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RESEARCH ARTICLE

Heat Transport in low-dimensional systems

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Recent results on theoretical studies of heat conduction in low-dimensional systems are presented. These studies are on simple, yet nontrivial, models. Most of these are classical systems, but some quantum-mechanical work is also reported. Much of the work has been on lattice models corresponding to phononic systems, and some on hard particle and hard disc systems. A recently developed approach, using generalized Langevin equations and phonon Green's functions, is explained and several applications to harmonic systems are given. For interacting systems, various analytic approaches based on the Green-Kubo formula are described, and their predictions are compared with the latest results from simulation. These results indicate that for momentum-conserving systems, transport is anomalous in one and two dimensions, and the thermal conductivity κ, diverges with system size L, as $\kappa \sim L^{\alpha}$. For one dimensional interacting systems there is strong numerical evidence for a universal exponent $\alpha = 1/3$, but there is no exact proof for this so far. A brief discussion of some of the experiments on heat conduction in nanowires and nanotubes is also given.

1. Introduction

It is now about two hundred years since Fourier first proposed the law of heat conduction that goes by his name. Consider a macroscopic system subjected to different temperatures at its boundaries. One assumes that it is possible to have a

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coarse-grained description with a clear separation between microscopic and macroscopic scales. If this is achieved, it is then possible to define, at any spatial point $\mathbf{x}$ in the system and at time t, a local temperature field $T(\mathbf{x},t)$ which varies slowly both in space and time (compared to microscopic scales). One then expects heat currents to flow inside the system and Fourier argued that the local heat current density $\mathbf{J}(\mathbf{x},t)$ is given by

$$\mathbf{J}(\mathbf{x},t) = -\kappa \nabla \mathbf{T}(\mathbf{x},\mathbf{t}) \ , \tag{1}$$

where κ is the thermal conductivity of the system. If $u(\mathbf{x},t)$ represents the local energy density then this satisfies the continuity equation $\partial u/\partial t + \nabla.\mathbf{J} = \mathbf{0}$. Using the relation $\partial u/\partial T = c$, where c is the specific heat per unit volume, leads to the heat diffusion equation:

$$\frac{\partial T(\mathbf{x},t)}{\partial t} = \frac{1}{c}\nabla.[\ \kappa \nabla T(\mathbf{x},t)\ ] \ . \tag{2}$$

Thus, Fourier's law implies diffusive transfer of energy. In terms of a microscopic picture, this can be understood in terms of the motion of the heat carriers, *i.e.* , molecules, electrons, lattice vibrations(phonons), etc., which suffer random collisions and hence move diffusively. Fourier's law is a phenomological law and has been enormously succesful in providing an accurate description of heat transport phenomena as observed in experimental systems. However there is no rigorous derivation of this law starting from a microscopic Hamiltonian description and this basic question has motivated a large number of studies on heat conduction in model systems. One important and somewhat surprising conclusion that emerges from these studies is that Fourier's law is probably not valid in one and two dimensional systems, except when the system is attached to an external substrate potential. For three dimensional systems, one expects that Fourier's law is true in generic models, but it is not yet known as to what are the neccessary conditions.

Since one is addressing a conceptual issue it makes sense to start by looking at the simplest models which incorporate the important features that one believes are necessary to see normal transport. For example, one expects that for a solid, anharmonicity and disorder play important roles in determining heat transport properties. Thus most of the theoretical studies have been on these simple models, rather than on detailed models including realistic interparticle potentials, etc. The hope is that the simple models capture the important physics, and understanding them in detail is the first step towards understanding more realistic models. This review almost exclusively will talk about simple models of heat conduction in low dimensional systems, mostly one dimensional ($1D$) and some two dimensional ($2D$). Also a lot of the models that have been studied are lattice models, where heat is transported by phonons, and are relevant for understanding heat conduction in electrically insulating materials. Some work on hard particle and hard disc systems will also be reviewed.

There are two very good earlier review articles on this topic, including those by Bonetto et al. [1] and Lepri et al. [2]. Some areas that have not been covered in much detail here can be found in those reviews. Another good review, which also gives some historic perspective, is that by Jackson [3]. Apart from being an update on the older reviews, one area which has been covered extensively in this review is the use of the nonequilibrium Green's function approach for harmonic systems. This approach nicely shows the connection between results from various studies on heat transport in classical harmonic chain models, and results obtained from methods such as the Landauer formalism, which is widely used in mesoscopic

physics. As we will see, this is one of the few methods where explicit results can be obtained for the quantum case also.

The article is organized as follows. In Sec. (2), some basic definitions and a description of some of the methods used in transport studies is given. In Sec. (3), results for the harmonic lattice are given. The nonequilibrium Green's function theory will be developed using the Langevin equation approach and various applications of this method are described. The case of interacting particles ((nonharmonic inter-particle interactions) in one dimension is treated in Sec. (4). This section briefly summarizes the analytic approaches, and then gives results of the latest simulations in momentum-conserving and momentum non-conserving one dimensional systems. The next section [Sec. (5)] looks at the joint effect of disorder and interactions in one dimensional systems. In Sec. (6) results on two dimensional interacting systems are presented while Sec. (7) gives results for billiard like systems of noninteracting particles. Some of the recent experimental results on nanowires and nanotubes are discussed in Sec. (8). Finally the conclusions of the review are summarized in Sec. (9) and a list of some interesting open problems is provided.

2. Methods

The most commonly used approaches in heat transport studies have been: (i) those which look at the *nonequilibrium steady state* obtained by connecting a system to reservoirs at different temperatures, and (ii) those based on the *Green-Kubo relation* between conductivity and equilibrium correlation functions. In this section we will introduce some of the definitions and concepts necessary in using these methods [secs. (2.1,2.2)]. Apart from these two methods, an approach that has been especially useful in understanding ballistic transport in mesoscopic systems, is the nonequilibrium Green's function method and we will describe this method in sec. (2.3). Ballistic transport of electrons refers to the case where electron-electron interactions are negligible. In the present context ballistic transport means that phonon-phonon interactions can be neglected.

2.1. *Heat bath models, definitions of current, temperature and conductivity*

To study steady state heat transport in a Hamiltonian system, one has to connect it to heat reservoirs. In this section we will first discuss some commonly used models of reservoirs, and give the definitions of heat current, temperature and thermal conductivity. It turns out that there are some subtle points involved here and we will try to explain these.

First let us discuss a few models of heat baths that have been used in the literature. For simplicity we here discuss the $1D$ case since the generalization to higher dimension is straight-forward. We consider a classical $1D$ system of particles interacting through a nearest neighbour interaction potential U and which are in an external potential V. The Hamiltonian is thus:

$$H = \sum_{l=1}^{N} [\frac{p_l^2}{2m_l} + V(x_l)\ ] + \sum_{l=1}^{N-1} U(x_l - x_{l+1}) \tag{3}$$

where $\{m_l, x_l, p_l = m_l \dot{x}_l\}$ for $l = 1, 2, ...N$ denotes the masses, positions and momenta of the N particles. For the moment we will assume that the interparticle potential is such that the particles do not cross each other and so their ordering on the line is maintained.

To drive a heat current in the above Hamiltonian system, one needs to connect it to heat reservoirs. Various models of baths have been used in the literature and here we discuss three popular ones.

(i) **Langevin baths**: These are defined by adding additional force terms in the equation of motion of the particles in contact with baths. In the simplest form, the additional forces consist of a dissipative term, and a stochastic term, which is taken to be Gaussian white noise. Thus with Langevin reservoirs connected to particles $l = 1$ and $l = N$, the equations of motion are given by:

$$\begin{aligned} \dot{p}_1 &= f_1 - \frac{\gamma_L}{m_1} p_1 + \eta_L(t) \\ \dot{p}_l &= f_l \quad \text{for} \quad l = 2, 3 ... N-1 \\ \dot{p}_N &= f_N - \frac{\gamma_R}{m_N} p_N + \eta_R(t) \\ \text{where} \qquad f_l &= -\frac{\partial H}{\partial x_l} \end{aligned} \tag{4}$$

is the usual Newtonian force on the l^{th} particle. The noise terms given by $\eta_{L,R}$ are Gaussian, with zero mean, and related to the dissipation coefficients $\gamma_{L,R}$ by the usual fluctuation dissipation relations

$$\begin{aligned} \langle \eta_L(t)\eta_L(t') \rangle &= 2k_B T_L \gamma_L \delta(t-t') \\ \langle \eta_R(t)\eta_R(t') \rangle &= 2k_B T_R \gamma_R \delta(t-t') \\ \langle \eta_L(t)\eta_R(t') \rangle &= 0 \ , \end{aligned}$$

where T_L, T_R are the temperatures of the left and right reservoirs respectively.

