Effect of interaction range on phonon relaxation in Fermi-Pasta-Ulam β chain

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We study the effect of increasing the range of interactions on phonon relaxation in a chain of atoms with quartic anharmonicity. The study is motivated by recent numerical studies, showing that the value of the exponent α characterizing the divergence of conductivity with system size apparently depends on the presence of second neighbor couplings. We perform a quantum calculation of the wave-vector (q) dependent relaxation rate $\Gamma(q)$ in the second order perturbation theory. The nonanalytic dependence of $\Gamma(q)$ arises due to small-q singularity of the collision integral. We find that $\Gamma(q) \propto Aq^{5/3} + Bq^2$. This gives rise to an asymptotic value $\alpha = 0.4$, but the q^2 terms lead to a higher apparent value of α at small sizes of the chain.

Anomalous behavior of thermal conductivity in one dimension has been studied quite intensively in recent years [1]. Numerical studies on vibrational chains where nearest neighbor atoms interact with cubic and quartic anharmonic potentials [Fermi-Pasta-Ulam (FPU) chains] show that conductivity κ diverges with chain size N, the number of atoms, as $\kappa \sim N^{\alpha}$[1,2]. In the early studies on chains with N of the order of a few thousand, it was found that $\alpha \approx 2/5$, whereas a recent study on a much larger ($N \sim 65\,000$) chain claims $\alpha = 1/3$ [3]. The value of $1/3$ is expected on the basis of a renormalization group study due to Narayan and Ramaswamy [4], who considered a fluid system using hydrodynamic equations. They found that for this system $\alpha = 1/3$, but argued that the result applies generally to any system in which conditions of local thermal equilibrium and momentum conservation hold. Indeed, a numerical study on a gas of hard spheres showed the divergence of κ with $\alpha = 1/3$ [5]. However, conduction in a chain of coupled rotors [6] presents a counterexample: Conductivity approaches a finite value in the large N limit as expected from the Fourier law. The hydrodynamic consideration has been extended further by Lee-Dadswell *et al.* [7], who argue for two classes of behavior for the frequency-dependent conductivity $\kappa(\omega)$. These classes are characterized by the low frequency behavior of the longitudinal viscosity $\zeta(\omega)$. For systems in which $\gamma = c_p/c_v \neq 1$, $\zeta(\omega) \sim \omega^{-1/2}$ and then $\kappa(\omega) \sim \omega^{-1/3}$ as $\omega \to 0$. This in turn leads to $\alpha = 1/3$. The other class of systems are those for which $\gamma = 1$. Here $\zeta(\omega) \to \zeta_0$ as $\omega \to 0$ and this leads to $\kappa(\omega) \sim \omega^{-1/2}$, which in turn gives $\alpha = 1/2$. According to the criteria given by Lee-Dadswell *et al.*, vibrational chain with cubic nonlinear potential belongs to the former class whereas the chain with quartic nonlinear potential belongs to the latter class. In their own simulation of the quartic case, they observed the predicted behavior for viscosity $\zeta(\omega) \to \zeta_0$, but the conductivity did not show a single power law behavior. Over a large range $\kappa(\omega) \sim \omega^{-0.38}$, which seems to become $\omega^{-1/2}$ asymptotically as $\omega \to 0$.

Numerical studies on other systems confuse the issues of universality of the behavior further. For example, conductivity on the diatomic Toda lattice [8] yields $\alpha \approx 0.4$, while a study that allows both transverse and longitudinal vibrations [9] gives different exponents in different regimes of coupling. In a recent work, we considered two variations of the FPU problem [10]. In the first variation, we extended the

couplings to the next-to-nearest neighbors (NNN) and found that for a chain of a few thousand atoms α seems to depend on the ratio η of NNN coupling to the nearest neighbor coupling; as the value of η is increased, the value of α increase from about 0.4 and seemingly saturates to a value ≈ 0.6 as η approaches unity. In the second variation, we considered a ladder of two chains with interchain couplings and two-dimensional vibrations of atoms and again found that $\alpha \approx 0.6$.

