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Memory effects and heat transport in one-dimensional insulators

S. Lepri[a]

Dipartimento di Energetica "S. Stecco", Via Santa Marta 3, 50139 Firenze, Italy
and
Istituto Nazionale di Fisica della Materia, Unità di Firenze, L.go E. Fermi 2, 50125 Firenze, Italy

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Abstract. We study the dynamical correlation functions and heat conduction for the simplest model of quasi one-dimensional (1d) dielectric crystal *i.e.* a chain of classical particles coupled by quadratic and cubic intersite potential. Even in the weakly nonlinear regime, numerical simulation on long enough chains reveal sizeable deviations from the perturbative results in the form of a slower decay of correlations in equilibrium. Their origin can be traced back to the subtle nonlinear effects described by mode-coupling theories. Measures of thermal conductivity with nonequilibrium molecular-dynamics method confirm the relevance of such effects for low-dimensional lattices even at very low temperatures.

PACS. 63.10.+a General theory – 05.60.-k Transport processes – 44.10.+i Heat conduction

1 Introduction

The theoretical study of physical models in one spatial dimension is often justified by their mathematical simplicity [1]. Besides this, they display intriguing peculiarities that render them qualitatively different from their three-dimensional counterparts. Actually, a further and even more relevant motivation is the possibility of modern experimental techniques to produce a variety of real systems that could, at least in principle, be effectively described by 1d models. Furthermore, the latter are of great importance to approach the dynamical and statistical properties of biological molecules like DNA [2] or proteins [3].

In the present paper we wish to study the problem of relaxation and heat transport in a classical chain of oscillators with quadratic and cubic intersite potential. Although this is a truly textbook model of an insulating crystal, there is no, to the best of our knowledge, systematic analysis of the effects of anharmonicity. The results may be of interest to describe experimental systems like *e.g.* strongly anisotropic crystals [4,5], polymers [6] or nanowires [7]. Some theoretical investigations of thermal conductance for a quantum wire in ballistic [8] and anharmonic [9] regimes have been also recently presented.

The first issue that we address is the following: which difference should one observe in this case with respect to the usual 3d systems? One may argue that the cubic nonlinearity ("three phonon" scattering) must be less efficient due to the stronger constraints to be fulfilled in 1d, an argument that has been even invoked to explain several experimental results [4,5]. A signature of this fact on the dynamical correlations is thus to be expected. To substantiate this argument, we studied the model within the framework of the memory-function formalism [10]. A perturbative calculation shows that correlation functions display a power-law tail (Sect. 2), that we study in some detail in the long-wavelength limit and compare, to some extent, with molecular dynamics simulations. The latter show that, even for relatively small anharmonicity, strong non-perturbative effects due to subtle nonlinear interaction arise for long enough chains. These can be quantitatively accounted for by mode-coupling theories [11] akin to the ones usually applied for dense fluids [12].

The consequences of such a behaviour on nonequilibrium energy transport is discussed in Section 3. Even in absence of such strong memory effects, the thermal conductivity has been shown to diverge with the system size both for 1d [13,14] and 2d lattices [15]. The characteristic divergence law, a signature of the mentioned mode-coupling effects [14], is recovered also in the present case. This signals again the overwhelming role of nonlinearity and fluctuations in low spatial dimensions.

[a] e-mail: lepri@avanzi.de.unifi.it

2 Correlation functions for an anharmonic chain

We consider a set of atoms of mass m arranged on a ring of N sites with spacing a. Let u_l be the displacement of the lth particle from its equilibrium position la. The Lagrangian reads as

$$\mathcal{L} = \sum_{l=1}^{N} \left[\frac{m}{2}\dot{u}_l^2 - \frac{m\omega_0^2}{2}\left(u_{l+1}-u_l\right)^2 - \frac{g}{3}\left(u_{l+1}-u_l\right)^3 \right]; \quad (1)$$

where g is the coupling constant. This is the lowest-order approximation of a generic anharmonic potential which couples nearest neighbours. For historical reasons, it is sometimes referred to as the Fermi-Pasta-Ulam α-model (FPU-α). For convenience, from now on we will always work in dimensionless units, where a, m and the angular frequency ω_0 are set to unity. This implies, for instance, that the sound speed $a\omega_0$ is also unity and that the energy and coupling constant (that we still denote with g) are measured respectively in units of $m\omega_0 a^2$ and $m\omega_0 a^{-1}$.