More general Langevin baths where the noise is correlated will be described in sec. (3.2). Here we briefly discuss one particular example of a correlated bath, namely the Rubin model. This model is obtained by connecting our system of interest to two reservoirs which are each described by semi-infinite harmonic oscillator chains with Hamiltonian of the form $H_b = \sum_{l=1}^{\infty} P_l^2/2 + \sum_{l=0}^{\infty} (X_l - X_{l+1})^2/2$, where $\{X_l, P_l\}$ denote reservoir degrees of freedom and $X_0 = 0$. One assumes that the reservoirs are initially in thermal equilibrium at different temperatures and are then linearly coupled, at time $t = -\infty$, to the two ends of the system. Let us assume the coupling of system with left reservoir to be of the form $-x_1 X_1$. Then, following the methods to be discussed in sec. (3.2), one finds that the effective equation of motion of the left-most particle is a generalized Langevin equation of the form:

$$\dot{p}_1 = f_1 + \int_{-\infty}^{t} dt' \Sigma_L(t-t') x_1(t') + \eta_L(t) \ , \tag{5}$$

where the fourier transform of the kernel $\Sigma_L(t)$ is given by:

$$\begin{aligned} \tilde{\Sigma}_L(\omega) = \int_0^{\infty} dt \Sigma_L(t) e^{i\omega t} &= e^{iq} \quad \text{for} \quad |\omega| < 2 \\ &= -e^{-\nu} \quad \text{for} \quad |\omega| > 2 \ , \end{aligned}$$

and q, ν are defined through $\cos(q) = 1 - \omega^2/2$, $\cosh(\nu) = \omega^2/2 - 1$ respectively.

The noise correlations are now given by:

$$\langle \tilde{\eta}_L(\omega)\tilde{\eta}_L(\omega')\rangle = \frac{k_B T_L}{\pi\omega} Im[\tilde{\Sigma}_L(\omega)]\ \delta(\omega+\omega'), \tag{6}$$

where $\tilde{\eta}_L(\omega) = (1/2\pi)\int_{-\infty}^{\infty} dt \eta_L(t) e^{i\omega t}$. Similar equations of motion are obtained for the particle coupled to the right reservoir.

(ii) **Nosé-Hoover baths**: These are deterministic baths with *time-reversible* dynamics which however, surprisingly, have the ability to give rise to *irreversible* dissipative behaviour. In its simplest form, Nosé-Hoover baths attached to the end particles of the system described by the Hamiltonian Eq. (3), are defined through the following equations of motion for the set of particles:

$$\begin{aligned} \dot{p}_1 &= f_1 - \zeta_L p_1 \\ \dot{p}_l &= f_l \quad \text{for} \quad l = 2, 3 ... N-1 \\ \dot{p}_N &= f_N - \zeta_R p_N \ , \end{aligned} \tag{7}$$

where ζ_L and ζ_R are also dynamical variables which satisfy the following equations of motion:

$$\begin{aligned} \dot{\zeta}_L &= \frac{1}{\theta_L}\left(\frac{p_1^2}{m_1 k_B T_L} - 1\right) \\ \dot{\zeta}_R &= \frac{1}{\theta_R}\left(\frac{p_N^2}{m_N k_B T_R} - 1\right) \ , \end{aligned}$$

with θ_L and θ_R as parameters which control the strength of coupling to reservoirs.

Note that in both models (i) and (ii) of baths, we have described situations where baths are connected to *particular particles* and not located at fixed positions in space. These are particularly suited for simulations of lattice models, where particles make small displacements about equilibrium positions. Of course one could modify the dynamics by saying that particles experience the bath forces (Langevin or Nosé-Hoover type) whenever they are in a given region of space, and then these baths can be applied to fluids too. Another dynamics where the heat bath is located at a fixed position, and is particularly suitable for simulation of fluid systems, is the following:

(iii) **Maxwell baths**: Here we take particles described by the Hamiltonian Eq. (3),and moving within a closed box extending from $x = 0$ to $x = L$. The particles execute usual Hamiltonian dynamics except when any of the end particles hit the walls. Thus when particle $l = 1$ at the left end ($x = 0$) hits the wall at temperature T_L, it is reflected with a random velocity chosen from the distribution:

$$P(v) = \frac{m_1 v}{k_B T_L}\ \theta(v)\ e^{-m_1 v^2/(2k_B T_L)} \ , \tag{8}$$

where $\theta(v)$ is the Heaviside step function. A similar rule is applied at the right end.

There are two ways of defining a current variable depending on whether one is using a discrete or a continuum description. For lattice models, where every particle moves around specified lattice points, the discrete definition is appropriate. In a fluid system, where the motion of particles is unrestricted, one has to use the continuum definition. For the $1D$ hard particle gas, the ordering of particles is maintained, and in fact both definitions have been used in simulations to calculate

the steady state current. We will show here explicitly that they are equivalent. Let us first discuss the discrete definition of heat current.

For the Langevin and Nosé-Hoover baths, we note that the equation of motion has the form $\dot{p}_l = f_l + \delta_{l,1} f_L + \delta_{l,N} f_R$ where f_L and f_R are forces from the bath. The instantaneous rate at which work is done by the left and right reservoirs on the system are respectively given by:

$$j_{1,L} = f_L v_1$$
$$\text{and} \quad j_{N,R} = f_R v_N \ ,$$

and these give the instantaneous energy currents from the reservoirs into the system. To define the local energy current inside the wire we first define the local energy density associated with the l^{th} particle (or energy at the lattice site l) as follows:

$$\epsilon_1 = \frac{p_1^2}{2m_1} + V(x_1) + \frac{1}{2}U(x_1 - x_2) \ ,$$
$$\epsilon_l = \frac{p_l^2}{2m_l} + V(x_l) + \frac{1}{2}[\ U(x_{l-1} - x_l) + U(x_l - x_{l+1})\ ] \ , \quad \text{for} \ \ l = 2, 3...N-1$$
$$\epsilon_N = \frac{p_N^2}{2m_N} + V(x_N) + \frac{1}{2}U(x_{N-1} - x_N) \ . \tag{9}$$

Taking a time derivative of these equations, and after some straightforward manipulations, we get the discrete continuity equations given by:

$$\dot{\epsilon}_1 = -j_{2,1} + j_{1,L}$$
$$\dot{\epsilon}_l = -j_{l+1,l} + j_{l,l-1} \quad \text{for} \ \ l = 2, 3...N-1$$
$$\dot{\epsilon}_N = j_{N,R} + j_{N,N-1} \ , \tag{10}$$
$$\text{with} \ \ j_{l,l-1} = \frac{1}{2}(v_{l-1} + v_l) f_{l,l-1} \tag{11}$$
$$\text{and where} \quad f_{l,l+1} = -f_{l+1,l} = -\partial_{x_l} U(x_l - x_{l+1})$$

is the force that the $(l+1)^{\text{th}}$ particle exerts on the l^{th} particle and $v_l = \dot{x}_l$. From the above equations one can identify $j_{l,l-1}$ to be the energy current from site $l-1$ to l. The steady state average of this current can be written in a slightly different form which has a clearer physical meaning. We will denote steady state average of any physical quantity A by $\langle A \rangle$. Using the fact that $\langle dU(x_{l-1} - x_l)/dt \rangle = 0$ it follows that $\langle v_{l-1} f_{l,l-1} \rangle = \langle v_l f_{l,l-1} \rangle$ and hence:

$$\langle j_{l,l-1} \rangle = \langle \frac{1}{2}(v_l + v_{l-1}) f_{l,l-1} \rangle = \langle v_l f_{l,l-1} \rangle \ , \tag{12}$$

and this has the simple interpretation as the average rate at which the $(l-1)^{\text{th}}$ particle does work on the l^{th} particle. In the steady state, from Eq. (10), we get the equality of current flowing between any neighbouring pair of particles:

$$J = \langle j_{1,L} \rangle = \langle j_{2,1} \rangle = \langle j_{3,2} \rangle = ... \langle j_{N,N-1} \rangle = -\langle j_{N,R} \rangle \ , \tag{13}$$

where we have used the notation J for the steady state energy current per bond. In simulations one can use the above definition, which involves no approximations,

and a good check of convergence to steady state is to verify the above equality on all bonds. In the case where interaction is in the form of hard particle collisions we can write the expression for steady state current in a different form. Replacing the steady state average by a time average we get:

$$\langle j_{l,l-1}\rangle = \langle v_l f_{l,l-1}\rangle = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau dt v_l(t) f_{l,l-1}(t) = \lim_{\tau\to\infty}\frac{1}{\tau}\sum_{t_c}\Delta K_{l,l-1}\ , \quad (14)$$

where t_c denotes time instances at which particles l and $(l-1)$ collide and $\Delta K_{l,l-1}$ is the change in energy of the $l^{\rm th}$ particle as a result of the collision.

Next we discuss the continuum definition of current which is more appropriate for fluids but is of general validity. We will discuss it for the case of Maxwell boundary conditions with the system confined in a box of length L. Let us define the local energy density at position x and at time t as:

$$\epsilon(x,t) = \sum_{l=1}^{N}\epsilon_l\ \delta[x - x_l(t)]\ , \quad (15)$$

where ϵ_l is as defined in Eq. (9). Taking a time derivative we get the required continuum continuity equation in the form (for $0 < x < L$):

$$\frac{\partial\epsilon(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = j_{1,L}\delta(x) + j_{N,R}\delta(x-L) \quad (16)$$

where $j(x,t) = j_K(x,t) + j_I(x,t)$

with $j_K(x,t) = \sum_{l=1}^{N}\epsilon_l(t)v_l(t)\delta[x - x_l(t)]$

and $j_I(x,t) = \sum_{l=2}^{N-1}(j_{l+1,l} - j_{l,l-1})\ \theta[x - x_l(t)] + j_{2,1}\theta[x - x_1(t)] - j_{N,N-1}\theta[x - x_N(t)]\ .$