The analytic studies using classical dynamics for particles have followed two routes. One is the mode-coupling procedure in which one obtains a self-consistent equation for the correlator $G(q,t)$ of the normal mode of wave vector q [11–13]. This approach shows that $G(q,t)$ has a scaled form which depends on the nature of the nonlinear potential in the system [12,13]. For the cubic nonlinearity, $G(q,t) \propto e^{-i\omega_q t} g_3(tq^{3/2})$, whereas for the quartic nonlinearity $G(q,t) \propto e^{-i\omega_q t} g_4(tq^2)$, where ω_q denotes the renormalized frequency of vibration for the mode of wave vector q. Thus, for the cubic case, the relaxation rate $\Gamma(q)$ for the mode of wave vector q goes as $q^{3/2}$ implying $\alpha = 1/3$; whereas for the quartic case $\Gamma(q)$ goes as q^2 implying $\alpha = 1/2$. These results match with the analysis of Lee-Dadswell *et al.* [7].

The other route involves a detailed consideration of the specific modes in the system and their scattering properties to calculate relaxation times. The first such study is due to Pereverzev [14], who formulated a classical Boltzmann equation for the mode distribution function and made a study of the collision integral for quartic nonlinear interaction among the harmonic modes. The relaxation time was seen to be divergent as the wave vector q of the mode vanishes, with nonanalytic relaxation, $\Gamma(q) \propto q^{5/3}$. We have recently done a detailed study of the above model using quantum dynamics for obtaining the conductivity of the chain directly as well as the relaxation rates of the modes [16]. The results obtained for $\Gamma(q)$ agree with those of Pereverzev and show that even at low temperatures $\Gamma(q) \propto T^2 q^{5/3}$.

In this paper, motivated by the numerical result [10] for the chain with NNN coupling, which shows a change in the value of α as a function of NNN coupling strength (η), we extend our calculation for the relaxation rate to this case. The physical idea here is to examine the effect on the singularity of the collision integral due to a change in the dispersion of the modes. Our analytical result is limited to the situation where η is small.

We consider the system described by the following Hamiltonian

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

where $V(x) = (1/2)m\omega_0^2 x^2 + (g/4!)x^4$, m is the mass of the atom, and x_l and p_l are the position and the momentum of the atom, whose equilibrium position is la. The system is studied with the periodic boundary conditions. In terms of the usual creation and annihilation operators for the modes, the Hamiltonian is written as

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

where the units used are such that $\hbar = \omega_0 = a = 1$, and

$$\omega_k^2 = \tilde{\omega}_k^2 + \eta \tilde{\omega}_{2k}^2, \quad \tilde{\omega}_k = 2|\sin k/2|, \quad (3)$$

$$A_k = a_k + a_{-k}^\dagger, \quad (4)$$

$$v(k,q,p,s) = (\gamma_k^* \gamma_q^* \gamma_p \gamma_s / \sqrt{\omega_k \omega_q \omega_p \omega_s}$$
$$+ \eta \gamma_{2k}^* \gamma_{2q}^* \gamma_{2p} \gamma_{2s} / \sqrt{\omega_k \omega_q \omega_p \omega_s}) \Delta(k+q-p-s), \quad (5)$$

$$\gamma_q = 1 - e^{-iq}. \quad (6)$$

Furthermore, $\tilde{g}$ is the dimensionless coupling constant and $\Delta(q) = 1$ if q is an integer multiple of 2π; otherwise, it is zero.

The phonon Green's function is defined as

$$D(q,\tau) = -\langle T_\tau [A_q(\tau) A_{-q}(0)] \rangle, \quad D(i\omega_n) = \int_0^\beta D(\tau) e^{i\omega_n \tau} d\tau, \quad (7)$$

where $\omega_n = 2\pi n/\beta$ are the Matsubara frequencies and β the inverse of temperature measured in units of $\hbar\omega_0/k_B$. We use the standard perturbation theory formalism [15] to calculate the relaxation time, where the unperturbed Hamiltonian is taken as [16]

$$H_0 = \sum_q \omega_q \hat{n}_q + \frac{\tilde{g}}{12N} \sum_{k,q} v(k,q,k,q)(\hat{n}_k + \hat{n}_{-k} + 1)(\hat{n}_q + \hat{n}_{-q} + 1), \quad (8)$$

where $\hat{n}_q = a_q^\dagger a_q$ is the number operator. H_0 includes the harmonic term as well as the diagonal part of the anharmonic terms. The unperturbed energies and occupation numbers, within Hartree-Fock approximation, are taken as