A difficulty of model (1) is the unboundedness of the potential. Therefore, in order to avoid runaway instability of trajectories (which could anyhow be overcome by adding even terms of higher order) we will deal with sufficiently small coupling constant and/or energies.

Upon introducing the complex amplitudes U_k through the discrete Fourier transform

$$U_k = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} u_l \, \mathrm{e}^{\mathrm{i}\frac{2\pi k}{N} l}, \quad (2)$$

where k is an integer ranging between $-\frac{N}{2}+1$ and $\frac{N}{2}$ we can thus rewrite the equations of motion as

$$\ddot{U}_k + \omega_k^2 U_k \;=\; -g\omega_k \frac{1}{\sqrt{N}} \sum_{k_1+k_2=k} \omega_{k_1}\omega_{k_2} U_{k_1} U_{k_2} \;\equiv\; \mathcal{F}_k \quad (3)$$

with $\mathcal{F}_k$ being the interaction force among modes. The condition on the indices of the sum is intended to be modulo N while

$$\omega_k \;=\; 2\left|\sin\left(\frac{\pi k}{N}\right)\right|. \quad (4)$$

is the usual harmonic (phononic) dispersion law.

2.1 Memory effects

Let us consider the normalized correlation function

$$\mathcal{G}_k(t) \;=\; \beta\omega_k^2 \left\langle U_k(t) U_k^*(0)\right\rangle, \quad (5)$$

which is defined in such a way that $\mathcal{G}_k(0) = 1$ (β is the inverse temperature). In the framework of the Mori-Zwanzig projection approach, it can be shown that it satisfies the equation of motion [10]

$$\ddot{\mathcal{G}}_k + \int_0^t \Gamma_k(t-s)\,\dot{\mathcal{G}}_k(s)\mathrm{d}s + \omega_k^2 \mathcal{G}_k \;=\; 0. \quad (6)$$

The memory function Γ_k accounts for memory effects and can be connected to the nonlinear force by the fluctuation-dissipation relation

$$\Gamma_k(t) \;=\; \beta\langle \mathcal{F}_k(t)\mathcal{F}_k^*(0)\rangle. \quad (7)$$

Notice that here it is also implicitly assumed that slow terms possibly contained in $\mathcal{F}_k$ are negligible in the thermodynamic limit [11].

In the following we will evaluate the memory function to the lowest order of perturbation theory. This amounts to evaluating the average in (7) on the measure of the unperturbed system ($g = 0$). A straightforward calculation yields

$$\Gamma_k(t) \;\approx\; \frac{Cg^2\omega_k^2}{\beta}\frac{1}{N}\sum_{k_1+k_2=k} \cos\omega_{k_1} t \, \cos\omega_{k_2} t \quad (8)$$

where C is a suitable numerical constant. Rather remarkably, the Laplace transform of Γ_k can be evaluated exactly in the large N limit (see the Appendix for some details of the calculation). Indeed, if we let $2\pi k/N \to q$ and define

$$\Gamma(q,z) \;=\; \int_0^\infty \Gamma(q,t)\mathrm{e}^{-\mathrm{i}zt}\,\mathrm{d}t \quad (9)$$

we obtain the simple result

$$\Gamma(q,z) = K\omega^2(q)\left[\frac{1}{\sqrt{\Omega_+^2(q)-z^2}} + \frac{1}{\sqrt{\Omega_-^2(q)-z^2}}\right], \quad (10)$$

where we have introduced the new (small) coupling parameter $K = Cg^2/2\beta$ and

$$\Omega_+(q) = 4\cos\frac{q}{4} \quad , \quad \Omega_-(q) = 4|\sin\frac{q}{4}|. \quad (11)$$

