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Thermal conductivity of nonlinear waves in disordered chains

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Abstract. We present computational data on the thermal conductivity of nonlinear waves in disordered chains. Disorder induces Anderson localization for linear waves and results in a vanishing conductivity. Cubic nonlinearity restores normal conductivity, but with a strongly temperature-dependent conductivity $\kappa(T)$. We find indications for an asymptotic low-temperature $\kappa \sim T^4$ and intermediate temperature $\kappa \sim T^2$ laws. These findings are in accord with theoretical studies of wave packet spreading, where a regime of strong chaos is found to be intermediate, followed by an asymptotic regime of weak chaos (Laptyeva *et al*, *Europhys. Lett.* **91**, 30001 (2010)).

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1. Introduction

In the absence of nonlinearity (or many-body interactions in quantum systems), all eigenstates – normal modes (NM) – in one-dimensional random lattices with disorder are spatially localized. This is Anderson localization [1], which was discovered 50 years ago in disordered crystals as a localization of electronic wave functions. It can be interpreted as an interference effect between multiple scattering events of the electron and random defects of the potential. Recent experiments on the observation of Anderson localization were performed with light propagation in spatially random optical media [2,3], with noninteracting Bose–Einstein condensates expanding in random optical potentials [4,5], and with wave localization in a microwave cavity filled with randomly distributed scatterers [6].

In many situations, nonlinear terms in the wave equations (respectively, many-body interaction terms in quantum systems) have to be included. Thus, a fundamental question which has attracted the attention of many researchers is: what happens to an initial excitation of arbitrary shape in a nonlinear disordered lattice. Nonlinearity renormalizes excitation frequencies, and induces interactions between NMs. Numerical studies show that wave packets spread subdiffusively and Anderson localization is destroyed [7–10]. In the regime of strong nonlinearity, far from where it can be treated perturbatively, new localization effects of self-trapping occur [11]. A theoretical explanation of the subdiffusive spreading was offered in refs [7,9,12]. It is based on the fact that the considered models are in general non-integrable. Therefore deterministic chaos will lead to an incoherent spreading. Estimates of the excitation transfer rate across the packet tail are obtained by calculating probabilities of mode–mode resonances inside the packet. Some predictions of this approach include the effect of different degrees of nonlinearity and were successfully tested in [13]. First experimental data were recently presented for repulsively interacting Bose–Einstein condensates in quasiperiodic potentials [14,15] which, among others, confirm the basic theoretical findings.

While the above wave packets are spreading into an 'empty' system, another set of related problems concerns the thermal conductivity at finite temperature T (i.e. at finite energy density $\varepsilon \sim T$) [16,17]. In the absence of nonlinearity, Anderson localization of NMs leads to a vanishing conductivity. It was observed that even a small amount of anharmonicity leads to a diffusive transport of energy, and a finite thermal conductivity κ [18]. Some numerical studies indicated that for low temperatures $\kappa \sim T^{1/2}$ [18] which would indicate a singularity at zero temperatures. Other expectations claim that heat conductivity vanishes strictly for weak enough (but still finite) anharmonicity [17].

In this report we use the theoretical results on wave packet spreading and derive a connection between κ and T. We predict that for low temperatures $\kappa \sim T^4$ which corresponds to the regime of weak chaos. At higher temperatures an optional intermediate regime of strong chaos may lead to $\kappa \sim T^2$. We perform numerical simulations which indicate that our predictions are plausible.

