}$$

To calculate $W(\tau)$, we also need to evaluate the following propagators:

$$G(q,\tau) = -\langle T_\tau [a_q(\tau) a_q^\dagger(0)]\rangle, \tag{19}$$

$$D(q,\tau) = -\langle T_\tau [A_q(\tau) A_q^\dagger(0)]\rangle \tag{20}$$

$$= G(q,\tau) + G(-q,-\tau). \tag{21}$$

The perturbation expansion involves unperturbed versions of the above propagators, denoted as G_0 and D_0, respectively.

We now briefly summarize the standard formalism employed to calculate the transport coefficients. The set of dia-

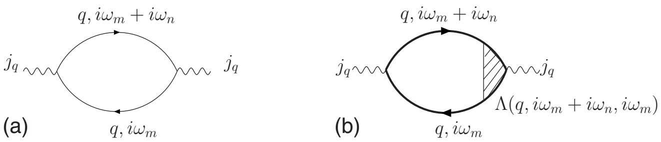

FIG. 1. (a) Zero-order diagram for $W^0(\tau)$. The lines represent factors of G_0 and wavy lines factors of current j_q. (b) Diagram for $W(i\omega_n)$. The thick lines stand for G and the shaded triangle for current vertex function Λ as defined in Eq. (23).

grams used to evaluate $W(\tau)$ or $W(i\omega_n)$ is shown in Fig. 1. Figure 1(a) shows the zero-order diagram. Its contribution is

$$W^0(i\omega_n) = -\frac{1}{N\beta}\sum_q \sum_{\omega_m} j_q^2 G_0(q,i\omega_m + i\omega_n)G_0(q,i\omega_m), \tag{22}$$

where $G_0(q,i\omega_m)$ is the frequency transform of $G(q,\tau)$, given by $(i\omega_m - \epsilon_q)^{-1}$. The higher-order terms in perturbation series (a) renormalize the propagators and (b) give rise to vertex corrections. This is shown in Fig. 1(b), in which the current vertex function $\Lambda(q,i\omega_m + i\omega_n,i\omega_m)$ is defined (see Fig. 2 also), and thicker lines represent the full propagators $G(q,i\omega_m)$. The diagrams that incorporate the self-energy corrections to each propagator independently renormalize the energies of the phonons, and more importantly give rise to finite lifetimes for these states. The decay of a one-particle state comes from all the processes that scatter the particle out of that state. The vertex corrections involve scattering processes involving both the particles together. These correspond physically to the processes in which the scattering events replenish the state [32,33]. Algebraically, one writes

$$W(i\omega_n) = -\frac{1}{N\beta}\sum_q \sum_{\omega_m} j_q G(q,i\omega_m + i\omega_n)G(q,i\omega_m) \times \Lambda(q,i\omega_m + i\omega_n,i\omega_m). \tag{23}$$

Note that, at zero order, $\Lambda(q,i\omega_m + i\omega_n,i\omega_m) = j_q$. One writes an integral equation for the current vertex function, which is

$$\Lambda(q,i\omega_m + i\omega_n,i\omega_m) = j_q - \frac{1}{N\beta}\sum_{q,\omega_l} U(q,p,q,p,i\omega_l - i\omega_m) \times G(p,i\omega_l + i\omega_n)G(p,i\omega_l) \times \Lambda(p,i\omega_l + i\omega_n,i\omega_l). \tag{24}$$

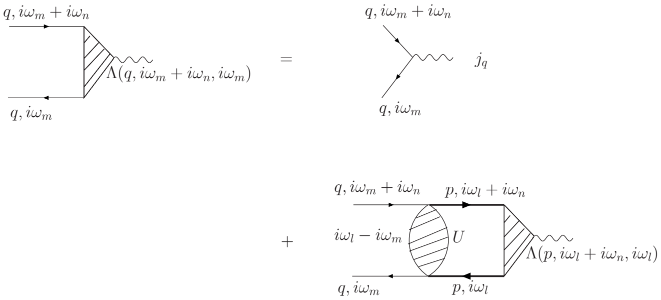

FIG. 2. Diagrammatic representation for the integral equation for the vertex function Λ as given in Eq. (24).