Here $j_{l,l-1},\ j_{1,L},\ j_{N,R}$ are as defined earlier in the discrete case, and we have written the current as a sum of two parts, j_K and j_I, whose physical meaning we now discuss. To see this, consider a particle configuration with $x_1, x_2, ...x_k < x < x_{k+1}, x_{k+2}, ...x_N$. Then we get

$$j_I(x,t) = j_{k+1,k}$$

which is thus simply the rate at which the particles on the left of x do work on the particles on the right. Hence we can interpret $j_I(x,t)$ as the contribution to the current density coming from interparticle interactions. The other part $j_K(x,t)$ arises from the physical flow of particles carrying energy across the point x. Note, however, that even in the absence of any net convection particle flow, both j_K and j_I can contribute to the energy flow. In fact for point particles interacting purely by hard elastic collisions $j_{k+1,k}$ is zero whenever the $k^{\rm th}$ and $(k+1)^{\rm th}$ particles are on the two sides of the point x and hence j_I is exactly zero. The only contribution to the energy current then comes from the part j_K and we thus for the steady-state current we obtain

$$\langle j(x,t)\rangle = \sum_{l=1}^{N}\langle\frac{m_l v_l^3}{2}\ \delta(x - x_l)\rangle\ . \quad (17)$$

In simulations either of expressions Eq. (14) or Eq. (17) can be used to evaluate the steady state current and will give identical results. For hard particle simulations one often uses a simulation which updates between collisions and in this case it is more efficient to evaluate the current using Eq. (14). We now show that, in the nonequilibrium steady state, the average current from the discrete and continuum definitions are the same, *i.e.* ,

$$\langle j_{l,l-1} \rangle = \langle j(x,t) \rangle = J \ . \tag{18}$$

Note that the steady state current is independent of l or x. To show this we first define the total current as:

$$\begin{aligned} \mathcal{J}(t) &= \int_0^L dx j(x,t) = \sum_{l=1,N} \epsilon_l v_l - \sum_{l=2,N-1} x_l (j_{l+1,l} - j_{l,l-1}) - x_1 j_{2,1} + x_N j_{N,N-1} \\ &= \sum_{l=1,N} \epsilon_l v_l + \sum_{l=1,N-1} (x_{l+1} - x_l) j_{l+1,l} \ . \end{aligned} \tag{19}$$

Taking the steady-state average of the above equation and using the fact that $\langle \epsilon_l v_l \rangle = -\langle \dot{\epsilon}_l x_l \rangle = \langle (j_{l+1,l} - j_{l,l-1}) x_l \rangle$, where $j_{1,0} = j_{1,L}, j_{N+1,N} = -j_{N,R}$ we get:

$$\langle \mathcal{J} \rangle = -\langle x_1 j_{1L} + x_N j_{NR} \rangle \ .$$

Since the Maxwell baths are located at $x = 0$ and $x = L$, the above then gives $\langle \mathcal{J} \rangle = L \langle j(x,t) \rangle = -L \langle j_{NR} \rangle$ and hence from Eq. (13), we get $\langle j(x,t) \rangle = J = \langle j_{l,l-1} \rangle$, which proves the equivalence of the two definitions.

The extensions of the current definitions, both the discrete and continuum versions, to higher dimensions is straightforward. Here, for reference, we outline the derivation for the continuum case since it is not easy to see a discussion of this in the literature. Consider a system in d-dimensions with Hamiltonian given by:

$$H = \sum_l \left[\ \frac{\mathbf{p}_l^2}{2m_l} + V(\mathbf{x}_l) \ \right] + \frac{1}{2} \sum_{l \neq n} \sum_n U(r_{ln}) \ , \tag{20}$$

where $\mathbf{x}_l = (x_l^1, x_l^2, ...x_l^d)$ and $\mathbf{p}_l = (p_l^1, p_l^2, ...p_l^d)$ are the vectors denoting the position and momentum of the l^{th} particle and $r_{ln} = |\mathbf{x}_l - \mathbf{x}_n|$. The particles are assumed to be inside a hypercubic box of volume L^d. As before we define the local energy density as:

$$\begin{aligned} \epsilon(\mathbf{x},t) &= \sum_l \delta(\mathbf{x} - \mathbf{x}_l) \epsilon_l \quad \text{where} \\ \epsilon_l &= \frac{\mathbf{p}_l^2}{2m_l} + V(\mathbf{x}_l) + \frac{1}{2} \sum_{n \neq l} U(r_{ln}) \ . \end{aligned}$$

Taking a derivative with respect to time (and suppressing the source terms arising

from the baths) gives:

$$\frac{\partial \epsilon(\mathbf{x},t)}{\partial t} = -\sum_{\alpha=1}^{d}\left[\frac{\partial}{\partial x_\alpha}\sum_l \delta(\mathbf{x}-\mathbf{x}_l)\ \epsilon_l v_l^\alpha\right] \ + \ \sum_l \delta(\mathbf{x}-\mathbf{x}_l)\dot{\epsilon}_l \qquad (21)$$
$$= -\sum_\alpha \frac{\partial}{\partial x^\alpha}[\ j_\alpha^K + j_\alpha^I\ ]\ ,$$

where

$$j_K^\alpha(\mathbf{x},t) = \sum_i \delta(\mathbf{x}-\mathbf{x}_l)\ \epsilon_l\ v_l^\alpha$$
$$\text{and}\ \ j_I^\alpha(\mathbf{x},t) = -\sum_l\sum_{n\neq l}\theta(x^\alpha - x_l^\alpha)\prod_{\nu\neq\alpha}\delta(x^\nu - x_l^\nu)\ j_{l,n} \qquad (22)$$
$$\text{where}\ \ j_{l,n} = \frac{1}{2}\sum_\nu(\ v_l^\nu + v_n^\nu\ )\ f_{l,n}^\nu\ ,$$

and $f_{l,n}^\alpha = -\partial U(r_{l,n})/\partial x_l^\alpha$ is the force, in the α^{th} direction, on the l^{th} particle due to the n^{th} particle. We have defined $j_{l,n}$ as the current, from particle n to particle l, analogously to the discrete $1D$ current. The part j_I^α gives the energy flow as a result of physical motion of particles across x^α. The part j_I^α also has a simple physical interpretation, as in the $1D$ case. First note that we need to sum over only those n for which $x_n^\alpha < x^\alpha$. Then the formula basically gives us the net rate, at which work is done, by particles on the left of x^α, on the particles to the right. This is thus the rate at which energy flows from left to right. By integrating the current density over the full volume of the system, we get the total current:

$$\mathcal{J}^\alpha(t) = \sum_l \epsilon_l v_l^\alpha + \frac{1}{2}\sum_{l\neq n}\sum_n (x_l^\alpha - x_n^\alpha)\ j_{l,n}\ . \qquad (23)$$

Thus we get an expression similar to that in $1D$ given by Eq. (19). In simulations making nonequilibrium measurements, any of the various definitions for current can be used to find the steady state current. However, it is not clear whether other quantities, such as correlation functions obtained from the discrete and continuum definitions, will be the same.

The local temperature can also be defined using either a discrete approach (giving T_l) or a continuum approach (giving $T(\mathbf{x},t)$). In the steady state these are respectively given by (in the $1D$ case):

$$k_B T_l = \left\langle \frac{p_l^2}{m_l}\right\rangle$$
$$k_B T(x) = \frac{\langle \sum_l \frac{p_l^2}{m_l}\delta(x-x_l)\rangle}{\langle \sum_l \delta(x-x_l)\rangle} \qquad (24)$$

Again it is not obvious that these two definitions will always agree. Lattice simulations usually use the discrete definition while hard particle simulations use the continuum definition.

The precise definition of thermal conductivity would be:

$$\kappa = \lim_{L\to\infty} \lim_{\Delta T\to 0} \frac{JL}{\Delta T} \ , \tag{25}$$

where $\Delta T = T_L - T_R$. In general κ would depend on temperature T. The finiteness of $\kappa(T)$, along with Fourier's law, implies that even for arbitrary fixed values of T_L, T_R the current J would scale as $\sim L^{-1}$ (or N^{-1}). What is of real interest is this scaling property of J with system size. We will typically be interested in the large N behaviour of the conductivity defined as:

$$\kappa_N = \frac{JN}{\Delta T} \ , \tag{26}$$

which will usually be denoted by κ. For large N, systems with normal diffusive transport give a finite κ while anomalous transport refers to the scaling

$$\kappa \sim N^{\alpha} \qquad \alpha \neq 0 \ , \tag{27}$$

and the value of the heat conduction exponent α is one of the main objects of interest. For the current, this implies $J \sim N^{\alpha-1}$.

The only examples where the steady state current can be analytically evaluated, and exact results are available for the exponent α, corresponds to harmonic lattices, using very specific methods that will be discussed in sec. (3).

Coupling to baths and contact resistance: In the various models of heat baths that we have discussed, the efficiency with which heat exchange takes place between reservoirs and system depends on the strength of coupling constants. For example, for the Langevin and Nosé-Hoover baths, the parameters γ and θ respectively determine the strength of coupling (for the Maxwell bath one could introduce a parameter which gives the probability that after a collision the particle's speed changes and this can be used to tune the coupling between system and reservoir). From simulations it is found that typically there is an optimum value of the coupling parameter for which energy exchange takes place most efficiently, and at this value one gets the maximum current for given system and fixed bath temperatures. For too high or too small values of the coupling strength the current is small. The coupling to bath can be thought of as giving rise to a contact resistance. An effect of this resistance is to give rise to boundary jumps in the temperature profile measured in simulations. One expects that these jumps will be present as long as the contact resistance is comparable to the systems resistance. We will later see that in order to be sure that one is measuring the true resistance of the system, it is necessary to be in parameter regimes where the contact resistances can be neglected.