$$\epsilon_q = \omega_q + \frac{\tilde{g}}{3N} \sum_k v(k,q,k,q)n_k, \quad (9)$$

$$n_q = n(\epsilon_q) = 1/[\exp(\beta\epsilon_q) - 1]. \quad (10)$$

The self-energy $\Sigma(q,i\omega_n)$ and the relaxation time $\tau(q,\omega) = \Gamma^{-1}(q,\omega)$ are related to the Green's function as

$$D(q,i\omega_n) = 1/[D_0^{-1}(q,i\omega_n) - \Sigma(q,i\omega_n)],$$
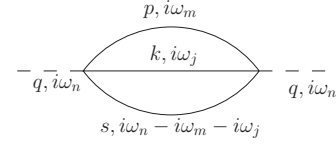

FIG. 1. Diagram for the second order contribution to the self-energy $\Sigma(q,i\omega_n)$. Solid lines represent bare phonon Green's functions D_0.

$$\Gamma(q,\omega) = -Im \lim_{\delta \to 0} \Sigma(q,i\omega_n \to \omega + i\delta), \quad (11)$$

where $D_0(q,i\omega_n) = -2\epsilon_q/(\epsilon_q^2 + \omega_n^2)$ is the unperturbed propagator. The self-energy is calculated up to second order and the contribution to $\Gamma(q,\omega)$ up to second order comes from the diagram in Fig. 1. This contribution is calculated as

$$\Sigma^{(2)}(q,i\omega_n) = \frac{\tilde{g}^2}{N^2\beta^2} \sum_{pks} \sum_{j,m} |v(q,k,p,s)|^2 D_0(p,i\omega_m) D_0(k,i\omega_j)$$
$$\times D_0(s,i\omega_n - i\omega_m - i\omega_j). \quad (12)$$

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

$$\Gamma^{(2)}(q,\epsilon_q) = \tilde{g}^2 \tilde{\omega}_q (e^{\beta\epsilon_q} - 1) \frac{2\pi}{N^2} \sum_{p,k,s} V(q,p,k,s) \tilde{\omega}_p \tilde{\omega}_k \tilde{\omega}_s n(\epsilon_p)$$
$$\times n(\epsilon_k)[1 + n(\epsilon_s)] \Delta(q+s-k-p) \delta(\epsilon_q + \epsilon_s - \epsilon_p - \epsilon_k), \quad (13)$$

where we have written

$$|v(q,k,p,s)|^2 = \tilde{\omega}_q \tilde{\omega}_p \tilde{\omega}_k \tilde{\omega}_s V(\tilde{\omega}_q, \tilde{\omega}_p, \tilde{\omega}_k, \tilde{\omega}_s),$$

$$V(\tilde{\omega}_q, \tilde{\omega}_p, \tilde{\omega}_k, \tilde{\omega}_s)$$
$$= \frac{1 + \eta(1+\eta)(4 - \tilde{\omega}_q^2)(4 - \tilde{\omega}_p^2)(4 - \tilde{\omega}_k^2)(4 - \tilde{\omega}_s^2)}{b(\tilde{\omega}_q)b(\tilde{\omega}_p)b(\tilde{\omega}_k)b(\tilde{\omega}_s)}, \quad (14)$$

where $b(\tilde{\omega}_q) = \{1 + \eta(4 - \tilde{\omega}_q^2)\}^{1/2}$.

For the evaluation of Eq. (13) we work within the Brillouin zone $(0, 2\pi)$. The calculation requires finding the roots of the argument of the δ function making use of the Δ function. These two represent the energy and momentum conservation in phonon collisions. For a general value of η, it is not possible to find an analytic solution. But for small η, we can obtain the solution to linear order in η. We first make the approximation on ω_q, as

$$\omega_q = \tilde{\omega}_q[1 + 2\eta \cos^2(q/2)]. \quad (15)$$

When η is small, ϵ_q is proportional to ω_q at high temperature. This proportionality factor which scales Γ_q is absorbed into $\tilde{g}$. So the energy conservation can be satisfied as $\omega_q + \omega_s = \omega_p + \omega_k$. The momentum conservation within this Brillouin zone requires $s = p + k - q + 2m\pi$ with $m = 0, \pm 1$. For $m = 0$, the normal processes, energy conservation leads to $s = k, p = q$ or $s = p, q = k$ which are diagonal terms that were taken out to be included in the unperturbed Hamiltonian. So the contribution from the normal processes is zero. For $m = \pm 1$, the Umklapp processes, energy conservation becomes

$$\sin(q/2) - \sin(p/2) - \sin(k/2) - \sin[(p + k - q)/2]$$
$$= 2\eta\{\cos^2(p/2)\sin(p/2) + \cos^2(k/2)\sin(k/2) - \cos^2[(p + k - q)/2]\sin[(p + k - q)/2]\}. \tag{16}$$