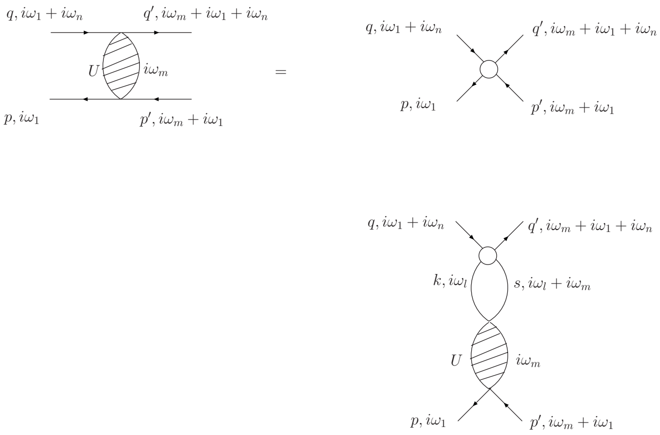

FIG. 3. Diagrammatic representation for the integral equation for the interaction vertex U obtained in a ladder approximation given in Eq. (25). The undirected lines represent factors of D_0.

The diagrammatic representation of this equation is shown in Fig. 2. The above equation involves the renormalized interaction vertex U. The renormalization of the interaction is necessary, as it is directly seen that, in the present case, the current vertex corrections become zero when U is replaced with the bare interaction v. We obtain $U(q,p',p,q';i\omega_m)$ in a ladder approximation that is shown in Fig. 3:

$$U(q,p',p,q';i\omega_m) = \tilde{g}v(q,p',p,q') - \frac{\tilde{g}}{N\beta}\sum_{k,s,\omega_l} v(q,s,k,q')D^0(k,i\omega_l) \times D^0(s,i\omega_l + i\omega_m)U(k,p',p,s;i\omega_m). \tag{25}$$

This integral equation can be solved as the interaction v is separable. Using Eq. (7), we can write

$$v(q,k,p,s) = u_2^*(q,k)u_2(p,s)\Delta(q+k-p-s), \tag{26}$$

where $u_2(q,p) = \gamma_q\gamma_p/\sqrt{\omega_q\omega_p}$. Now the following expression for U:

$$U(q,p',p,q';i\omega_m) = \tilde{U}(p-q;i\omega_m)u_2^*(q,p')u_2(p,q') \times \Delta(q+p'-p-q'), \tag{27}$$

solves the integral equation, with $\tilde{U}$ given by

$$\tilde{U}(p-q;i\omega_m) = \frac{\tilde{g}}{1+\tilde{g}K(p-q,i\omega_m)}. \tag{28}$$

Here $K(p-q,i\omega_m)$ is easily seen to be

$$K(p-q,i\omega_m) = \frac{1}{N\beta}\sum_{k,s,\omega_l} \omega_k\omega_s D_0(k,i\omega_l)D_0(s,i\omega_l + i\omega_m) \times \Delta(p+k-q-s), \tag{29}$$

where in the last equation the explicit form for the γ_p's has been used.

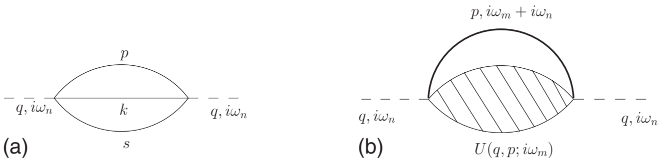

FIG. 4. (a) Diagram for self-energy Σ in the second-order perturbation theory. (b) Self-energy diagram with renormalized interaction vertex.

From Eq. (23) it is a standard exercise [32] to obtain the following expression for conductivity in terms of propagators and vertex function:

$$\kappa = \frac{1}{T}\int_{-\infty}^{\infty}\frac{d\epsilon}{2\pi}\left(-\frac{dn(\epsilon)}{d\epsilon}\right)\int\frac{dq}{2\pi}j_q\Lambda(q,\epsilon-i\delta,\epsilon+i\delta)\frac{A(q,\epsilon)}{2\Gamma(q,\epsilon)}. \tag{30}$$

The quantities $A(q,\epsilon)$ and $\Gamma(q,\epsilon)$ are related to the retarded Green's function $G(q,\epsilon)$ in the following way:

$$G(q,\epsilon) = G(q,i\omega_n \to \epsilon + i\delta) = \frac{1}{\epsilon - \epsilon_q - \Sigma(q,\epsilon + i\delta)}, \tag{31}$$

and the self-energy $\Sigma(q,\epsilon+i\delta)=\Sigma_R(q,\epsilon)-i\Gamma(q,\epsilon)$. Further,

$$A(q,\epsilon) = -2\ \mathrm{Im}\ G(q,\epsilon + i\delta) \tag{32}$$

is the spectral function. The above expression for conductivity is valid only when the decay rates $\Gamma(q,\epsilon) \ll \tilde{\epsilon}_q = \epsilon_q + \Sigma_R(q,\epsilon)$, a condition that is well satisfied for small q. Evaluation of the conductivity requires computation of the single-particle self-energy and the vertex function Λ. These calculations are presented in the next section, with some details relegated to the Appendix.