Inversion of the Laplace transform yields [16]

$$\Gamma(q,t) \;=\; K\omega^2(q)\,\left[J_0(\Omega_+(q)t) + J_0(\Omega_-(q)t)\right], \quad (12)$$

where J_0 is the Bessel function. With this result at hand, we can give a closed expression for $\mathcal{G}$ by solving equation (6) with the Laplace transform method that yields the formal solution (with $\dot{\mathcal{G}}(q,t=0)=0$)

$$\mathcal{G}(q,z) \;=\; \frac{\mathrm{i}z + \Gamma(q,z)}{z^2 - \omega^2(q) - \mathrm{i}z\Gamma(q,z)}\,. \quad (13)$$

If, like in the present case, the dissipative effects are weak, the latter expression can be approximated as

$$\mathcal{G}(q,z) \;=\; \frac{-\mathrm{i}/2}{z-\omega(q)-\mathrm{i}\Gamma(q,z)/2} + \frac{-\mathrm{i}/2}{z+\omega(q)-\mathrm{i}\Gamma(q,z)/2} \quad (14)$$

and the correlation function are determined for every q by the standard methods of inverse Laplace transformation *i.e.* by determining the singularities in the complex plane of $\mathcal{G}$.

2.2 Long wavelengths

Let us focus on the effective dynamics of the long-wavelength modes. The latter are the slowest ones and are directly responsible of energy transport and therefore of main interest here. For $q \to 0$ one has from equation (11) $\Omega_+ \approx 4$ and $\omega \approx \Omega_- \approx |q|$. This implies that the first term of the memory function decays on a much faster time scale and can be neglected so that

$$\Gamma(q,z) \;\approx\; \frac{Kq^2}{\sqrt{q^2-z^2}}\,. \tag{15}$$

Therefore, in this limit, the transform of the mode autocorrelation satisfies the scaling relation

$$\mathcal{G}(q,z) \;=\; \frac{1}{|q|}G\left(\frac{z}{|q|}\right), \tag{16}$$

where, from equation (14)

$$G(w)=\frac{-\mathrm{i}/2}{w-1-\mathrm{i}K/2\sqrt{1-w^2}}+\frac{-\mathrm{i}/2}{w+1-\mathrm{i}K/2\sqrt{1-w^2}}\,. \tag{17}$$

From equations (16) and (15) it follows immediately that $\mathcal{G}(q,t)$ depends only on the product $|q|t$.

To estimate the behaviour of $\mathcal{G}(q,t)$ in a more detailed way one has to study the properties of the function $G(w)$. Besides of the branch cut in $z=\pm 1$, the latter has two simple poles in the upper part of the complex plane that, for small K, are approximatively given by $\pm 1 + \mathrm{i}\frac{\sqrt{3}}{4}K^{2/3}$ (we neglect the term $\mathcal{O}(K^{2/3})$ in the real part since this gives only a small correction to the unperturbed frequency). Accordingly, the inversion of the Laplace transform (17) yields two contributions to the decay, the exponential plus some power-law tails. More precisely, the calculation yields

$$\mathcal{G}(q,t) \;\propto\; \exp(-\gamma(q)|t|)\,\cos qt \;-\; Kf(K,|q|t) \tag{18}$$

where we have introduced the (short times) relaxation rate

$$\gamma(q) \;=\; \frac{\sqrt{3}}{4}K^{2/3}\,|q|. \tag{19}$$

Notice how the square-root in (17) affects the functional dependence of the relaxation time on the coupling constant and therefore on temperature. The behaviour of the slowly decaying correction

$$f(K,\tau)=\frac{1}{2\pi}\int_{-1}^{+1}\mathrm{d}w\frac{\sqrt{1-w^2}}{(1-w^2)(w+1)^2+K^2/4}\,\cos w\tau. \tag{20}$$

has been evaluated numerically finding that, as expected, the latter oscillates with a period close to 2π while its envelope decays for large τ as $K^{-2}\tau^{-3/2}$.

