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Heat transport in one dimension

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Abstract. We review the state of the art of the problem of heat conduction in one dimensional nonlinear lattices. The peculiar role of finite size and time corrections to the predictions of the hydrodynamic theory is discussed. The emerging scenario indicates that when dealing with systems, whose spatial size is comparable with the mean-free path of peculiar nonlinear excitations, hydrodynamic predictions at leading order are no more predictive. We can conjecture that one should take into account estimates of subleading contributions, which could play a major role in some regions of the parameter space in 'small' systems.

Keywords: transport processes / heat transfer

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Contents

1. Introduction

In the last decades heat transport in low-dimensional systems has been quite a debated problem, being characterized by unusual features like divergence of heat conductivity, superdiffusion, the peculiar role played by nonlinearity, integrability and disorder, etc. We can summarize the overall scenario by saying that, at variance with what was first naively conjectured on the basis of chaos theory in spatially extended dynamical systems, heat conduction in low-dimensional systems exhibits anomalous behavior, characterized by a power-law divergence of the heat conductivity κ with the system size L, namely

$$\kappa \sim L^{\gamma} \;, \tag{1}$$

with $\gamma > 0$. This important physical property was first pointed out in [1, 2]. Nowadays we have realized that it emerges as a combined effect of reduced space dimensionality and conservation laws, yielding non standard relaxation properties even in a linear response regime. For instance, anomalous heat conductivity has been typically observed in hamiltonian lattices where energy and momentum are conserved, with some remarkable exception, like in the case of the rotor model [3], or similar models with a bounded potential. A typical setup adopted to check relations like (1) is a hamiltonian chain with a moderate temperature gradient applied at its boundaries. By varying the size L of the system one can directly check the dependence of κ on L. Alternatively, one can exploit the linear-response approach and measure the correlation function of the total energy-current $J(t)$ of the same hamiltonian chain in equilibrium conditions. This quantity is found to behave as [2]

$$\langle J(t)J(0)\rangle \propto t^{-(1-\delta)} \tag{2}$$

with $0 \leqslant \delta < 1$. Making use of the Green–Kubo formula one can conclude that the heat conductivity κ diverges, while the relation between the space and time exponents boils down to $\gamma = \delta$.

J. Stat. Mech. (2020) 034001

Nowadays we have come to a satisfactory theoretical explanation of such power-law divergences. For instance, fluctuating hydrodynamics accounts for the basic features of anomalous heat conduction in chains of nonlinearly coupled oscillators [4, 5], while rigorous predictions of the anomalous behaviour in stochastic conservative evolution of similar chains have been obtained [6, 7].

In order to provide a more detailed account of the standard scenario expected for anomalous heat conduction in low dimensions, in the next section we shortly review the results obtained for widely analyzed models, discussing also a case with long range interactions. Then we shall describe various examples where finite-size effects yield non-standard scenarios for what heat conduction is concerned.

2. Models and results: the standard scenario

A widely investigated model is the celebrated Fermi–Pasta–Ulam (FPU) chain, whose Hamiltonian reads

$$H = \sum_{n=1}^{L} \frac{p_n^2}{2m} + V(q_{n+1} - q_n) \tag{3}$$

with

$$V(x) = \frac{1}{2}x^2 + \frac{\alpha}{3}x^3 + \frac{\beta}{4}x^4. \tag{4}$$

The canonically conjugated variables q_n and p_n represent the displacement of the n-th anharmonic oscillator from its equilibrium position and its momentum, respectively. The predicted value of the divergence exponent is $\gamma = \frac{1}{3}$ [8]. This exponent identifies a universality class of models, including the alternate-mass hard-point gas [9, 10], the alternate-mass hard-point chain [11] and any other model exhibiting a leading cubic nonlinearity. When the cubic nonlinearity is suppressed (i.e. $\alpha = 0$) the predicted divergence exponent is $\gamma = \frac{1}{2}$ [12], which has been found to be in common with other models like the harmonic chain with conservative noise [13], the alternate-mass hard-point chain at zero pressure [11] and the FPU chain with zero compressibility [14]. It can be argued that all of the latter models have in common an effective leading quartic nonlinearity, at variance with the previously mentioned models.