IV. EVALUATION OF CONDUCTIVITY

We begin our discussion by first considering the approximation in which vertex corrections are neglected by replacing $\Lambda(q,\epsilon-i\delta,\epsilon+i\delta)$ by j_q. Under the valid assumption that $A(q,\epsilon)$ is sharply peaked at $\tilde{\epsilon}_q$, one finds

$$\kappa = \frac{1}{T}\int\frac{dq}{2\pi}\left(-\frac{dn(\epsilon)}{d\epsilon}\right)_{\tilde{\epsilon}_q}\omega_q^2 v_q^2 \tau_q = \int\frac{dq}{2\pi}v_q^2\tau_q C_q, \tag{33}$$

where C_q denotes the mode specific heat, and $\tau_q=\Gamma^{-1}(q,\tilde{\epsilon}_q)$. With this identification, one just gets the familiar formula of kinetic theory.

The lowest-order contribution to $\Gamma(q,\omega)$ comes from the second-order self-energy diagram shown in Fig. 4(a). The schematic form for the self-energy containing all the other contributions can be drawn in terms of renormalized propagators and the renormalized interaction vertex, as shown in Fig. 4(b). We first discuss the contribution of Fig. 4(a). It turns out that it contains crucial aspects of the physics of the problem. This self-energy is

$$\Sigma(q,i\omega_n) = \frac{\tilde{g}^2}{N\beta^2}\sum_{pks}\sum_{j,m}|v(q,k,p,s)|^2 \times D_0(p,i\omega_m)D_0(k,i\omega_j)D_0(s,i\omega_n - i\omega_m - i\omega_j). \tag{34}$$

The imaginary part of this self-energy on shell is seen to be

$$\Gamma^{(2)}(q,\epsilon_q) = \tilde{g}^2\omega_q(e^{\beta\epsilon_q}-1)\frac{1}{N}\sum_{p,k,s}\omega_p\omega_k\omega_s n_p n_k(1+n_s) \times\Delta(q+s-k-p)\,\delta(\epsilon_q+\epsilon_s-\epsilon_p-\epsilon_k). \tag{35}$$

To analyze the energy-momentum conditions in the above formula, we note that the Hartree energy has the same dispersion as the linear mode, due to the nature of the interaction, i.e., $\epsilon_q=2\tilde{\omega}_0|\sin q/2|$. For the low-temperature expansion that we develop here, the temperature-dependent Hartree correction give only higher-order terms in temperature, and we can replace $\epsilon_q=\omega_q$. In one dimension, the energy-momentum conditions permit few solutions. For normal processes, only the diagonal terms for which $p=q,k=s$ or $p=s,k=q$ are allowed. But these are excluded from the perturbation Hamiltonian. This leaves contributions from only umklapp processes, for which $s=p+k-q+2\pi m$ with $m=\pm1$. The analysis of umklapp processes is long but straightforward, as many subcases need to be considered in the regions of the Brillouin zone where umklapp processes are allowed. For example, using the zone $(0-2\pi)$, $s=p+k-q+2\pi$ would hold when $p+k-q<0$, for which the energy conservation condition is

$$\sin\left(\frac{k}{2}-\frac{q-p}{4}\right) = \tan\left(\frac{q-p}{4}\right)\cos\left(\frac{q+p}{4}\right). \tag{36}$$