2. Models

We study two different Hamiltonian models. The first model describes interacting anharmonic oscillators in a quartic Klein–Gordon (KG) chain, given as

$$\mathcal{H}_K = \sum_l \frac{p_l^2}{2} + \frac{\tilde{\epsilon}_l}{2}u_l^2 + \frac{1}{4}u_l^4 + \frac{1}{2W}(u_{l+1} - u_l)^2, \tag{1}$$

where u_l and p_l are respectively the generalized coordinate/momentum on the site l, and $\tilde{\epsilon}_l$ are the disordered potential strengths chosen uniformly in the interval $[1/2, 3/2]$. Likewise, $\partial_t^2 u_l = -\partial\mathcal{H}_K/\partial u_l$ generates the equations of motion

$$\ddot{u}_l = -\tilde{\epsilon}_l u_l - u_l^3 + \frac{1}{W}(u_{l+1} + u_{l-1} - 2u_l). \tag{2}$$

By neglecting the nonlinear terms, the KG model (1) reduces to a linear eigenvalue problem. This leads to a set of NM amplitudes, $A_{\nu,l}$, with NM squared frequencies $\omega_\nu^2 \in [1/2, 3/2 + 4/W]$ and $\Delta = 1 + 4/W$ being the width of the squared eigenfrequency spectrum. The NM asymptotic spatial decay is given by $A_{\nu,l} \sim \mathrm{e}^{-l/\xi(\omega_\nu^2)}$ where $\xi(\omega_\nu^2)$ is the localization length. It is approximated [19] in the limit of weak disorder ($W \ll 1$) as $\xi(\omega_\nu^2) \leq 96W^{-2}$. The NM participation number $P_\nu = 1/\sum_l A_{\nu,l}^4$ characterizes the NM spatial extent. An average measure of this extent is the localization volume V, which is on the order of $3.3\xi(0)$ for weak disorder and unity in the limit of strong disorder [20]. The average squared frequency spacing of NMs within a localization volume is then $d \approx \Delta/V$.

The two squared frequency scales d and Δ with $d < \Delta$ are thus expected to determine the dynamics details in the presence of nonlinearity.

Nonlinearity induces an interaction between NMs. Since all NMs are exponentially localized in space, each of them is effectively coupled to a finite number of neighbour modes, i.e. the interaction range is finite. However, the strength of this coupling is proportional to the characteristic energy density, ε. The squared frequency shift due to the nonlinearity is then $\delta \sim \varepsilon$.

The KG model is suitable for studies of the dynamics for weak and intermediate disorder $W < 20$, since otherwise the coupling strength between nearest-neighbour oscillators becomes too weak and the required computation times too long. In the limit of strong disorder, the NMs become localized on a single site, and will be coupled by nonlinearity to their nearest neighbour. Therefore this limit can be modelled by a chain of harmonic oscillators with random frequencies and purely anharmonic nearest-neighbour coupling:

$$\mathcal{H}_{\mathrm{FSW}} = \sum_l \frac{p_l^2}{2} + \frac{\tilde{\epsilon}_l}{2} u_l^2 + \frac{1}{4}(u_{l+1} - u_l)^4 \tag{3}$$

which is an example from a class of models studied by Fröhlich, Spencer and Wayne [21] and therefore called here as the FSW model. It follows qualitatively from the KG model by first transforming into NM space, dropping secular terms [12], and finally through the limits of strong disorder, and of high temperatures (energies). Its quartic potential part however is invariant under homogeneous coordinate shifts, contrary to the KG case.

3. Thermal conductivity

The thermal conductivity is measured by a standard approach, when the thermal baths attached to the ends generate a temperature gradient and heat current along the chain [16]. For the KG model we implement Langevin thermostats with two next-to-end atoms coupled to Langevin heat baths with $\ddot{u}_{1,N} = -\partial H/\partial u_{1,N} + \xi_{1,N} - \lambda \dot{u}_{1,N}$ with white noise $\langle \xi_{1,N} \rangle = 0$ and $\langle \xi_{1,N}(t)\xi_{1,N}(0) \rangle = 2\lambda T_{1,N}\delta(t)$ where $\langle\cdot\rangle$ denotes ensemble averages. T is the temperature, and λ denotes the coupling strength between the system and the heat bath. For the FSW model we use Nosé–Hoover thermostats adding the terms $-\zeta_\pm \dot{u}_{1,N}$ to the respective equations of motion, where $\dot{\zeta}_\pm = \dot{u}_{1,N}^2/T_{1,N} - 1$.