Some efforts have been devoted also to study heat transport in chains with long-range interactions (e.g. see [15–18]). This problem has been investigated for Hamiltonian chains of the form (3), with interaction potential

$$V = \frac{1}{2N_0(\alpha)} \sum_{i=1}^{N} \sum_{i \neq j}^{N} \frac{v(q_i - q_j)}{|i-j|^{\alpha}}, \tag{5}$$

where the generalized Kac factor

$$N_0(\alpha) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \frac{1}{|i-j|^{\alpha}} \tag{6}$$

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J. Stat. Mech. (2020) 034001

guarantees the extensivity of the Hamiltonian. Note that for $\alpha = 0$ (mean-field interaction) $N_0(0) = N - 1$ reproduces the standard Kac prescription, while for $\alpha \to +\infty$ (nearest-neighbor interaction) one has $N_0(+\infty) = 1$. Overall, for any fixed chain size N, $N_0(\alpha)$ is a monotonic decreasing function of α, while the interval $0 < \alpha < 1$ identifies the parameter region corresponding to non-additive interactions in one dimension.

In two recent papers [19, 20] the authors considered the long-range versions of the rotors chain, namely

$$v(q_i - q_j) = 1 - \cos(q_i - q_j) \tag{7}$$

and of the FPU-β model

$$v(q_i - q_j) = \frac{1}{2}(q_i - q_j)^2 + \frac{1}{4}(q_i - q_j)^4 \,. \tag{8}$$

In fact, the nearest-neighbor versions (i.e. $\alpha \to +\infty$) of the former model exhibits standard diffusion of energy [3], while the latter is characterized by anomalous diffusion with $\gamma = \frac{1}{2}$.

Nonequilibrium measurements of the rotors chain (7), with thermal reservoirs at different temperature, $T_1 > T_2$, acting at the chain ends, indicate that for $\alpha > 1$ the resulting temperature profile interpolates linearly between T_1 and T_2. Despite the long range nature of the interaction this is a strong indication that a standard diffusive process still governs energy transport through the chain, as in the limit $\alpha \to +\infty$. For $\alpha < 1$ the temperature profile progressively flattens, until reaching a constant bulk temperature $T = (T_1 + T_2)/2$ in the 'mean-field' limit $\alpha \to 0^+$. In fact, in this limit the energy exchanged among rotors is irrelevant with respect to the amount of energy directly exchanged by each rotor with the thermal baths. Accordingly, any rotor eventually have to compromise between the two different temperatures imposed by the reservoirs [19]. In this sense, the heat transport process is dominated by a sort of 'parallel' energy transport mechanism, because the transfer of energy from the reservoirs to the rotors is instantaneous, irrespectively of the distance of any rotor from the reservoirs. Said differently, in this regime the mechanism of energy transport by sound waves is practically immaterial.

For $\alpha < 1$ a similar scenario characterizes model (8). In fact, flat temperature profiles are observed also in this case and it has been checked that the same 'parallel' energy transport mechanism observed for rotors is at work. On the other hand, the scenario is definitely more complex for $\alpha > 1$ and it seems to be strongly affected by finite size effects. In the next section we discuss this case as a first example of a gallery of cases where such effects play a crucial role in determining sizable deviation of transport properties from the standard scenario.

3. The role of finite size effects

In this section we illustrate several examples of how finite size effects may yield sizable modifications of heat transport in low-dimensional systems.

J. Stat. Mech. (2020) 034001

3.1. The FPU-β model with long-range interactions

This model, introduced at the end of the previous section, for $\alpha > 1$ should be expected to reproduce the standard anomalous behavior with $\gamma = \frac{1}{2}$, predicted for its short range version ($\alpha \to +\infty$). On the other hand, careful numerical investigations provide an overall scenario, where an anomalous diffusion mechanism sets in, characterized by an exponent γ, which is much closer to the value $\frac{2}{5}$, the one predicted by first-order mode-coupling theory [21]. Only for very large values of α (e.g. $\alpha = 5$) and by performing very long numerical simulations on systems with very large values of L one can observe a slow increase of the estimate of γ from $\frac{2}{5}$. This testifies at the strong effect of finite size corrections in the long-range version of this model, with respect to the standard scenario characterizing its short-range version, although no theoretical argument is presently available to explain the reason why the long-range version of the FPU-β model singles out the first order mode-coupling exponent, rather the expected one. As a further 'surprise', for $\alpha = 2$ one finds that a flat temperature profile sets in, although, as clearly shown by numerics, the mechanism of transport along the chain certainly dominates over the parallel transport process. One could conjecture that this apparently 'ballistic' regime (similar to the one characterizing integrable models) emerges because for $\alpha = 2$ the model is close to some (presently unknown) integrable approximation. Anyway, even by increasing the chain size L to the largest numerically available values the flat shape of the temperature profile is quite robust. In this sense we can guess that if finite size effects are again at work, in this case they are definitely more relevant than for any other value of $\alpha > 1$.