2.2. *Green-Kubo Formula*

The Green-Kubo formula provides a relation between transport coefficients, such as the thermal conductivity κ or the electrical conductivity σ, and *equilibrium* time correlation functions of the corresponding current. For the thermal conductivity in a classical $1D$ system, the Green-Kubo formula gives:

$$\kappa = \frac{1}{k_B T^2} \lim_{\tau\to\infty} \lim_{L\to\infty} \frac{1}{L} \int_0^{\tau} dt \langle \mathcal{J}(0)\mathcal{J}(t)\rangle \ , \tag{28}$$

where $\mathcal{J}$ is the total current as defined in Eq. (19) and $\langle ... \rangle$ denotes an average over initial conditions chosen from either a micro-canonical ensemble or a canonical one at temperature T. Two important points to be remembered with regard to use of the above Green-Kubo formula are the following:

(i) It is often necessary to subtract a convective part from the current definition or, alternatively, in the microcanonical case one can work with initial conditions chosen such that the centre of mass velocity is zero (see also discussions in [7, 8]). To understand this point, let us consider the case with $V(\mathbf{x}) = 0$. Then for a closed system that is not in contact with reservoirs, we expect the time average of the total current to vanish. But this is true only if we are in the centre of mass frame. If the centre of mass is moving with velocity $\mathbf{v}$ then the average velocity of any particle $\langle \mathbf{v}_l \rangle = \mathbf{v}$. Transforming to the moving frame let us write $\mathbf{v}_l = \mathbf{v}'_l + \mathbf{v}$. Then the average total current in the rest frame is given by (in d-dimensions):

$$\langle \mathcal{J}^\alpha \rangle = \left[\frac{M}{2}\mathbf{v}^2 + \sum_l \langle \epsilon'_l \rangle \right] v^\alpha + \sum_\nu \left[\sum_l \langle m_l v_l'^\alpha v_l'^\nu \rangle + \frac{1}{2} \sum_{\substack{l,n \\ l \neq n}} \langle \ (x_l^\alpha - x_n^\alpha) \ f_{l,n}^\nu \ \rangle \right] v^\nu$$

$$= (E + PV) \ v^\alpha \ , \tag{29}$$

where $M = \sum m_l$ and E is the average total energy of the system as measured in the rest frame and $V = L^d$. In deriving the above result we have used the standard expression for equilibrium stress-tensor given by:

$$V\sigma_{\alpha\nu} = \sum \langle m_l v_l'^\alpha v_l'^\nu \rangle + \frac{1}{2} \sum_{l \neq n} \langle \ (x_l^\alpha - x_n^\alpha) \ f_{l,n}^\nu \ \rangle \ \ , \tag{30}$$

and assumed an isotropic medium. Thus, in general, to get the true energy current in an arbitrary equilibrium ensemble one should use the expression:

$$\mathcal{J}_c^\alpha = \mathcal{J}^\alpha - (E + PV) v^\alpha \ . \tag{31}$$

The corresponding form in $1D$ should be used to replace $\mathcal{J}$ in Eq. (28).

(ii) The second point to note is that in Eq. (28) the order of limits $L \to \infty$ *and then* $\tau \to \infty$ has to be strictly maintained. In fact for a system of particles inside a finite box of length L it can be shown exactly that:

$$\int_0^\infty dt \langle \mathcal{J}_c(0) \mathcal{J}_c(t) \rangle = 0 \ . \tag{32}$$

To prove this, let us consider a microcanonical ensemble (with $\langle \mathcal{J} \rangle = 0$, so that $\mathcal{J}_c = \mathcal{J}$), in which case from Eq. (19) we get:

$$\mathcal{J}(t) = \frac{d}{dt} \left[\sum_{l=1}^N \epsilon_l(t) x_l(t) \right] \ . \tag{33}$$

Multiplying both sides of the above equation by $\mathcal{J}(0)$, integrating over t and noting that both the boundary terms on the right hand side vanish, we get the required result in Eq. (32). With the correct order of limits in Eq. (28), one can calculate the correlation functions with arbitrary boundary conditions and apply the formula to obtain the response of an open system with reservoirs at the ends.

Derivation of the Green-Kubo formula for thermal conductivity: There have been a number of derivations of this formula by various authors including Green, Kubo, Mori, McLennan, Kadanoff and Martin, Luttinger, and Visscher [4, 5, 6, 7, 8, 9, 10, 11, 12]. None of these derivations are rigorous and all require certain assumptions. Luttinger's derivation was an attempt at a mechanical derivation and involves introducing a fictitious 'gravitational field' which couples to the energy density and drives an energy current. However one now has to relate the response of the system to the field and its response to imposed temperature gradients. This requires additional inputs such as use of the Einstein relation relating diffusion coefficient (or thermal conductivity) to the response to the gravitational field. We believe that this derivation, as is also the case for most other derivations , implicitly assumes local thermal equilibrium. Although these derivations are not rigorous, they are quite plausible, and it is likely that the assumptions made are satisfied in a large number of cases of practical interest. Thus the wide use of the Green-Kubo formula in calculating thermal conductivity and transport properties of different systems is possibly justified in many situations.

Here we give an outline of a non-mechanical derivation of the Green-Kubo formula, one in which the assumptions can be somewhat clearly stated and their physical basis understood. The assumptions we will make here are:

(a) The nonequilibrium state with energy flowing in the system can be described by coarse-grained variables and the condition of local thermal equilibrium is satisfied.

(b) There is no particle flow, and energy current is equal to heat current. The energy current satisfies Fourier's law which we write in the form $J(x,t) = -D\partial u(x,t)/\partial x$ where $D = \kappa/c$, c is the specific heat capacity, and $u(x,t) = \bar{\epsilon}(x,t)$, $J(x,t) = \bar{j}(x,t)$ are macroscopic variables obtained by a coarse-graining (indicated by bars) of the microscopic fields.

(c) Finally, we assume that regression of equilibrium energy fluctuations occurs in the same way as nonequilibrium flow of energy.

We consider a macroscopic system of size L. Fluctuations in energy density in equilibrium can be described by the correlation function $S(x,t) = \langle \epsilon(x,t)\epsilon(0,0)\rangle - \langle \epsilon(x,t)\rangle \langle \epsilon(0,0)\rangle$. Assumption (c) above means that the decay of these fluctuations is determined by the heat diffusion equation and given by:

$$\frac{\partial S(x,t)}{\partial t} = D\frac{\partial^2 S(x,t)}{\partial x^2} \qquad \text{for} \quad t > 0 \ ,$$

where we have also assumed temperature fluctuations to be small enough so that the temperature dependence of D can be neglected. From time reversal invariance we have $S(x,t) = S(x,-t)$. Using this and the above equation we get:

$$\tilde{S}(k,\omega) = \int_{-\infty}^{\infty} dt \hat{S}(k,t) e^{-i\omega t} = \frac{2Dk^2 \hat{S}(k,t=0)}{D^2k^4 + \omega^2} \ ,$$

where $\hat{S}(k,t) = \int_{-\infty}^{\infty} dx S(x,t) e^{ikx}$. Now, from equilibrium statistical mechanics we have $\hat{S}(k=0,t=0) = ck_BT^2$ and using this in the above equation we obtain:

$$\kappa = cD = \frac{1}{2k_BT^2} \lim_{\omega\to 0}\lim_{k\to 0} \frac{\omega^2}{k^2}\tilde{S}(k,\omega) \ . \tag{34}$$

One can relate the energy correlator to the current correlator using the continuity

equation $\partial\epsilon(x,t)/\partial t + \partial j(x,t)/\partial x = 0$ and this gives:

$$\langle\tilde{j}(k,\omega)\tilde{j}(k',\omega')\rangle = (2\pi)^2\frac{\omega^2}{k^2}\tilde{S}(k,\omega)\ \delta(k+k')\delta(\omega+\omega')\ ,$$

where $\tilde{j}(k,\omega) = \int_{-\infty}^{\infty} dxdtj(x,t)e^{i(kx-\omega t)}$. Integrating the above equation over k' gives:

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dt\ \langle j(x,t)j(0,0)\rangle\ e^{i(kx-\omega t)} = \frac{\omega^2}{k^2}\tilde{S}(k,\omega)\ . \tag{35}$$

From Eq. (34) and Eq. (35) we then get:

$$\kappa = \lim_{\omega\to 0}\lim_{k\to 0}\frac{1}{2k_BT^2}\int_{-\infty}^{\infty} dx\ \int_{-\infty}^{\infty} dt\ \langle j(x,t)j(0,0)\rangle\ e^{i(kx-\omega t)}\ . \tag{36}$$

Finally, using time-reversal and translational invariance and interpreting the $\omega \to 0,\ k \to 0$ limits in the alternative way (as $\tau \to \infty,\ L \to \infty$) we recover the Green-Kubo formula in Eq. (28) .

Limitations on use of the Green-Kubo formula: There are several situations where the Green-Kubo formula in Eq. (28) is not applicable. For example, for the small structures that are studied in mesoscopic physics, the thermodynamic limit is meaningless, and one is interested in the conductance of a specific finite system. Secondly, in many low dimensional systems, heat transport is anomalous and the thermal conductivity diverges. In such cases it is impossible to take the limits as in Eq. (28); one is there interested in the thermal conductance as a function of L instead of an L-independent thermal conductivity. The usual procedure that has been followed in the heat conduction literature is to put a cut-off at $t_c \sim L$, in the upper limit in the Green-Kubo integral [2]. The argument is that for a finite system connected to reservoirs, sound waves traveling to the boundaries at a finite speed, say v, lead to a decay of correlations in a time $\sim L/v$. However there is no rigorous justification of this assumption. A related case is that of integrable systems, where the infinite time limit of the correlation function in Eq. (28) is non-zero.