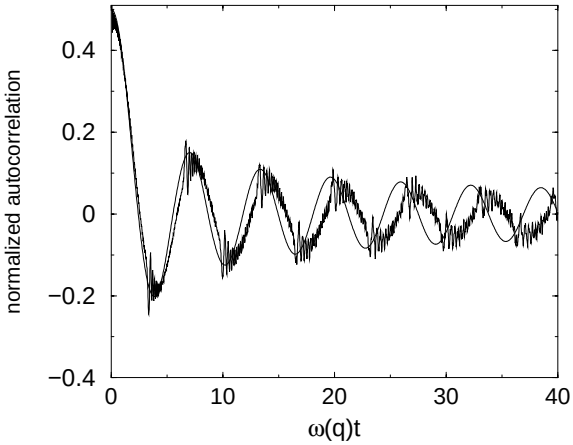

Fig. 1. The normalized autocorrelation function of the nonlinear force $\mathcal{F}_k$ for $\beta = 10^4$, $g = 1.0$, $N = 128$, $k = 1$ (corresponding to $q = 0.0490$). The thick solid line is the (approximate) perturbative result $J_0/2$ (see Eq. (12)).

2.3 Comparison with the numerical simulations

In the present section we compare the results of the perturbative calculation with the outcomes of molecular dynamics simulations. The latter were performed at equilibrium and in the microcanonical ensemble by integrating the equations of motion with a third order symplectic algorithm [17] and starting from random initial conditions. We then let the system evolve for a certain transient time in order to start the measures from a generic phase-space point. The energy per particle has been fixed in every computation and the corresponding temperature has been measured as twice the average kinetic energy density. In computing spectra and correlations functions a Fast Fourier Transform routine has been used, and the data are usually averaged over an ensemble of several trajectories (typically between 20 and 200) to reduce statistical fluctuations.

As a first check we compared the perturbative expression of the memory function (12) with the correlation of the nonlinear force appearing in equation (7) (see Fig. 1). The two agree well on short times, but some deviation is observed after a few oscillation periods. Furthermore, the temperature and wavenumber dependence of the relaxation rates has been checked by measuring the initial decay rate of the envelope of $\mathcal{G}(q,t)$. As seen in Figures 2 and 3, a reasonable agreement with the result of perturbation theory is obtained for $q > 0.006$ (corresponding to $N < 10^3$). However, for smaller wavenumbers (longer chains) the data crossover to a different behaviour that is consistent with the law $q^{5/3}$. The latter is the result expected from mode-coupling theory and has been numerically observed for the model with quartic nonlinearity at much larger temperatures [11].

We can therefore conclude that, despite the smallness of the perturbative parameter ($K \sim 0.01$), the dynamical effects of nonlinear mode interaction take over on longer

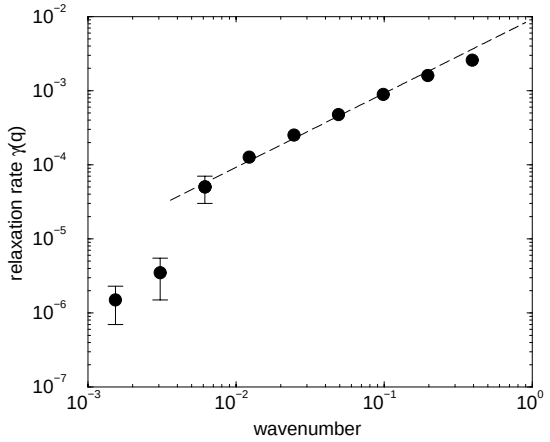

Fig. 2. Scaling of the relaxation rates with the wavenumber q for $g = 0.25$ and $\beta = 10.0$. The straight line is the result of perturbation theory.

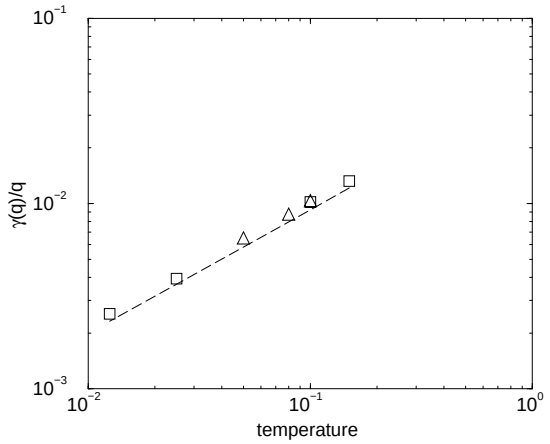

Fig. 3. Scaling of the relaxation rates with temperature for the first Fourier mode of a chain of length $N = 256$ (triangles) and $N = 512$ (squares). The straight line is the result of perturbation theory.