Moreover, the structure factors of this long-range model for $\alpha > 1$ indicate that the dynamical exponent z depends on α in a way that is certainly different form the one that could be expected on the basis of the theory of Lévy processes [20]. Last, but not least, by adding to potential (8) the cubic term $v(q_i - q_j) = \frac{1}{3}(q_i - q_j)^3$ one recovers the same dependence of z on α, up to $\alpha = 5$. This is also a surprise, because in the limit $\alpha \to +\infty$ the cubic and quartic versions of the short-range FPU-model should converge to different values of z. It is a matter of fact that no theoretical explanation is, at present, available to cope with this puzzling scenario.

3.2. Anharmonic chains with nearest-neighbor asymmetric interactions

Several numerical investigations (e.g. see [22]) have pointed out that finite size corrections are particularly relevant in anharmonic chains with asymmetric interactions, represented by Hamiltonian models of the following form:

$$H = \sum_{n=1}^{L} \frac{p_n^2}{2m} + V(q_{n+1} - q_n) \tag{9}$$

with $V(x) \neq V(-x)$. A typical example in the Fermi–Pasta–Ulam model (4). For instance, there is a range of parameters where out of equilibrium measurements of the heat conductivity of this specific model are consistent with Fourier's law, i.e. with a finite thermal conductivity. As shown in [23, 24] this effect is quite robust and persists for relatively large values of L (and, consistently, for large values of the simulation times). In fact, the expected theoretical prediction of a diverging heat conductivity (1) with $\gamma = \frac{1}{3}$ can be recovered in simulations performed only for exceedingly large values of L in this region of the parameter space. It has been argued that this crossover from standard diffusion to the expected anomalous regime can be read as a consequence of the relatively long relaxation time of mass inhomogeneities induced by the asymmetry of the interaction potential. Such density fluctuations are supposed to behave as scatterers of phonon-like waves and they are sizable only over large but finite space and time scales, until they are eventually relaxed. Anyway, a reliable theoretical estimate of these scales, based on the computation of higher order corrections to the hydrodynamics in this regime, is stil lacking.

The intricate scenario of heat transport in anharmonic chains has been enriched by the contribution contained in [25], where the authors study a model where the Hamiltonian (9) has an additional local 'pinning' potential of the form

$$U(q_i) = \frac{1}{2}\sum_{n=1}^{L} q_n^2. \tag{10}$$

By varying the nonlinear coupling β one observes a crossover from a ballistic transport, typical of an integrable model, to an anomalous diffusive regime ruled by and exponent of the time correlation function, which corresponds to a value of $\gamma \sim 0.2$. The crossover occurs in the parameter region $0.1 < \beta < 1$. Numerical simulations performed for a chain of a few thousands of oscillators show that by further increasing β, also γ seems to increase. The overall outcome completely challenges the basic theoretical argument, which predicts that an anharmonic chain equipped by a local potential should exhibit normal diffusion. For the sake of completeness it is worth mentioning that in this paper the model under scrutiny is compared with the so-called ϕ^4-model, where the nonlinear term in Hamiltonian (9), $\beta(q_{n+1} - q_n)^4$ is substituted with βq_n^4. Also for this model one observes, in the same parameter region, a crossover from a ballistic regime to an anomalous diffusive regime, but, for $\beta > 1$, the exponent γ seems to vanish, so that the expected diffusive behavior is recovered. Also these results have a logical interpretation only if we invoke the role of finite size corrections combined with nonlinearity. Actually, in the ϕ^4-model there is no way to argue that a ballistic regime should be observed for any finite, even if small, value of β. The ballistic behavior observed in both models for $\beta < 0.1$ seems to suggest that for small nonlinearities one needs to explore definitely much larger chains and integrate the dynamics over much longer times, than those employed in [25], before in both chains phonon-like waves may experience the scattering effects due to the local potential. Moreover, the weaker quadratic pinning potential of the original model seems to be still affected by finite size corrections, even in the region $\beta > 1$. A problem that one should investigate systematically is the dependence on β of the chain length and of the integration time necessary to recover standard diffusive transport, at least in the crossover region $0.1 < \beta < 1$, where one can expect to perform proper numerical analysis in an accessible computational time.