For the KG model the heat flux along the chain is defined as the time average of $j_{\mathrm{KG}} = -(1/2W)\sum_l (\dot{u}_{l+1} + \dot{u}_l)(u_{l+1} - u_l)$ [16]. For the FSW model the heat flux follows from the time average of $j_{\mathrm{FSW}} = -\frac{1}{2}\sum_l (\dot{u}_{l+1} + \dot{u}_l)(u_{l+1} - u_l)^3$ [16]. Then the thermal conductivity coefficient $\kappa = jN/(T_N - T_1)$ [16]. We use the mean temperature $T = (T_N + T_1)/2$ as a parameter corresponding to the energy density $\langle\varepsilon\rangle = T$, and $(T_N - T_1)/T = 0.5$ further on.

4. Predictions

The numerical evolution of a wave packet spreading into an empty system [7–10] yields subdiffusive growth of the second moment. This implies that the diffusion rate is depending on the energy density (temperature). A theoretical approach [7,9,12] postulates that the wave packet evolves chaotically, and estimates the diffusion rate for the KG model to be [12]

$$D \sim \varepsilon^2 \mathcal{P}^2(\varepsilon) \tag{4}$$

with the resonance probability [20]

$$\mathcal{P}(\varepsilon) \approx 1 - \mathrm{e}^{-a\varepsilon/d} \tag{5}$$

a being an unknown constant of order one.

For small temperatures $\varepsilon \sim T$. Therefore, and assuming that the thermal conductivity is proportional to the diffusion rate [10], we conclude that for the KG model

$$\kappa \sim T^2 \left(1 - \mathrm{e}^{-bT/d}\right)^2 \tag{6}$$

with b another constant of order one. In particular, we find that

$$\kappa \sim T^4 \ , \ T \ll d \ \text{(weak chaos)}, \tag{7}$$

$$\kappa \sim T^2 \ , \ T \gg d \ \text{(strong chaos)}. \tag{8}$$

Note that for larger energy densities (temperatures) the KG model enters the regime of self-trapping, and the above predictions do not apply anymore. The self-trapping regime is expected when $\varepsilon \sim T \approx 2/(3W)$ [10]. It is the asymptotic high-temperature limit of the KG model, where the thermal conductivity should drop with increasing temperature [17]. Thus, depending on the strength of disorder, we expect that the thermal conductivity grows with temperature as T^4, then (for not too strong disorder) it grows as T^2, and finally goes through a maximum and starts to decrease with further increase of temperature. The three phases are summarized in the inset of figure 3 in ref. [10].

The application of the above approach to the FSW model leads to $d \sim 1$ and to the absence of a self-trapped regime. Instead, for large temperatures, the leading order anharmonic potential terms of the FSW model bring it close to the momentum conserving β-Fermi–Pasta–Ulam chain (FPU). The FPU chain has a thermal conductivity which diverges with increasing system size [16]. Therefore, κ will increase with system size also for the FSW model for large temperatures, until the harmonic oscillator potential parts cannot be neglected anymore, leading to a final saturation of the thermal conductivity with a further increase in system size. Indeed, the harmonic oscillator potential parts are violating total momentum conservation, and therefore the thermal conductivity stays finite for large enough system size [10,17]. Since the momentum conserving terms of the FSW model become more dominant at larger temperatures, it follows that the higher the temperature, the larger the system sizes needed, and the larger the saturated conductivity value. The cross-over to this pseudo-FPU regime can be expected when the temperature is of order unity (since all relevant FSW model parameters are of order unity). Therefore, we conclude that we shall not see a pronounced regime of strong chaos, instead the regime of weak chaos at low temperatures should gradually transform into the pseudo-FPU regime.

5. Numerical results

The thermal conductivity is computed along the above lines, with additional averaging over disorder realizations.