Another way of using the Green-Kubo formula for finite systems is to include the infinite reservoirs also while applying the formula and this was done, for example, by Allen and Ford [13] for heat transport and by Fisher and Lee [14] for electron transport. Both these cases are for non-interacting systems and the final expression for conductance (which is more relevant than conductivity in such systems) is basically what one also obtains from the Landauer formalism [15], or the nonequilibrium Green's function approach [see sec. (2.3)].

It has been shown that Green-Kubo like expressions for the linear response heat current for finite open systems can be derived rigorously by using the steady state fluctuation theorem [16, 17, 18, 19, 20, 21, 22]. This has been done for lattice models coupled to stochastic Markovian baths and the expression for linear response conductance of a one dimensional chain is given as:

$$\lim_{\Delta T\to 0}\frac{J}{\Delta T} = \frac{1}{k_BT^2}\int_0^{\infty}\langle j_l(0)j_l(t)\rangle\ , \tag{37}$$

where j_l is the discrete current defined in sec. (2.1). Some of the important differences of this formula with the usual Green-Kubo formula are worth keeping in mind: (i) the dynamics of the system here is non-Hamiltonian since they are for a system coupled to reservoirs, (ii) one does not need to take the limit $N \to \infty$ first,

the formula being valid for a finite system, (iii) the discrete bond current appears here, unlike the continuum one in the usual Green-Kubo formula. Recently, an exact linear response result similar to Eq. (37), for the conductance of a finite open system has been derived using a different approach [23]. This has been done for quite general classical Hamiltonian systems and for a number of implementations of heat baths.

It appears that the linear response formula given by Eq. (37) is the correct one to use to evaluate the conductance in systems where there is a problem with the usual Green-Kubo formula, *e.g.* in finite systems or low dimensional systems showing anomalous transport (because of slow decay of $\langle \mathcal{J}(0)\mathcal{J}(t)\rangle$. We note here the important point that the current-current correlation can have very different scaling properties, for a purely Hamiltonian dynamics, as compared to a heat bath dynamics. This has been seen in simulations by Deutsche and Narayan [24] for the random collision model [defined in sec. (4.2.1)]. Of course this makes things somewhat complicated since the usefulness of the Green-Kubo formalism arises from the fact that it allows a calculation of transport properties from equilibrium properties of the system, and without any reference to heat baths, etc. In fact, as we will see in sec. (4.1), all the analytic results for heat conduction in interacting one dimensional systems rely on Eq. (28) and involve a calculation of the current-current correlator for a closed system. Some of the simulation results discussed later suggest that, for interacting (nonlinearly) systems, in the limit of large system size the heat current is independent of details of the heat baths. This means that, in the linear response regime and the limit of large system sizes, a description which does not take into account bath properties may still be possible.

2.3. *Nonequilibrium Green's function method*

The nonequilibrium Green's function method (NEGF) is a method, first invented in the context of electron transport, to calculate steady state properties of a finite system connected to reservoirs which are themselves modeled by noninteracting Hamilitonians with infinite degrees of freedom [46, 47, 48]. Using the Keldysh formalism, one can obtain formal expressions for the current and other observables such as electron density, in models of electrons such as those described by tight-binding type Hamiltonians. Recently this approach has been applied both to phonon [50, 51] and photon [55, 56] transport.

The main idea in the formalism is as follows. One starts with an initial density matrix describing the decoupled system, and two infinite reservoirs which are in thermal equilibrium, at different temperatures and chemical potentials. The system and reservoirs are then coupled together and the density matrix is evolved with the full Hamiltonian for an infinite time so that one eventually reaches a nonequilibrium steady state. Various quantitites of interest such as currents and local densities, etc can be obtained using the steady state density matrix and can be written in terms of the so called Keldysh Green's functions. An alternative and equivalent formulation is the Langevin approach where, instead of dealing with the density matrix, or in the classical case with the phase space density, one works with equations of motion of the phase space variables of the full Hamiltonian (system plus reservoirs). Again the reservoirs, which are initially in thermal equilibrium, are coupled to the system in the remote past. It is then possible to integrate out the reservoir degrees of freedom, and these give rise to generalized Langevin terms in the equation of motion. For non-interacting systems, one can show that it is possible to recover all the results of NEGF exactly, both for electrons and phonons. Here we will discuss this approach for the case of phonons, and describe the main results that have been

obtained [sec. (3.2)].

For non-interacting systems, the formal expressions for current obtained from the NEGF approach is in terms of transmission coefficients of the heat carriers (electrons, phonons or photons) across the system, with appropriate weight factors corresponding to the population of modes in the reservoirs. These expressions are basically what one also obtains from the Landauer formalism [15]. We note that in the Landauer approach one simply thinks of transport as a transmission problem and the current across the system is obtained directly using this picture. In the simplest set-up one thinks of one-dimensional reservoirs (leads) filled with non-interacting electrons at different chemical potentials. On connecting the system in between the reservoirs, electrons are transmitted through the system from one reservoir to the other. The net current in the system is then the sum of the currents from left-moving and right-moving electron states from the two reservoirs respectively.

3. Heat conduction in harmonic lattices

The harmonic crystal is a good starting point for understanding heat transport in solids. Indeed in the equilibrium case we know that studying the harmonic crystal already gives a good understanding of, for example, the specific heat of an (electrically) insulating solid. In the nonequilibrium case, the problem of heat conduction in a classical one dimensional harmonic crystal was studied for the first time by Rieder, Lebowitz and Lieb (RLL) [25]. They considered the case of stochastic Markovian baths and were able to obtain the steady state exactly. The main results of this paper were: (i) the temperature in the bulk of the system was constant and equal to the mean of the two bath temperatures, (ii) the heat current approaches a constant value for large system sizes and an exact expression for this was obtained. These results can be understood physically when one realizes that in the ordered crystal, heat is carried by freely propagating phonons. RLL considered the case where only nearest neighbour interparticle interactions were present. Nakazawa (NK) [26] extended these results to the case with a constant onsite harmonic potential at all sites and also to higher dimensions. The approach followed in both the RLL and NK papers was to obtain the exact nonequilibrium stationary state measure which, for this quadratic problem, is a Gaussian distribution. A complete solution for the correlation matrix was obtained and from this one could obtain both the steady state temperature profile and the heat current.

In sec. (3.1) we will briefly describe the RLL formalism. In sec. (3.2) we will describe a different and more powerful formalism. This is the Langevin equation and nonequilibrium Green's function method and various applications of this will be discussed in secs. (3.3,3.4,3.5).

3.1. *The Rieder-Lebowitz-Lieb method*

Let us consider a classical harmonic system of N particles with displacements about the equilibrium positions described by the vector $X = \{x_1, x_2, ...x_N\}^T$, where T denotes transpose. The particles can have arbitrary masses and we define a diagonal matrix $\hat{M}$ whose diagonal elements $M_{ll} = m_l$, for $l = 1, 2...N$, give the masses of the particles. The momenta of the particles are given by the vector $P = (M\dot{X}) = \{p_1, p_2, ...p_N\}^T$. We consider the following harmonic Hamiltonian for

the system:

$$H = \frac{1}{2}P^T\hat{M}^{-1}P + \frac{1}{2}X^T\hat{\Phi}X \ , \tag{38}$$

where $\hat{\Phi}$ is the force matrix. Let us consider the general case where the l^{th} particle is coupled to a white noise heat reservoir at temperature T_l^B with a coupling constant γ_l. The equations of motion are given by:

$$\begin{aligned} \dot{x}_l &= \frac{p_l}{m_l} \\ \dot{p}_l &= -\sum_n \Phi_{ln}x_n - \frac{\gamma_l}{m_l}p_l + \eta_l \quad \text{for} \ \ l = 1, 2...N \end{aligned} \tag{39}$$

with the noise terms satisfying the usual fluctuation dissipation relations

$$\langle \eta_l(t)\eta_n(t')\rangle = 2\gamma_l k_B T_l^B \delta_{l,n}\delta(t-t') \ . \tag{40}$$

Defining new variables $q = \{q_1, q_2...q_{2N}\}^T = \{x_1, x_2...x_N, p_1, p_2...p_N\}^T$ we can rewrite Eqs. (39,40) in the form:

$$\begin{aligned} \dot{q} &= -\hat{A}\ q + \eta \\ \langle \eta(t)\eta^T(t')\rangle &= \hat{D}\delta(t-t') \end{aligned} \tag{41}$$

where the $2N$ dimensional vector $\eta^T = (0, 0, ..0, \eta_1, \eta_2...\eta_N)$ and the $2N \times 2N$ matrices $\hat{A}, \hat{D}$ are given by:

$$\hat{A} = \begin{pmatrix} 0 & -\hat{M}^{-1} \\ \hat{\Phi} & \hat{M}^{-1}\hat{\Gamma} \end{pmatrix} \qquad \hat{D} = \begin{pmatrix} 0 & 0 \\ 0 & \hat{E} \end{pmatrix}$$

and $\hat{\Gamma}$ and $\hat{E}$ are $N \times N$ matrices with elements $\Gamma_{ln} = \gamma_l\delta_{l,n}$, $E_{ln} = 2k_BT_l^B\gamma_l\delta_{ln}$ respectively. In the steady state, time averages of total time derivatives vanish, hence we have $\langle d(qq^T)/dt\rangle = 0$. From Eq. (41) we get

$$\begin{aligned} \langle \frac{d}{dt}(qq^T)\rangle &= \langle (-\hat{A}q + \eta)q^T + q(-q^T\hat{A}^T + \eta^T)\rangle \\ &= -\hat{A}.\hat{B} - \hat{B}.\hat{A}^T + \langle \eta q^T + q\eta^T\rangle = 0 \end{aligned} \tag{42}$$

where $\hat{B}$ is the correlation matrix $\langle qq^T\rangle$. To find the average of the term involving noise we first write the formal solution of Eq. 41:

$$q(t) = \hat{G}(t-t_0)q(t_0) + \int_{t_0}^{t} dt'\hat{G}(t-t')\eta(t') \quad \text{where} \quad \hat{G}(t) = e^{-\hat{A}t}. \tag{43}$$