("hydrodynamic") time/length scales. Eventually, this originates substantial deviations from the results obtained in the previous section.

3 Thermal conduction

In the present section we will study the consequences on the phenomenon of stationary heat transport along the chain. Let us discuss the case of linear response *i.e.* small thermal gradients. We first evaluate the asymptotic decay of the Green-Kubo integrand in the framework of the perturbative calculation described above and compare the results with numerical simulations.

3.1 The Green-Kubo formula

If we neglect the anharmonic term (which contributes to the conductivity only to order g^2), the heat current J is approximated by its harmonic part [14]

$$J \approx J_H = \frac{\mathrm{i}}{2N} \sum_{k=-N/2+1}^{N/2} v_k \omega_k \left(U_k \dot{U}_k^* - U_k^* \dot{U}_k \right) \quad (21)$$

where $v_k = \omega_k'$ is the phase velocity. It is convenient to recast the above expression in the new variables $A_k = \mathrm{e}^{\mathrm{i}\omega_k t} U_k$. Taking into account the fact that $\sum_k v_k \omega_k |A_k|^2 = 0$ for symmetry reasons ($v_k = -v_{-k}$), one finds

$$J_H = \frac{\mathrm{i}}{2N} \sum_k v_k \omega_k \left(A_k \dot{A}_k^* - A_k^* \dot{A}_k \right). \quad (22)$$

The integrand appearing in the Green-Kubo formula for thermal conductivity

$$\kappa = k_\mathrm{B} \beta^2 N \int_0^\infty \langle J(t) J(0) \rangle \mathrm{d}t \quad (23)$$

contains correlation functions of quantities that are quadratic in A_k. As the latter quantities are slowly varying ($\dot{A}_k \ll \omega_k A_k$) we get the approximate expression

$$N \langle J(t) J(0) \rangle \approx \frac{1}{4\beta N} \sum_k v_k^2 \langle \dot{A}_k(t) \dot{A}_k^*(0) \rangle + \text{c.c.} \quad (24)$$

where we have also taken into account the equipartition of energy $\langle \omega_k^2 |A_k|^2 \rangle = 1/\beta$.

Let us assume that the large t behaviour of (24) is dominated by long-wavelength modes. On the basis of the above discussion one expects that in this limit the autocorrelation of $\dot{A}(q,t)$ will depend only on $|q|t$, *i.e.*

$$\langle \dot{A}(q,t) \dot{A}^*(q,0) \rangle = \frac{1}{\beta} \mathcal{A}(|q|t), \quad (25)$$

where $\mathcal{A}$ is a suitable function. Replacing the sum in (24) with an integral and taking into account the fact that $v(q) \to 1$ for $q \to 0$ one gets

$$N \langle J(t) J(0) \rangle \propto \frac{1}{t\beta^2} \int_0^{+\infty} \mathcal{A}(x) \mathrm{d}x. \quad (26)$$

Since that the integral in this formula is convergent because of the asymptotic behaviour of (20), we can conclude that the Green-Kubo integrand decays as $1/t$ for large t and that the thermal conductivity is infinite.

To estimate the divergence law for a finite chain, one can cut off the integral in the formula (23) up to some time proportional to the length N [14]. As a result, κ should diverge logarithmically with the system size. In the next subsection we will compare this prediction with numerical results.

3.2 Nonequilibrium simulations and finite-size conductivity

A simple and efficient way to compute transport coefficients is to use nonequilibrium molecular dynamics.

First of all we consider the chain with fixed ends ($u_0 = u_{N+1} = 0$) and let the first and the Nth oscillators interact with two reservoirs operating at different temperatures $T_{\rm R} = T + \Delta T/2$ and $T_{\rm L} = T - \Delta T/2$, respectively. In such a way a net heat current flows through the lattice. The thermal conductivity for the finite chain can thus be measured as the ratio between such a flux and the applied temperature gradient.