3.3. Toda lattice with a harmonic substrate potential

We conclude this section by discussing the case of a Toda lattice, equipped with a substrate potential, whose hamiltonian reads

$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + \exp(q_{i+1} - q_i) + \frac{\nu^2}{z} |q_i|^z \right]. \tag{11}$$

Let us recall that the unpinned Toda chain (i.e. $\nu = 0$) is integrable and, accordingly, heat transport is ballistic due to the finite–speed propagation of Toda solitons. These are localized nonlinear excitations which are known to interact with each other by a non–dissipative diffusion mechanism, due to the stochastic sequence of spatial shifts experienced by a soliton as it moves through the lattice and interacts with other excitations without momentum exchange [26]. Actually, the calculation of the transport coefficients by the Green–Kubo formula indicates the presence of a finite Onsager coefficient, which corresponds to a diffusive process on top of the dominant ballistic one (e.g. see [27] and [28]).

When the pinning term is at work for any integer value of $z \geqslant 2$ the Toda chain becomes chaotic, as one can easily conclude by measuring the spectrum of characteristic Lyapunov exponents (see [29]).

Anyway, the case $z = 2$ exhibits some peculiar features. In fact, only in this case one can easily check that, only in this case, the 'center of mass'

$$h_c = \frac{1}{2} \sum_{n=1}^{L} (p_n^2 + q_n^2)$$

is an additional conserved quantity, beyond total energy. Nonequilibrium simulations of model (11), where heat reservoirs at different temperature, $T_1 > T_2$ act at its boundaries, yield, as expected, a linear profile of temperature, compatible with standard Fourier's law, apart the remarkable exception of the case $z = 2$, where the temperature profile in the bulk of the chain flattens at $T = (T_1 + T_2)/2$. The latter scenario is the one expected for the unpinned Toda chain, but it is fully inconsistent with the basic consideration that the presence of any pinning term breaks translation invariance and total momentum is no more conserved. This notwithstanding, in order to observefor $z = 2$ a temperature profile in the form of a linear interpolation between T_1 and T_2 (i.e. Fourier's law) one has to simulate the dynamics of very large chains over very long times: typically $L \sim \mathcal{O}(10^4)$ and $t \sim \mathcal{O}(10^6)$, when all the parameters of the model are set to unit.

Equilibrium measurements based on the Green–Kubo relation, i.e. on the behavior of the energy current correlator, provide further interesting facets of this scenario. By comparing the Toda chain with quadratic and quartic pinning potentials one observes in the latter case clear indications of a diffusive regime, i.e. a finite heat conductivity, and a practically negligible influence of finite size corrections, while in the former case the power spectrum (i.e. the Fourier transform of the energy current correlator) is found to exhibit a peculiar scaling regime (with a power $-5/3$), before eventually reaching a plateau that indicates a standard diffusion. In the same region of the spectrum the FPU model (where the parameters α and β have been chosen in such a way to correspond to a Taylor series expansion of the Toda chain) with the addition of (10) is found to converge to a plateau, in the absence of any preceeding power-law scaling.

Further details about the unexpected transport regimes encountered in the Toda chain equipped with the quadratic pinning can be found in [29, 30].

One should point out that many of them are still waiting for a convincing theoretical interpretation.

4. Conclusions

In this short review we have summarized the standard scenario of heat transport in nonlinear lattices, based on numerical investigations and nonlinear fluctuating hydrodynamics. We have also discussed a series of typical cases where strong finite size effects significantly modify this standard scenario. We want to point out that this is not a purely academic problem. When dealing with low dimensional materials one typically has in mind nano-wires and polymers, that are usually made of a relatively small number of atoms. Accordingly, we can expect that a reliable theory of heat conduction in these real materials should take seriously into account the role of finite size corrections, which, as we have discussed here, is typically amplified by peculiar long-living nonlinear excitations.

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J. Stat. Mech. (2020) 034001

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J. Stat. Mech. (2020) 034001