5.1 *KG chain*

We first present results for the disorder strength $W = 2$. Here the localization length $\xi \approx 25$ and the localization volume $V \approx 75$. The thermal conductivity κ_N is plotted for various temperatures vs. system size N in figure 1. For large temperatures, $T \geq 0.1$, the conductivity reaches its saturated level κ at system size $N \approx \xi$. For the linear wave equation, exponentially localized NMs induce a dependence $\kappa_{\text{linear}} \sim \mathrm{e}^{-N/\xi}$. In the presence of nonlinearity the exponential decay with N will stop at the saturated value of κ. Assuming that $\kappa \sim T^\alpha$ it follows that the system size for saturated conductivity values scales as $N \sim -\alpha\xi \ln T$. Thus, for lower temperatures the system size needed to reach saturated values of κ increases. This is due to the dropping of the saturated value of κ with T. We were able to reach temperatures as low as $T = 0.005$ and conductivity values $\kappa = 0.008$. According to ref. [10] (inset in figure 3) the regime of strong chaos is realized for $0.01 < T < 0.3$. Therefore we expect to observe $\kappa \sim T^2$ for $0.01 < T < 1$, followed by a maximum and a further dropping with increasing temperatures. These predictions are indeed compatible with the numerical results in figure 2. We also compute the conductivity for a reference ordered chain with $\tilde{\epsilon}_l = 1$, which coincides with the high-temperature part of $\kappa(T)$ for the disordered case. Therefore, the observed maximum is due to disorder, as well as the decrease of κ with further lowering of the temperature. The low-temperature data are also consistent with the T^2 law. However the temperature window is too narrow to conclude about a confirmation. Also, we expect that at even lower temperatures (so far not reachable with our computational means) the conductivity should cross over into the weak chaos regime and follow the T^4 law.

To find evidence for the asymptotic low-temperature behaviour $\kappa \sim T^4$ we chose a stronger disorder $W = 6$. In that case $\xi \approx 3$ and $V \approx 10$. The conductivity is reduced by two orders of magnitude. We are therefore quite limited in the temperature window, and do not obtain conclusive data (see figure 2). We again find a maximum in the $\kappa(T)$ dependence, and a clear indication that the small-temperature conductivity drops faster than

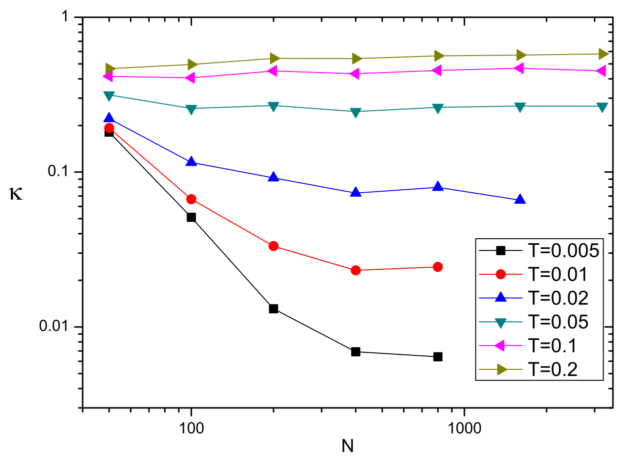

Figure 1. KG chain: the size-dependent thermal conductivity κ_N vs. N for different temperatures and $W = 2$.