Working out all the contributions, we find the following result:

$$\Gamma^{(2)}(q,\epsilon_q) = \tilde{g}^2\omega_q(e^{\beta\epsilon_q}-1)\int_0^{2\pi} \times\frac{dp}{2\pi}\frac{n_p\omega_p n(\omega_1)\omega_1[n(\omega_2)+1]\omega_2}{J_a(q,p)}, \tag{37}$$

where

$$J_a(q,p) = \left(\frac{1}{4}[\cos(q/2)+\cos(p/2)]^2 + \sin(q/2)\sin(p/2)\right)^{1/2} \tag{38}$$

and

$$\omega_{1,2} = 2\sin\left(\frac{q-p}{4}\right)\left\{\left[1-\tan^2\left(\frac{q-p}{4}\right)\cos^2\left(\frac{q+p}{4}\right)\right]^{1/2} \pm\cos\left(\frac{q+p}{4}\right)\right\}. \tag{39}$$

We first note that, if we replace the Bose factors $n(\omega)$ by their high-temperature form T/ω in the above formula, it reduces exactly to the energy relaxation rate obtained by Pereverzev [30], in the classical version of the Peierls equation approach. The denominator $J_a(q,p)$ inside the integral, which comes from the Jacobian of the energy conservation δ function for umklapp processes, is identical to the one found in Pereverzev's calculation. The denominator diverges as $q \to 0$, and, to leading order in small q, the integral diverges as $q^{-1/3}$. This, as shown by Pereverzev [30], leads to the relaxation rate $\Gamma^{(2)}(q,\tilde{\epsilon}_q) \propto T^2 q^{5/3}$.

We now go beyond the second-order result and obtain a low-temperature expansion. This requires summing all diagrams with a fixed number of phonon lines carrying the Bose factor n_q, which results in a power of temperature. To the lowest order in density, this can be done by using the ladder approximation for the interaction vertex in the self-energy diagram of Fig. 4(b).

The contribution for the self-energy diagram in this approximation can be written as

$$\Sigma(q,i\omega_n) = -\frac{1}{\beta N}\sum_{p,\omega_m} D_0(p,i\omega_m + i\omega_n)U(q,p,q,p;i\omega_m). \tag{40}$$

Following Harris [35], who derived the low-temperature result for the relaxation rate of magnons, we use the spectral representation for U given by

$$U(q,p,q,p;i\omega_n) = -\int \frac{d\omega}{\pi}\frac{\mathrm{Im}\,U(q,p,q,p;\omega)}{i\omega_n - \omega}, \tag{41}$$

and perform the frequency sum. This leads to the following expression for the relaxation rate:

$$\Gamma(q,\epsilon_q) = -\frac{1}{N}\sum_p \mathrm{Im}\,U(q,p,q,p;\epsilon_p - \epsilon_q)[n(\epsilon_p) - n(\epsilon_p - \epsilon_q)] - (\epsilon_p \to -\epsilon_p). \tag{42}$$

To go further, we use the optical theorem for Im U, which follows straightforwardly from Eqs. (28) and (29), to write

$$\Gamma(q,\epsilon_q) = -\frac{1}{N}\sum_p [n(\epsilon_p) - n(\epsilon_p - \epsilon_q)]\omega_q\omega_p K_I(p-q,\epsilon_p - \epsilon_q) \times |\tilde{U}(p-q,\epsilon_p - \epsilon_q)|^2 - (\epsilon_p \to -\epsilon_p), \tag{43}$$

where

$$K_I(p,\omega) = \mathrm{Im}\,K(p,i\omega_n \to \omega + i\delta) = -\frac{n(\omega_1)\omega_1[n(\omega_2)+1]\omega_2}{n(\epsilon_q - \epsilon_p)J_a(q,p)}. \tag{44}$$

This expression for $\Gamma(q,\epsilon_q)$ differs from the second-order expression evaluated above just by the factor of $|\tilde{U}|^2$. This form is particularly useful for the low-q and low-temperature expansion ($\hbar\Omega_q \ll k_B T \ll \hbar\omega_0$). Again as argued by Harris [35], we replace the $\tilde{U}$ factors by their zero-temperature and zero-frequency values. This is because the Bose factors associated with the internal lines in $\tilde{U}$ contribute higher-order factors of temperature, and frequency-dependent terms contribute higher-order factors in momentum. From Eq. (28) we see that this requires evaluation of $K(p-q,i\omega)$ at zero temperature and zero frequency. Denoting this value by $K_0(p-q)$, we find

$$K_0(p) = \frac{2}{\pi}\{1 - \cot(p/4)\cos(p/4)\ln[\tan(\pi/4 + p/8)]\}. \tag{45}$$