Among the several possible choices, we simulated the effect of the reservoirs by means of Nosé-Hoover thermostatting method [18]. The latter preserves the deterministic nature of the dynamics and is simply implemented by adding the force terms $-\zeta_{\rm L}\,\dot{u}_1$ and $-\zeta_{\rm R}\,\dot{u}_N$ to the equation of motion of the first and last oscillator respectively. The "thermal" variables $\zeta_{\rm L}$, $\zeta_{\rm R}$, evolve according to the dynamical equations [18]

$$\dot{\zeta}_{\rm L} = \frac{1}{\tau^2}\left(\frac{\dot{u}_1^2}{T_{\rm L}} - 1\right)$$
$$\dot{\zeta}_{\rm R} = \frac{1}{\tau^2}\left(\frac{\dot{u}_N^2}{T_{\rm R}} - 1\right), \qquad (27)$$

where τ is the thermostat response time and controls the strength of the coupling between the reservoirs and the chain. The above prescriptions imply that the kinetic energy of the boundary particles fluctuates around the imposed average value, thus mimicking an interaction with a reservoir in canonical equilibrium.

The simulations were performed integrating the equation of motion for the bulk particles together with the (27) with a fourth-order Runge-Kutta algorithm. The boundary temperatures were kept fixed so that upon increasing the lattice length the applied temperature gradient $\Delta T/N$ is decreased and the Green-Kubo formula becomes more and more accurate. Both the time averaged kinetic temperatures $T_l = \overline{\dot{u}_l^2}$ and heat flux $\overline{J}$ where [19,20]

$$J = \frac{1}{2N}\sum_l (\dot{u}_{l+1} + \dot{u}_l)\,\left[u_{l+1} - u_l + g(u_{l+1} - u_l)^2\right], \qquad (28)$$

have been computed over a single trajectory (approximatively 10^6 time units) started from random initial conditions. In every run, a suitably long transient (about 10^4 time units) has been discarded in order to let the system reach a statistically stationary state with each oscillator in local equilibrium.

The thermal conductivity is thus computed as $\kappa = |\overline{J}|N/\Delta T$. It has to be noted that the latter quantity represents an effective transport coefficient including both boundary and bulk scattering mechanisms. Alternatively, one could as well consider, say, a subchain far enough from the ends and compute a bulk conductivity as the ratio between $|\overline{J}|$ and the actual temperature gradient measured there. Since the latter will also be inversely proportional to N, the resulting scaling with size (which is the main issue here) will be of course the same with both definitions. Besides this, the first choice avoids the difficulty of dealing with very small gradients (see below).

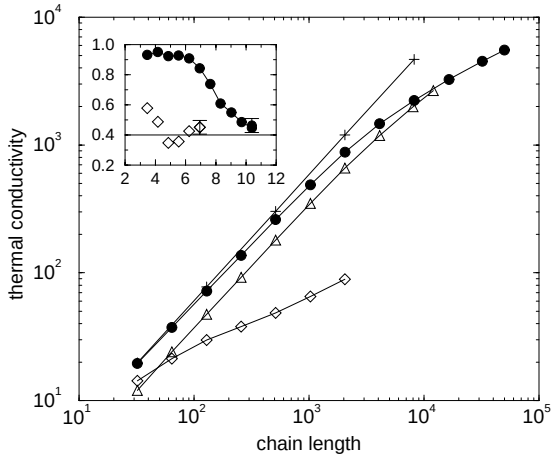

Fig. 4. Thermal conductivity of the FPU-α model *versus* lattice length N for $g = 0.25$, $T = 0.1$, $\tau = 1.0$ and $\Delta T = 0.1$ (triangles), $\Delta T = 0.02$ (full circles). The crosses (resp. diamonds) refer to the harmonic (resp. FPU-β) models for $T = 0.1$ and $\Delta T = 0.02$. The inset shows the logarithmic derivative $\Delta \log \kappa / \Delta \log N$ *versus* $\log N$ of the data for the FPU-α (full circles) and FPU-β (diamonds) respectively.