Setting $t_0 \to -\infty$ and assuming $\hat{G}(\infty) = 0$ (so that a unique steady state exists), we get $q(t) = \int_{-\infty}^{t} dt' \hat{G}(t-t')\eta(t')$ and hence

$$\begin{aligned} \langle q\eta^T \rangle &= \int_{-\infty}^{t} dt' \hat{G}(t-t') \langle \eta(t')\eta^T(t) \rangle \\ &= \int_{-\infty}^{t} dt' \hat{G}(t-t')\hat{D}\delta(t-t') = \frac{1}{2}\hat{D} \end{aligned} \tag{44}$$

where we have used the noise correlations given by Eq. (40), and the fact that $\hat{G}(0) = \hat{I}$, a unit matrix. Using Eq. (44) in Eq. (42), we finally get

$$\hat{A}.\hat{B} + \hat{B}.\hat{A}^T = \hat{D} \tag{45}$$

The solution of this equation gives the steady state correlation matrix $\hat{B}$ which completely determines the steady state since we are dealing with a Gaussian process. In fact the steady state is given by the Gaussian distribution

$$P(\{q_l\}) = (2\pi)^{-N} Det[\hat{B}]^{-1/2} e^{-\frac{1}{2}q^T \hat{B}^{-1} q} \ . \tag{46}$$

Some of the components of the matrix equation Eq. (45) have simple physical interpretations. To see this we first write $\hat{B}$ in the form

$$\hat{B} = \begin{pmatrix} \hat{B}_x & \hat{B}_{xp} \\ \hat{B}_{xp}^T & \hat{B}_p \end{pmatrix}$$

where $\hat{B}_x$, $\hat{B}_p$ and $\hat{B}_{xp}$ are $N \times N$ matrices with elements $(\hat{B}_x)_{ln} = \langle x_l x_n \rangle$, $(\hat{B}_p)_{ln} = \langle p_l p_n \rangle$ and $(\hat{B}_{xp})_{ln} = \langle x_l p_n \rangle$. From Eq. (45) we then get the set of equations:

$$\hat{M}^{-1}\hat{B}_{xp}^T + \hat{B}_{xp}\hat{M}^{-1} = 0 \tag{47}$$

$$\hat{B}_x\hat{\Phi}^T - \hat{M}^{-1}\hat{B}_p + \hat{B}_{xp}\hat{M}^{-1}\hat{\Gamma} = 0 \tag{48}$$

$$\hat{M}^{-1}\hat{\Gamma}\hat{B}_p + \hat{B}_p\hat{\Gamma}\hat{M}^{-1} + \hat{\Phi}\hat{B}_{xp} + \hat{B}_{xp}^T\hat{\Phi} = \hat{E} \tag{49}$$

From Eq. 47 we get the identity $\langle x_l p_n/m_n \rangle = -\langle x_n p_l/m_l \rangle$. Thus $\langle x_l p_l \rangle = 0$. The diagonal terms in Eq. 48 give

$$\begin{aligned} &\sum_n \langle x_l(\Phi_{ln}x_n) \rangle - \frac{1}{m_l}\langle p_l^2 \rangle + \langle x_l p_l \rangle \frac{\gamma_l}{m_l} = 0 \\ &\Rightarrow \langle x_l \frac{\partial H}{\partial x_l} \rangle = \langle \frac{p_l^2}{m_l} \rangle = k_B T_l \end{aligned}$$

where we have defined the local temperature $k_B T_l = \langle p_l^2/m_l \rangle$. This equation has the form of the 'equipartition' theorem of equilibrium physics. It is in fact valid quite generally for any Hamiltonian system at all bulk points and simply follows from the fact that $\langle (d/dt) x_l p_l \rangle = 0$. Finally let us look at the diagonal elements of Eq. 49. This gives the equation

$$\sum_n \langle (\Phi_{ln}x_n)\frac{p_l}{m_l} \rangle = \frac{\gamma_l}{m_l} k_B (T_l^B - T_l) \tag{50}$$

which again has a simple interpretation. The right hand can be seen to be equal to $\langle(-\gamma_l p_l/m_l + \eta_l)p_l/m_l\rangle$ which is simply the work done on the lth particle by the heat bath attached to it (and is thus the heat input at this site). On the left hand side $\langle(-\Phi_{ln}x_n)p_l/m_l\rangle$ is the rate at which the $n^{\rm th}$ particle does work on the $l^{\rm th}$ particle and is therefore the energy current from site n to site l. The left side is thus is just the sum of the outgoing energy currents from the lth site to all the sites connected to it by $\hat{\Phi}$. Thus we can interpret Eq. (50) as an energy-conservation equation. The energy current between two sites is given by

$$J_{n\to l} = -\langle(\Phi_{ln}x_n)\frac{p_l}{m_l}\rangle \ . \tag{51}$$

Our main interests are in computing the temperature profile and the energy current in the steady state. This requires solution of Eq. (45) and this is quite difficult and has been achieved only in a few special cases. For the one-dimensional ordered harmonic lattice, RLL were able to solve the equation exactly and obtain both the temperature profile and the current. The extension of their solution to higher dimensional lattices is straightforward and was done by Nakazawa. More recently Bonetto et al [67] have used this approach to solve the case with self-consistent reservoirs attached at all the bulk sites of a ordered harmonic lattice.

A numerical solution of Eq. (45) requires inversion of a $N(2N+1)\times N(2N+1)$ matrix which restricts one to rather small system sizes. The RLL approach is somewhat restrictive since it is not easily generalizable to other kinds of heat baths or to the quantum case. Besides, except for the ordered lattice, it is difficult to obtain useful analytic results from this approach. In the next section we discuss a different approach which is both analytically more tractable, as well as numerically more powerful.

3.2. *Langevin equations and Green's function (LEGF) formalism*

This approach involves a direct solution of generalized Langevin equations. Using this solution one can evaluate various quantities of interest such as steady state current and temperature profiles. Compact formal expressions for various quantities of interest can be obtained and, as pointed out earlier, it turns out that these are identical to results obtained by the nonequilibrium Green's function (NEGF) method described in sec. (2.3). The method can be developed for quantum mechanical systems, in which case we deal with quantum Langevin equations (QLE), and we will see that the classical results follow in the high temperature limit. In all applications we will restrict ourselves to this approach which we will henceforth refer to as the Langevin equations and Green's function (LEGF) method. As we will see, for the ordered case to be discussed in sec. (3.3), one can recover the standard classical results as well as extend them to the quantum domain using the LEGF method. For the disordered case too [sec. (3.4)], one can make significant progress. Another important model that has been well studied in the context of harmonic systems is the case where self-consistent heat reservoirs are attached at all sites of the lattice. In sec. (3.5) we will review results for this case obtained also from the LEGF approach. All examples in this section deal with the case where particle displacements are taken to be scalars. The generalization to vector displacements is straightforward.

The LEGF formalism has been developed in the papers by [40, 41, 42, 43, 44] and relies on the approach first proposed by Ford, Kac and Mazur [45] of modeling a heat bath by an infinite set of oscillators in thermal equilibrium. Here we will outline the basic steps as given in [44]. One again considers a harmonic system

which is coupled to reservoirs which are of a more general form than the white noise reservoirs studied in the last section. The reservoirs are now themselves taken to be a collection of harmonic oscillators, whose number will be eventually taken to be infinite. As we will see, this is equivalent to considering generalized Langevin equations where the noise is still Gaussian but in general can be correlated. We will present the discussion for the quantum case and obtain the classical result as a limiting case.

We consider here the case of two reservoirs, labeled as L (for left) and R (right) , which are at two different temperatures. It is easy to generalize to the case where there are more than two reservoirs. For the system let $X = \{x_1, x_2, ...x_N\}^T$ now be the set of Heisenberg operators corresponding to the displacements (assumed to be scalars) of the N particles, about equilibrium lattice positions. Similarly let X_L and X_R refer to position operators of the particles in the left and right baths respectively. The left reservoir has N_L particles and the right has N_R particles. Also let P, P_L, P_R be the corresponding momentum variables satisfying usual commutation relations with the position operators (*i.e.* $[x_l, p_n] = i\hbar\delta_{l,n}$, etc.). The Hamiltonian of the entire system and reservoirs is taken to be:

$$
\begin{aligned}
H &= H_S + H_L + H_R + H_L^I + H_R^I \qquad (52)\\
\text{where} \quad H_S &= \frac{1}{2}P^T\hat{M}^{-1}P + \frac{1}{2}X^T\hat{\Phi}X \ ,\\
H_L &= \frac{1}{2}P_L^T\hat{M}_L^{-1}P_L + \frac{1}{2}X_L^T\hat{\Phi}_L X_L \ ,\\
H_R &= \frac{1}{2}P_R^T\hat{M}_R^{-1}P_R + \frac{1}{2}X_R^T\hat{\Phi}_R X_R \ ,\\
H_L^I &= X^T\hat{V}_L X_L, \qquad H_R^I = X^T\hat{V}_R X_R \ ,
\end{aligned}
$$

where $M,\ M_L,\ M_R$ are real diagonal matrices representing masses of the particles in the system, left, and right reservoirs respectively. The quadratic potential energies are given by the real symmetric matrices $\hat{\Phi},\ \hat{\Phi}_L,\ \hat{\Phi}_R$ while $\hat{V}_L$ and $\hat{V}_R$ denote the interaction between the system and the two reservoirs respectively. It is assumed that at time $t = t_0$, the system and reservoirs are decoupled and the reservoirs are in thermal equilibrium at temperatures T_L and T_R respectively.