The zero order solution obtained by putting $\eta=0$ is $\sin[k_0/2-(q-p)/4]=\cos[(q+p)/4]\tan[(q-p)/4]$. To first or-

der in η solutions for k are obtained by putting $k=k_0$ in the right-hand side (RHS) of Eq. (16) and is

$$\sin[k/2 - (q - p)/4] = \cos[(q + p)/4]\tan[(q - p)/4]\zeta(q,p),$$

$$\zeta(q,p) = 1 - 6\eta \sin\left(\frac{q}{2}\right)\sin\left(\frac{p}{2}\right)\left[1 - \tan^2\left(\frac{q - p}{4}\right)\right]. \tag{17}$$

Substituting this solution in Eq. (13), one obtains

$$\Gamma^{(2)}(q,\epsilon_q) = \tilde{g}^2\tilde{\omega}_q(e^{\beta\epsilon_q} - 1)\int_0^{2\pi}\frac{dp}{2\pi}V(\tilde{\omega}_q,\tilde{\omega}_p,\tilde{\omega}_1,\tilde{\omega}_2)\frac{n(\omega_p)\tilde{\omega}_p n(\omega_1)\tilde{\omega}_1[n(\omega_2) + 1]\tilde{\omega}_2}{J(q,p)}, \tag{18}$$

where $\tilde{\omega}_{1,2}=2\sin[(q-p)/4](\{1-\tan^2[(q-p)/4]\cos^2[(q+p)/4]\zeta^2(q,p)\}^{1/2}\pm\cos[(q+p)/4]\zeta(q,p))$, with $\omega_{1,2}=\tilde{\omega}_{1,2}b(\tilde{\omega}_{1,2})$. $J(q,p)$ is the Jacobian of the argument of the δ function, and is given by

$$J(q,p) = [\tfrac{1}{4}\{\cos(q/2) + \cos(p/2)\}^2 + \sin(q/2)\sin(p/2) + \eta S_1(q,p) + \eta^2 S_2(q,p)]^{1/2}[2 + \eta S_3(q,p)],$$

$$S_1(q,p) = 12 \sin^2[(q - p)/4]\cos^2[(q + p)/4]\sin(q/2)\sin(p/2)\{1 - \tan^2[(q - p)/4]\},$$

$$S_2(q,p) = -36 \sin^2[(q - p)/4]\cos^2[(q + p)/4]\sin^2(q/2)\sin^2(p/2)\{1 - \tan^2[(q - p)/4]\}^2,$$

$$S_3(q,p) = 1 + 3\{1 - 4\sin^2[(q - p)/4]\}\{1 - 4\tan^2[(q - p)/4]\cos^2[(q + p)/4]\zeta^2(q,p)\}.$$

The expression under the square root is non-negative for small η. Consistent with the approximation of Eq. (15), we keep only the leading order term of η in J. Then, in the high temperature limit, the q dependence of Γ is given by $\Gamma(q,\epsilon_q) \propto \tilde{\omega}_q(e^{\beta\epsilon_q} - 1)I(q)$, where

$$I(q) = \int_0^{2\pi}\frac{dp}{[\tfrac{1}{4}\{\cos(q/2) + \cos(p/2)\}^2 + \sin(q/2)\sin(p/2) + \eta S_1(q,p)]^{1/2}}. \tag{19}$$