We now evaluate Eq. (43) by substituting for the $\tilde{U}$ factors

$$\tilde{U}(p-q,0) = \frac{\tilde{g}}{1 + \tilde{g}K_0(p-q)}. \tag{46}$$

The factor K_0 varies between 0 and $2/\pi$ over the range of integration. We have seen, in the evaluation of the second-order term, that the most important contribution to the integral comes from the low-momentum singularity of K_I. Thus, with little error, we can replace $\tilde{U}(p-q,\tilde{\epsilon}_p - \tilde{\epsilon}_q)$ by a constant $\tilde{g}_R = \tilde{g}/(1+\tilde{g}K_0)$. In the Appendix, we have given the evaluation of this term in the low-temperature limit, and indeed find the qualitative dependence $\Gamma(q) \propto q^{5/3}T^2$. To check this result and also obtain $\Gamma(q)$ for higher values of q, we have also evaluated the integral numerically. Apart from numerical factors, this requires the evaluation of the integral given in Eq. (37). As a first step toward this evaluation, we reduce the range of integration to $0-\pi$. Then the denominator tends to zero schematically as $(qp)^{1/2} + q^2$ as $q,p \to 0$. Such singular integrals can be evaluated by the method of Gaussian quadratures with weight function proportional to $p^{-1/2}$. We found that our procedure yields convergent answers, and the result are exhibited in Fig. 5.

Finally, we turn to examine the effect of vertex corrections. First, as a general remark, we mention that the physical role of vertex corrections in the calculation of transport relaxation time is to give weight to scattering processes dependent on the scattering angle. The smaller the weight, the smaller is the scattering angle. However, in one dimension, this feature is already taken care of, as our relaxation rate contains contributions from only umklapp processes, as discussed above. Nevertheless, $\Lambda(q,\epsilon_q - i\delta,\epsilon_q + i\delta)$ can have nontrivial wave-vector dependence, which can affect the evaluation of κ in a qualitative manner. One can derive an integral equation for this quantity directly from Eq. (24). After performing the frequency sum on the right-hand side of this equation [34], one obtains

$$\Lambda(q,\epsilon_q - i\delta,\epsilon_q + i\delta) = j_q - \frac{1}{N}\sum_p \omega_q\omega_p \frac{n(\omega_p)}{\Gamma(p,\tilde{\epsilon}_p)}\,\mathrm{Im}\,\tilde{U}(p-q,\omega_p - \omega_q - i\delta) \times\Lambda(p,\epsilon_p - i\delta,\epsilon_p + i\delta). \tag{47}$$

Using the same low-temperature approximation as was used for Eq. (43), we get

$$\Lambda(q) = j_q - \frac{\tilde{g}_R^2}{N}\sum_p \omega_q\omega_p \frac{n(\omega_p)}{\Gamma(p,\tilde{\epsilon}_p)}K_I(p-q,\omega_p - \omega_q)\Lambda(p), \tag{48}$$

where $\Lambda(q)$ denotes $\Lambda(q,\epsilon_q - i\delta,\epsilon_q + i\delta)$ here. The kernel of this integral equation is not separable and singular, due to the