The dependence of κ on the chain length is reported in Figure 4 for two different series of simulations with $T = 0.1$ and for relatively small ($\Delta T = 0.02$) and large ($\Delta T = 0.1$) applied temperature differences. In both cases κ increases linearly with N for $N < 10^3$. Moreover, no sizable temperature gradient forms along the chain. Both facts are a signature of the weakness of the anharmonic effects up to this time/length scales, as confirmed by comparing with data obtained (using the same setup and parameters) for the pure harmonic ($g = 0$) chain. The latter displays the expected linear increase of κ with N [21] and differ by less than a few percent from the anharmonic case in this range of system sizes (compare full dots and crosses in Fig. 4). The fact that κ is smaller for larger ΔT can be thus be attributed to stronger boundary scattering that, in turn, tends to reduce the conductivity.

For larger N the bulk anharmonic scattering takes over and, accordingly, the two curves for different ΔT approach one the other. The conductivity increases more slowly with the size, and we can tentatively measure the effective divergence law of the form N^α. The data in the inset of Figure 4 (full dots) are consistent with a convergence to the asymptotic value $\alpha = 2/5$ expected from the theory and observed in previous works on other 1d models [14,22]. Notice also that the crossover size is in reasonable agreement with the behavior reported in Figure 2.

In order to clarify the role of different anharmonic interactions, we also compared the above results with some measurements for a chain with quartic potential. More precisely, we considered the so-called Fermi-Pasta-Ulam $\beta-$model (FPU-β) where the cubic term in the Lagrangian (1) is replaced by $(u_{l+1} - u_l)^4/4$. The corresponding coupling constant has been set to the value 1.0 to have about the same ratio between the average

anharmonic and harmonic potential energies as in the previous case (approximatively 0.04 for $T = 0.1$). With such a choice, the strength of the nonlinear terms (as measured by the suitable perturbative parameters) are of the same order and a comparison between the two models makes sense. As shown again in Figure 4, the values of κ are now definitely smaller (about one order of magnitude at $N = 1024$). Moreover, a linear temperature profile sets in along the chain and the data neatly approach a power-law behaviour with an exponent very close to 2/5 already for $N > 64$ (diamonds in the inset of Fig. 4). We therefore conclude that, consistently with the general argument given in the Introduction, the cubic nonlinearity is much less effective for what concerns the process of energy diffusion and transport in 1d.

In conclusion, we have shown that the dynamical correlations and transport in 1d lattice are strongly affected by nonlinear effects which are not accounted for by the simple perturbative analysis reported above even in the weakly anharmonic regime. For the model with cubic intersite potential, they manifest themselves *e.g.* in a faster divergence (N^α rather than $\log N$) of the thermal conductivity with the size N. Further consequences of those issues on other physical phenomena like energy diffusion or wavepacket propagation will be subject of future research.

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Appendix: Evaluation of the memory function

In this Appendix we sketch some details of the perturbative calculation of the memory function for the quadratic force. One wants to evaluate the Laplace transform of the sum appearing in equation (8). As a first step, we replace the sum for large N by the integral over the Brillouin zone

$$\frac{1}{2\pi}\int_{-\pi}^{+\pi} \mathrm{d}q' \, \cos\omega(q')t \, \cos\omega(q-q')t. \tag{A.1}$$

Its transform is thus given by

$$\frac{\mathrm{i}z}{4\pi}\int_{-\pi}^{+\pi} \mathrm{d}q' [\frac{1}{(\omega(q')+\omega(q-q'))^2 - z^2} + \frac{1}{(\omega(q')-\omega(q-q'))^2 - z^2}]. \tag{A.2}$$

It is convenient to perform the change of variable $u = \mathrm{e}^{\mathrm{i}(q'-q/2)/2}$. After some algebra, the integral reads as

$$\frac{z}{2\pi}\int \frac{\mathrm{d}u}{u}\left[\frac{1}{\Omega_-^2(u+1/u)^2/4 + z^2} + \frac{1}{\Omega_+^2(u-1/u)^2/4 + z^2}\right] \tag{A.3}$$

where the frequencies $\Omega_\pm(q)$ are defined in equation (11) and the integration is along a path joining the points $\pm\exp(-\mathrm{i}q/2)$. By means of the further change of variable $u^2 = \zeta$, the integration can be performed on the unit circle. The result (10) is thus obtained by means of the theorem of residues.

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