The Heisenberg equations of motion for the system (for $t > t_0$) are:

$$
\hat{M}\ddot{X} = -\hat{\Phi}X - \hat{V}_L X_L - \hat{V}_R X_R \ , \qquad (53)
$$

and the equations of motion for the two reservoirs are

$$
\hat{M}_L\ddot{X}_L = -\hat{\Phi}_L X_L - \hat{V}_L^T X \ , \qquad (54)
$$

$$
\hat{M}_R\ddot{X}_R = -\hat{\Phi}_R X_R - \hat{V}_R^T X \ . \qquad (55)
$$

One first solves the reservoir equations by considering them as linear inhomogeneous equations. Thus for the left reservoir the general solution to Eq. (54) is (for

$t > t_0$):

$$X_L(t) = \hat{f}_L^+(t-t_0)\hat{M}_L X_L(t_0) + \hat{g}_L^+(t-t_0)\hat{M}_L\dot{X}_L(t_0) - \int_{t_0}^{t} dt'\ \hat{g}_L^+(t-t')\hat{V}_L^T X(t')\ , \quad (56)$$

$$\text{with} \quad \hat{f}_L^+(t) = \hat{U}_L \cos(\hat{\Omega}_L t)\hat{U}_L^T\ \theta(t), \quad \hat{g}_L^+(t) = \hat{U}_L \frac{\sin(\hat{\Omega}_L t)}{\hat{\Omega}_L}\hat{U}_L^T\ \theta(t)\ ,$$

where $\theta(t)$ is the Heaviside function, and $\hat{U}_L,\ \hat{\Omega}_L$ are the normal mode eigenvector and eigenvalue matrices respectively, corresponding to the left reservoir Hamiltonian H_L, and which satisfy the equations:

$$\hat{U}_L^T\hat{\Phi}_L\hat{U}_L = \hat{\Omega}_L^2\ , \quad \hat{U}_L^T\hat{M}_L\hat{U}_L = \hat{I}\ .$$

A similar solution is obtained for the right reservoir. Plugging these solutions back into the equation of motion for the system, Eq. (53), one gets the following effective equations of motion for the system:

$$\hat{M}\ddot{X} = -\hat{\Phi}X + \eta_L + \int_{t_0}^{t} dt'\hat{\Sigma}_L(t-t')X(t') + \eta_R + \int_{t_0}^{t} dt'\hat{\Sigma}_R(t-t')X(t'), \quad (57)$$

where $\hat{\Sigma}_L(t) = \hat{V}_L\ \hat{g}_L^+(t)\ \hat{V}_L^T, \quad \hat{\Sigma}_R(t) = \hat{V}_R\ \hat{g}_R^+(t)\ \hat{V}_R^T$

$$\text{and} \quad \eta_L = -\hat{V}_L\ \left[\ \hat{f}_L^+(t-t_0)\hat{M}_L X_L(t_0)\ +\ \hat{g}_L^+(t-t_0)\hat{M}_L\dot{X}_L(t_0)\ \right]$$

$$\eta_R = -\hat{V}_R\ \left[\ \hat{f}_R^+(t-t_0)\hat{M}_R X_R(t_0)\ +\ \hat{g}_R^+(t-t_0)\hat{M}_R\dot{X}_R(t_0)\ \right]\ .$$

This equation has the form of a generalized quantum Langevin equation. The properties of the noise terms η_L and η_R are determined using the condition that, at time t_0, the two isolated reservoirs are described by equilibrium phonon distribution functions. At time t_0, the left reservoir is in equilibrium at temperature T_L and the population of the normal modes (of the isolated left reservoir) is given by the distribution function $f_b(\omega, T_L) = 1/[e^{\hbar\omega/k_B T_L} - 1]$. One then gets the following correlations for the left reservoir noise:

$$\langle \eta_L(t)\eta_L^T(t')\rangle = \hat{V}_L\hat{U}_L\ \left[\cos\hat{\Omega}_L(t-t')\frac{\hbar}{2\hat{\Omega}_L}\coth\left(\frac{\hbar\hat{\Omega}_L}{2k_B T_L}\right) - i\sin\hat{\Omega}_L(t-t')\frac{\hbar}{2\hat{\Omega}_L}\right]\ \hat{U}_L^T\hat{V}_L^T\ , \quad (58)$$

and a similar expression for the right reservoir. The limits of infinite reservoir sizes ($N_L, N_R \to \infty$) and $t_0 \to -\infty$ are now taken. One can then solve Eq. (57) by taking Fourier transforms. Let us define the Fourier transforms $\tilde{X}(\omega) = (1/2\pi)\int_{-\infty}^{\infty} dt\ X(t)e^{i\omega t},\ \tilde{\eta}_{L,R}(\omega) = (1/2\pi)\int_{-\infty}^{\infty} dt\ \eta_{L,R}(t)e^{i\omega t},\ \hat{g}_{L,R}^+(\omega) = \int_{-\infty}^{\infty} dt\ \hat{g}_{L,R}^+(t)e^{i\omega t}$. One then gets the following stationary solution to the equations

of motion Eq. (57):

$$X(t) = \int_{-\infty}^{\infty} d\omega \tilde{X}(\omega) e^{-i\omega t} \ , \tag{59}$$

$$\text{with} \quad \tilde{X}(\omega) = \hat{G}^{+}(\omega) \ [\tilde{\eta}_L(\omega) + \tilde{\eta}_R(\omega)] \ ,$$

$$\text{where} \quad \hat{G}^{+}(\omega) = \frac{1}{[-\omega^2 \hat{M} + \hat{\Phi} - \hat{\Sigma}_L^{+}(\omega) - \hat{\Sigma}_R^{+}(\omega)]} \ ,$$

$$\text{and} \quad \hat{\Sigma}_L^{+}(\omega) = \hat{V}_L \hat{g}_L^{+}(\omega) \hat{V}_L^T, \quad \hat{\Sigma}_R^{+}(\omega) = \hat{V}_R \hat{g}_R^{+}(\omega) \hat{V}_R^T \ .$$

For the reservoirs one obtains [using Eq. (56)]

$$-\hat{V}_L \tilde{X}_L(\omega) = \tilde{\eta}_L(\omega) + \hat{\Sigma}_L^{+} \tilde{X}(\omega) \ ,$$

$$-\hat{V}_R \tilde{X}_R(\omega) = \tilde{\eta}_R(\omega) + \hat{\Sigma}_R^{+} \tilde{X}(\omega) \ . \tag{60}$$

The noise correlations, in the frequency domain, can be obtained from Eq. (58) and we get (for the left reservoir):

$$\langle \tilde{\eta}_L(\omega) \tilde{\eta}_L^T(\omega') \rangle = \delta(\omega + \omega') \ \hat{\Gamma}_L(\omega) \ \frac{\hbar}{\pi} [1 + f_b(\omega, T_L)] \tag{61}$$

$$\text{where} \quad \hat{\Gamma}_L(\omega) = Im[\hat{\Sigma}_L^{+}(\omega)]$$

which is a fluctuation-dissipation relation. This also leads to the more commonly used correlation:

$$\frac{1}{2} \langle \ \tilde{\eta}_L(\omega) \tilde{\eta}_L^T(\omega') + \tilde{\eta}_L(\omega') \tilde{\eta}_L^T(\omega) \ \rangle = \delta(\omega + \omega') \ \hat{\Gamma}_L(\omega) \ \frac{\hbar}{2\pi} \ \coth(\frac{\hbar\omega}{2k_B T_L}). \tag{62}$$

Similar relations hold for the noise from the right reservoir. The identification of $\hat{G}^{+}(\omega)$ as a phonon Green function, with $\hat{\Sigma}_{L,R}^{+}(\omega)$ as self energy contributions coming from the baths, is the main step that enables a comparison of results derived by the LEGF approach with those obtained from the NEGF method. This has been demonstrated in refn. [44].

Steady state properties: The simplest way to evaluate the steady state current is to evaluate the following expectation value for current from left reservoir into the system:

$$J = -\langle \ \dot{X}^T \hat{V}_L X_L \ \rangle. \tag{63}$$

This is just the rate at which the left reservoir does work on the wire. Using the solution in Eq. (59,60,61) one obtains, after some manipulations:

$$J = \frac{1}{4\pi} \int_{-\infty}^{\infty} d\omega \ \mathcal{T}(\omega) \hbar\omega \ [f(\omega, T_L) - f(\omega, T_R)] \ . \tag{64}$$

$$\text{where} \ \ \mathcal{T}(\omega) = 4 \ Tr[\ \hat{G}^{+}(\omega) \ \hat{\Gamma}_L(\omega) \hat{G}^{-}(\omega) \ \hat{\Gamma}_R(\omega)] \ ,$$

and $\hat{G}^{-}(\omega) = \hat{G}^{+\dagger}(\omega)$. This expression for current is of identical form as the NEGF expression for electron current (see for example [46, 47, 48, 49]) and has also been derived for phonons using the NEGF approach in refns.[50, 51]. In fact this expression was first proposed by Angelescu et al.[52] and by Rego and Kirczenow [53] for

a $1D$ channel and they obtained this using the Landauer approach. Their result was obtained more systematically later by Blencowe [54]. Note that Eq. (64) above can also be written as an integral over only positive frequencies using the fact that the integrand is an even function of ω. The factor $\mathcal{T}(\omega)$ is the transmission coefficient of phonons at frequency ω through the system, from the left to right reservoir. The usual Landauer result for a $1D$ channel precisely corresponds to Rubin's model of bath, to be discussed in sec. (3.4.1).