Note that the integral diverges at $q=0$. To study this divergence [14], it is convenient to make the substitution $x=\tan(p/2)$ in Eq. (19). Thus

$$I(q) = \int_0^\infty dx\frac{\sqrt{1 + x^2}[\cos(q/4) + x \sin(q/4)]}{\sqrt{P(q,x)}}, \tag{20}$$

where

$$P(q,x) = \{[1 - \cos(q/2)]^2 x^4 + 8 \sin(q/2)x^3 - 2 \sin^2(q/2)x^2 + 8 \sin(q/2)x + [1 + \cos(q/2)]^2\}[x^2\sin^2(q/4) + 2x \sin(q/2) + \cos^2(q/4)]$$
$$\times [1 + x^2] + 24\eta x \sin(q/2)\{x^4\sin^2(q/2) - 4x^3\sin(q/2) + [4 + 2 \sin^2(q/2)]x^2 - 4x \sin(q/2) + \sin^2(q/2)\}[-x^2\cos(q/2)$$
$$+ 2x \sin(q/2) + \cos(q/2)]. \tag{21}$$

To derive the nature of divergence at small q, we need to retain only terms with the lowest power of q in the coefficients of each power of x. Thus, for small q,

$$I(q) \propto \int_0^\infty \frac{\sqrt{1 + x^2}[1 + (q/4)x + \text{higher order terms in } q]}{\sqrt{P_0(q,x)}}$$

$$= I_1(q) + qI_2(q), \tag{22}$$

where

$$P_0(q,x) = (q^6/1024)x^8 + (\tfrac{1}{4} - 3\eta)q^3 x^7 + (2 + 24\eta)q^2 x^6$$
$$+ (4 - 48\eta)qx^5 + (\tfrac{15}{4} + 48\eta)q^2 x^4 + (10 + 48\eta)qx^3$$
$$+ 4x^2 + 6qx + 4. \tag{23}$$

It is easily seen that both $I_1(q)$ and $I_2(q)$ diverge as $q\to 0$.

The divergence of $I_1(q)$ can be extracted by using the transformation $y=xq^{1/3}$ [14]. Then

$$I_1(q) \propto \frac{1}{q^{1/3}}\int_0^\infty dy\frac{\sqrt{q^{2/3} + y^2}}{\sqrt{\tilde{P}_0(q,y)}},$$

$$\tilde{P}_0(q,y) = (q^4/1024)y^8 + (\tfrac{1}{4} - 3\eta)q^{4/3}y^7 + (2 + 24\eta)q^{2/3}y^6$$
$$+ (4 - 48\eta)y^5 + (\tfrac{15}{4} + 48\eta)q^{4/3}y^4 + (10$$
$$+ 48\eta)q^{2/3}y^3 + 4y^2 + 6q^{4/3}y + 4q^{2/3}. \tag{24}$$

Now setting $q=0$ inside the integral,

$$I_1(q) \propto \frac{1}{q^{1/3}}\int_0^\infty dy\frac{y}{\sqrt{(4 - 48\eta)y^5 + 4y^2}} \tag{25}$$

and the integrand on the RHS is finite for $\eta<1/12$. Note that this divergence is the same as for the nearest neighbor case,
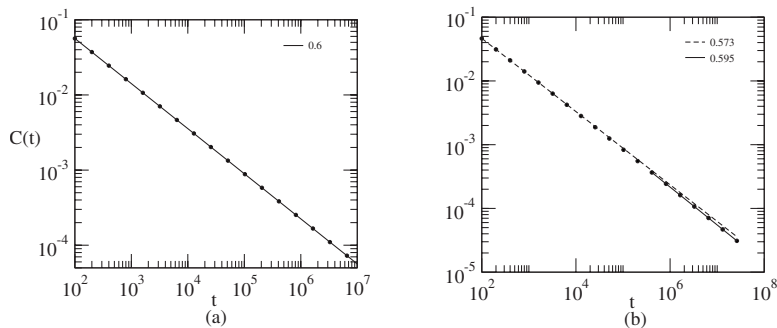
FIG. 2. Behavior of $C(t)$. (a) For $B/A = 0$, $C(t)$ decreases as $t^{-0.6}$. (b) For $B/A = 1$, at smaller times $C(t) \sim t^{-0.573}$ and at large values of t, $C(t) \sim t^{-0.595}$.

even though the Jacobians involved are different. This leads to rather different forms for the polynomials $P_0(q, x)$; for the $\eta \neq 0$ case, it is of four orders higher, but its q dependence and the numerator lead to the same exponent.