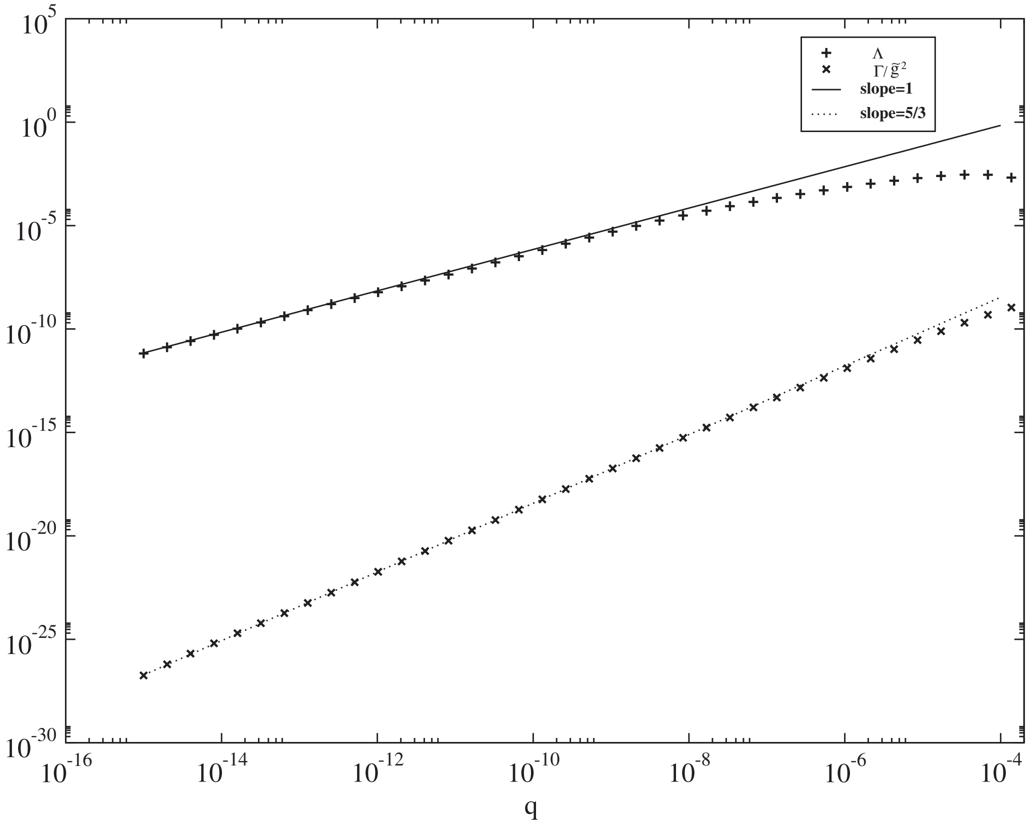

FIG. 5. Numerical solutions of $\Lambda(q)$ and $\Gamma(q)/\tilde{g}^2$ as functions of q for $T=0.1$.

presence of the factor $J_a(q,p)$ in the denominator through K_I. Note that this is the factor that also gave rise to the singular behavior of $\Gamma(q,\tilde{\epsilon}_q)$. We have solved this equation numerically. The solution is shown in Fig. 5, and is seen to be linear in q over a wide range. We have checked the convergence of the solution by raising the number of points in the Gaussian quadrature formula. This implies that the transport relaxation time also varies as $q^{-5/3}$. Then, following the arguments of Lepri *et al.*, one argues the value of α to be 0.4.

V. SUMMARY

In this paper, we have studied thermal transport in a chain of anharmonically coupled particles using quantum dynamics. We have obtained the phonon relaxation rate $\Gamma(q)$ in the low-temperature limit by including all diagrams of the lowest order in phonon density, and find that $\Gamma_q \propto q^{5/3}T^2$. Like the earlier result of Pereverezev on energy relaxation of the mode using classical Boltzmann equation, in our result the relaxation arises due to umklapp scattering and is specific to the phonon dispersion. We have used the Kubo formula to calculate the conductivity directly. We use self-energy corrections as well as vertex corrections in this evaluation, and find that the conductivity diverges with exponent $\alpha=0.4$.

This is at variance with recent numerical results on classical chains, which give $\alpha=1/3$, in agreement with the hydrodynamic arguments of Narayan and Ramaswamy [26], though the generality of these arguments has been questioned by later arguments of Lee-Dadswell *et al.* [29]. We would further like to point out that the hydrodynamic arguments use density and momentum conservation equations for particles, whereas both these equations do not apply to a phonon gas, as may be easily checked from the Boltzmann equation for phonons. Further investigations are needed to resolve these issues.

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APPENDIX

In this appendix, we give the details of the numerical and analytical evaluations of $\Gamma(q,\epsilon_q)$, followed by details of the procedure used for numerically solving the integral equation of the vertex function.

Using Eq. (43) after replacing $\tilde{U}$ by a constant as discussed in the text, one gets

$$\Gamma(q,\omega_q) = \tilde{g}_R^2 \frac{\omega_q(e^{\beta\omega_q}-1)}{\beta}\int_0^{2\pi} dp\ \omega_p n(\omega_p) \times \frac{\omega_1 n(\omega_1)\omega_2[1+n(\omega_2)]}{J_a(q,p)}. \tag{A1}$$