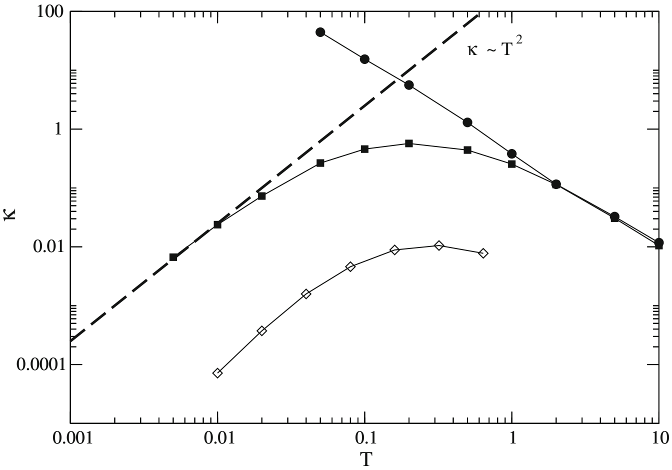

Figure 2. KG chain: $\kappa(T)$ for $W = 2$ (filled squares). For comparison we also show the data for $\tilde{\epsilon}_l \equiv 1$ (filled circles). Thin solid lines guide the eye. The dashed line corresponds to the power law T^2. The stronger disorder case $W = 6$ corresponds to the open diamond data points.

T^2 with temperature. Yet we do not have enough low-temperature data to conclude about the exponent.

5.2 *FSW chain*

To observe the asymptotic low-temperature behaviour of conductivity, we explore the strong disorder limit and study the FSW chain. Since the localization length $\xi = 0$ for

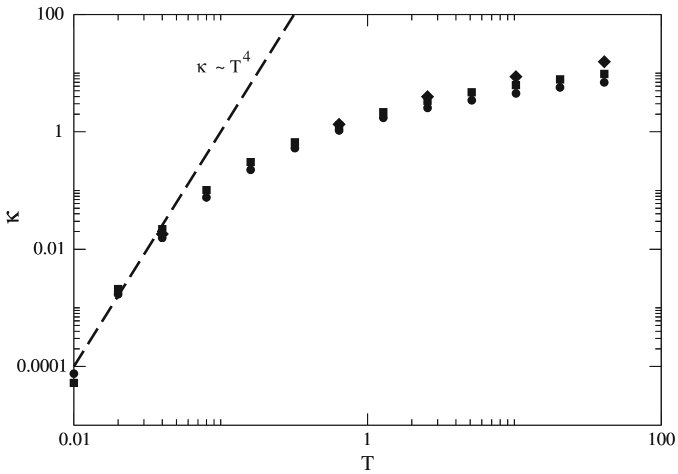

Figure 3. FSW chain: $\kappa(T)$ for system sizes $N = 16$ (filled circles), $N = 64$ (filled squares) and $N = 256$ (filled diamonds). The dashed line corresponds to the T^4 law.

the FSW chain, we can use small system sizes for small temperatures, while (as discussed above) we shall need larger system sizes to obtain the saturated conductivity values for larger temperatures. In figure 3 we plot the conductivity κ vs. temperature for different system sizes $N = 16, 64, 256$. Indeed, we observe a significant difference between the data for temperatures $T > 1$, while the data agree well for lower temperatures. Therefore we can reach lower values of the conductivity as compared to the KG chain case. Yet for $\kappa < 10^{-4}$ (which corresponds to $T \approx 0.01$) we again reach our computational limitations, since the number of realizations and the integration times, which are needed to reduce the impact of fluctuations, increase drastically. The numerical results in figure 3 indicate that for low temperatures the conductivity behaves as $\kappa \sim T^4$. Also at larger temperatures we observe a cross-over to the predicted pseudo-FPU regime. Again we need more data in the low-temperature regime to be more conclusive about the conductivity data.

6. Discussion and outlook

We computed the thermal conductivity for nonlinear disordered chains and obtained results which indicate that theoretical predictions based on wave packet spreading are plausible. In particular, we find indications for an asymptotic low-temperature $\kappa \sim T^4$ and intermediate temperature $\kappa \sim T^2$ laws. To be more conclusive, we need data at even lower temperatures than those presented here. The needed CPU times are however currently exceeding our capabilities. Possible solutions include the usage of massive parallel computing equipment, or the search for other models which will allow to make the needed observations with standard computational equipment.

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