For $I_2(q)$, the divergence can be obtained using the transformation $y = xq$. Setting $q = 0$ inside the integrand in a similar way, one finds

$$I_2(q) \propto \frac{1}{q} \int_0^\infty dy \frac{1}{\sqrt{(\frac{1}{4} - 3\eta)y^3 + (2 + 24\eta)y^2 + (4 - 48\eta)y}}. \tag{26}$$

The integral is again finite. Thus, as $q \to 0$, the relaxation rate behaves as

$$\Gamma^{(2)}(q) = Aq^{5/3} + Bq^2. \tag{27}$$

In a strict power-law behavior one would expect $\Gamma(q)$ to be proportional to $q^{5/3}$ multiplied by an analytic function. The fact that it is different here suggests different relaxation behavior in different regimes of time. To understand the effect on the divergence of conductivity qualitatively, we take $\Gamma^{(2)}(q)$ to be the transport relaxation rate τ_q^{-1} in the following formula for conductivity [17]:

$$\kappa = \int \frac{dq}{2\pi} v_q^2 \tau_q C_q = \int \frac{dq}{2\pi} v_q^2 C_q \int_0^\infty dt \exp(-t/\tau_q), \tag{28}$$

where C_q is the mode specific heat and v_q is the group velocity of the mode with wave number q. Following the previous works [2,14], the N dependence of conductivity is obtained by limiting the time integral to N/v_0, the time taken by the mode with the largest relaxation time to traverse the chain. Since the integral is dominated by the $q \to 0$ modes, we may use constant values for specific heat and group velocity in the integral. This leads to

$$\kappa \propto \int_0^{NA/v_0} dt \, C(t),$$

$$C(t) = \int_0^{2\pi} dq \exp\{-t[q^{5/3} + (B/A)q^2]\}. \tag{29}$$

The behavior of $C(t)$ is obtained numerically and is shown in Fig. 2. For $B/A = 1$, one notices that initially $C(t)$ decreases with an exponent ≈ 0.573. Only at very large times does the exponent become 0.6, the value obtained for $B = 0$. So for finite chains, as the integral for conductivity is limited by NA/v_0, the effective exponent α may depend on the value of B/A. It is also noted that, for not so large times, the exponent is ≈ 0.57 close to the asymptotic value of 0.6. So in the $\eta \to 0$ limit that we are working, we expect α to be close to 0.4, even for finite chains. In the numerical results [10], one finds that for $\eta \ll 1$, α is close to 0.4. The calculation here suggests that for small values of η the asymptotic value of α is 0.4, but there are crossover effects which are important at small sizes of chain. At larger values of η, whether there is a true change in the asymptotic value of α or the numerical results reflect stronger size-dependent crossover effect is not established by our calculation due to its limitation to small values of η.

[1] S. Lepri *et al.*, Phys. Rep. **1**, 377 (2003).
[2] S. Lepri *et al.*, Phys. Rev. Lett. **78**, 1896 (1997).
[3] T. Mai *et al.*, Phys. Rev. Lett. **98**, 184301 (2007).
[4] O. Narayan and S. Ramaswamy, Phys. Rev. Lett. **89**, 200601 (2002).
[5] P. Grassberger *et al.*, Phys. Rev. Lett. **89**, 180601 (2002).
[6] C. Giardina *et al.*, Phys. Rev. Lett. **84**, 2144 (2000).
[7] G. R. Lee-Dadswell *et al.*, Phys. Rev. E **72**, 031202 (2005).
[8] T. Hatano, Phys. Rev. E **59**, R1 (1998).
[9] J. Wang and B. Li, Phys. Rev. Lett. **92**, 074302 (2004).
[10] Santhosh G. *et al.*, J. Stat. Mech.: Theory Exp. 2005, P07005 (2005).
[11] S. Lepri, Phys. Rev. E **58**, 7165 (1998).

[12] L. Delfini *et al.*, Phys. Rev. E **73**, 060201(R)(2006).
[13] L. Delfini *et al.*, J. Stat. Mech.: Theory Exp. 2007, P02007 (2007).
[14] A. Pereverzev, Phys. Rev. E **68**, 056124 (2003).
[15] See, for example, G. D. Mahan, *Many Particle Physics* (Kluwer Academic/Plenum, New York, 2000).
[16] Santhosh G. and D. Kumar (unpublished).
[17] To calculate the transport relaxation rate one needs to evaluate the vertex corrections. For the nearest-neighbor couplings we have reported such a calculation in [16]. There we find that the q dependence of the relaxation rate is the same as found in the second order perturbation theory. A similar calculation here is very tedious and has not been performed.