We first change the range of integration to 0-π to write

$$\Gamma(q,\omega_q) = \tilde{g}_R^2 \frac{\omega_q(e^{\beta\omega_q}-1)}{\beta}\int_0^{\pi} dp\ \omega_p n(\omega_p)\omega_1 n(\omega_1) \times \omega_2[1+n(\omega_2)]\frac{J_a'(q,p)+J_a(q,p)}{J_a(q,p)J_a'(q,p)}, \tag{A2}$$

where $J_a'(q,p)=J_a(q,2\pi-p)$. The denominator now reads

$$J_aJ_a' = \frac{1}{4}\{[\cos^2(q/2)+\cos^2(p/2)+4\sin(q/2)\sin(p/2)]^2 - 4\cos^2(p/2)\cos^2(q/2)\}^{1/2}. \tag{A3}$$

To perform the integration numerically, we note that the integrand assumes very large values as $p,q\rightarrow 0$, as in this domain the denominator is proportional to $(pq)^{1/2}+q^4$. To handle this singular variation, we adopt the procedure of Gaussian quadrature. The integrand is written as $F(p)/p^{1/2}$, and the the integral is obtained as the sum, $\Sigma F(p_i)H_i$, where the points p_i and weights H_i correspond to the Gaussian quadrature formula with weight function $p^{-1/2}$ [36].

To obtain the analytical behavior at small q, we note that, for small q, $\omega_1\rightarrow\omega_p$ and $\omega_2\propto\omega_q$, and the relaxation rate can be written as

$$\Gamma(q,\omega_q) = \tilde{g}_R^2 \frac{\omega_q(e^{\beta\omega_q}-1)}{\beta}\int_0^{2\pi} dp\ \omega_p^2 n_p[n_p+1] \times \frac{J_a'(q,p)+J_a(q,p)}{J_a(q,p)J_a'(q,p)}. \tag{A4}$$

Changing the integration variable to $y=\sin(p/2)$ and retaining terms to the lowest order in q, one arrives at the following expression:

$$\Gamma(q,\omega_q) = 2\tilde{g}_R^2\omega_q^2\int_0^1 \frac{dy}{\sqrt{1-y^2}} \times \frac{y^2e^{\beta y}}{(e^{\beta y}-1)^2}\frac{N(q,y)}{(y^4-2qy^3+4q^2y^2+4qy)^{1/2}}, \tag{A5}$$

where $N(q,y)=J_a'(q,p(y))+J_a(q,p(y))$. Now it is easily seen that the integral diverges as $q\rightarrow 0$. Furthermore, we note that $N(q,y)$ is a slowly varying function and can be replaced by a constant value $N(0,0)$. The divergence with respect to q can be extracted by making the substitution $y=q^{1/3}x$ and setting $q=0$ in the integrand. This leaves us with

$$\Gamma(q,\omega_q) = 2N(0,0)\tilde{g}_R^2\frac{\omega_q^2(k_BT)^2}{q^{1/3}}\int_0^{\pi q^{-1/3}}\frac{dx}{(x^4+4x)^{1/2}}. \tag{A6}$$

Since the integral has a weak dependence on q we obtain the result given in the text.

In order to solve Eq. (48) for the vertex function $\Lambda(q)$, we note that the kernel diverges due to the presence of the factor $\Gamma(p,\tilde{\epsilon}_p)$ in the denominator. This divergence can be softened by the transformation $\Lambda(p)=p\chi(p)$. The equation for $\chi(q)$ is

$$\chi(q) = \frac{j_q}{q} - \tilde{g}_R^2\frac{\omega_q}{q}\int_0^{2\pi}\frac{dp}{2\pi} \times \frac{\omega_p n_p(e^{\beta(\omega_q-\omega_p)}-1)\omega_1\omega_2 n(\omega_1)[1+n(\omega_2)]p\chi(p)}{\Gamma(p,\omega_p)J_a(q,p)}. \tag{A7}$$

The integration range is again changed to 0-π. To solve this integral equation numerically, we again use the Gaussian quadrature method [36]. Here we can solve the equation by using the weight function $p^{-1/6}$. The equation is schematically written as

$$\chi(q_i) = j(q_i)/q_i + \sum_{j=1}^{N} K_{i,j}W_j\chi(p_j), \tag{A8}$$

where $K(q,p)p^{1/6}$ denotes the kernel of the equation. The discrete values p_j and the weights W_j are again determined by the Gaussian quadrature method with weight function $w(p)=p^{-1/6}$. Now the solution is obtained by inversion of the matrix equation. Note that, with this procedure, the sum gives the correct analytical limit to the integral, which is essential to obtain the correct inversion. Finally, the solution is checked for consistency and convergence by increasing N.

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