For small temperature differences $\Delta T = T_L - T_R << T$, where $T = (T_L + T_R)/2$, *i.e.* , in the linear response regime the above expression reduces to:

$$J = \frac{\Delta T}{4\pi} \int_{-\infty}^{\infty} d\omega \ \mathcal{T}(\omega)\hbar\omega \ \frac{\partial f(\omega, T)}{\partial T} \ . \tag{65}$$

$$\tag{66}$$

The classical limit is obtained by taking the high temperature limit $\hbar\omega/k_B T \to 0$. This gives:

$$J = \frac{k_B \ \Delta T}{4\pi} \ \int_{-\infty}^{\infty} d\omega \ \mathcal{T}(\omega) \ . \tag{67}$$

One can similarly evaluate various other quantities such as velocity-velocity correlations and position-velocity correlations. The expressions for these in the classical case are respectively:

$$\begin{aligned} K &= \langle \dot{X}\dot{X}^T \rangle \\ &= \frac{k_B T_L}{\pi} \int_{-\infty}^{\infty} d\omega \ \omega \ G^+(\omega)\Gamma_L(\omega)G^-(\omega) + \frac{k_B T_R}{\pi} \int_{-\infty}^{\infty} d\omega \ \omega \ G^+(\omega)\Gamma_R(\omega)G^-(\omega) \ , \\ C &= \langle X\dot{X}^T \rangle \\ &= \frac{ik_B T_L}{\pi} \int_{-\infty}^{\infty} d\omega \ G^+(\omega)\Gamma_L(\omega)G^-(\omega) + \frac{ik_B T_R}{\pi} \int_{-\infty}^{\infty} d\omega \ G^+(\omega)\Gamma_R(\omega)G^-(\omega) \ . \end{aligned}$$

The correlation functions K can be used to define the local energy density which can in turn be used to define the temperature profile in the non-equilibrium steady state of the wire. Also we note that the correlations C give the local heat current density. Sometimes it is more convenient to evaluate the total steady state current from this expression rather than the one in Eq. (64).

For one-dimensional wires the above results can be shown [32] to lead to expressions for current and temperature profiles obtained in earlier studies of heat conduction in disordered harmonic chains [28, 30, 32].

In our derivation of the LEGF results we have *implicitly assumed that a unique steady state will be reached*. One of the necessary conditions for this is that no modes outside the bath spectrum are generated for the combined model of system and baths. These modes, when they exist, are localized near the system and any initial excitation of the mode is unable to decay. This has been demonstrated and discussed in detail in the electronic context [49].

We note that unlike other approaches such as the Green-Kubo formalism and Boltzmann equation approach, the Langevin equation approach explicitly includes the reservoirs. The Langevin equation is physically appealing since it gives a nice picture of the reservoirs as sources of noise and dissipation. Also just as the Landauer formalism and NEGF have been extremely useful in understanding electron transport in mesoscopic systems it is likely that a similar description will be useful

for the case of heat transport in (electrically) insulating nanotubes, nanowires, etc. The LEGF approach has some advantages over NEGF. For example, in the classical case, it is easy to write Langevin equations for nonlinear systems and study them numerically. Unfortunately, in the quantum case, one does not yet know how to achieve this, and understanding steady state transport in interacting quantum systems is an important open problem.

3.3. *Ordered harmonic lattices*

As mentioned above, heat conduction in the ordered harmonic chain was first studied in the Rieder, Lebowitz and Lieb (RLL) paper and its higher dimensional generalization was obtained by Nakazawa. The approach followed in both the RLL and Nakazawa papers was to obtain the exact nonequilibrium stationary state measure which, for this quadratic problem, is a Gaussian distribution. A complete solution for the correlation matrix was obtained and from this one could obtain both the steady state temperature profile and the heat current.

Here we follow refn. [57] to show how the LEGF method, discussed in the previous section, can be used to calculate the heat current in ordered harmonic lattices connected to Ohmic reservoirs (for a classical system this is white noise Langevin dynamics). We will see how exact expressions for the asymptotic current ($N \to \infty$) can be obtained from this approach. We also briefly discuss the model in the quantum regime and extensions to higher dimensions.

3.3.1. One dimensional case

The model considered in [57] is a slightly generalized version of those studied by RLL and Nakazawa. An external potential is present at all sites and the pinning strength at the boundary sites are taken to be different from those at the bulk sites. Thus both the RLL and Nakazawa results can be obtained as limiting cases. Also it seems that this model more closely mimics the experimental situation. In experiments the boundary sites would be interacting with fixed reservoirs, and the coupling to those can be modeled by an effective spring constant that is expected to be different from the interparticle spring constant in the bulk. We also note here that the constant onsite potential present along the wire relates to experimental situations such as that of heat transport in a nanowire attached to a substrate or, in the two-dimensional case, a monolayer film on a substrate. Another example would be the heat current contribution from the optical modes of a polar crystal.

Consider N particles of equal masses m connected to each other by harmonic springs of equal spring constants k. The particles are also pinned by onsite quadratic potentials with strengths k_o at all sites except the boundary sites where the pinning strengths are $k_o + k'$. The Hamiltonian is thus:

$$H = \sum_{l=1}^{N} [\frac{p_l^2}{2m} + \frac{1}{2} k_o x_l^2] + \sum_{l=1}^{N-1} \frac{1}{2} k (x_{l+1} - x_l)^2 + \frac{1}{2} k' (x_1^2 + x_N^2) \ , \tag{68}$$

where x_l denotes the displacement of the l^{th} particle from its equilibrium position. The particles 1 and N at the two ends are connected to heat baths at temperature T_L and T_R respectively, assumed to be modeled by Langevin equations corresponding to Ohmic baths ($\Sigma(\omega) = i\gamma\omega$). In the classical case the steady state heat current

from left to right reservoir can be obtained from Eq. (67) and given by [29, 32]:

$$J = \frac{k_B(T_L - T_R)}{4\pi} \int_{-\infty}^{\infty} d\omega \mathcal{T}_N(\omega), \tag{69}$$
$$\text{where } \mathcal{T}_N(\omega) = 4\,\Gamma^2(\omega)|\hat{G}_{1N}(\omega)|^2,\ \hat{G}(\omega) = \hat{Z}^{-1}/k$$
$$\text{and } \hat{Z} = [-m\omega^2\hat{I} + \hat{\Phi} - \hat{\Sigma}(\omega)]/k\ ,$$

where $\hat{I}$ is a unit matrix, $\hat{\Phi}$ is the force matrix corresponding to the Hamiltonian in Eq. (68). The $N \times N$ matrix $\hat{\Sigma}$ has mostly zero elements except for $\Sigma_{11} = \Sigma_{NN} = i\Gamma(\omega)$ where $\Gamma(\omega) = \gamma\omega$. The matrix $\hat{Z}$ is tri-diagonal matrix with $Z_{11} = Z_{NN} = (k+k_o+k'-m\omega^2-i\gamma\omega)/k$, all other diagonal elements equal to $2+k_o/k-m\omega^2/k$ and all off-diagonal elements equal to -1. Then it can be shown easily that $|G_{1N}(\omega)| = 1/(k\ |\Delta_N|)$ where Δ_N is the determinant of the matrix $\hat{Z}$. This can be obtained exactly. For large N, only phonons within the spectral band of the system can transmit, and the integral over ω in Eq. (69) can be converted to one over q to give:

$$J = \frac{2\gamma^2 k_B(T_L - T_R)}{k^2\pi} \int_0^{\pi} dq |\frac{d\omega}{dq}|\ \frac{\omega_q^2}{|\Delta_N|^2}\ , \tag{70}$$

with $m\omega_q^2 = k_o + 2k[1 - \cos(q)]$. Now using the result:

$$\lim_{N\to\infty} \int_0^{\pi} dq \frac{g_1(q)}{1 + g_2(q)\sin Nq} = \int_0^{\pi} dq \frac{g_1(q)}{[1 - g_2^2(q)]^{1/2}}\ , \tag{71}$$

where $g_1(q)$ and $g_2(q)$ are any two well-behaved functions, one can show that in the limit $N \to \infty$, Eq. (70) gives

$$J = \frac{\gamma k^2 k_B(T_L - T_R)}{m\Omega^2}(\Lambda - \sqrt{\Lambda^2 - \Omega^2})\ , \tag{72}$$
$$\text{where } \Lambda = 2k(k-k') + k'^2 + \frac{(k_o+2k)\gamma^2}{m} \text{ and } \Omega = 2k(k-k') + \frac{2k\gamma^2}{m}\ .$$

Two different special cases lead to the RLL and Nakazawa results. First in the case of fixed ends and without onsite potentials, *i.e.* $k' = k$ and $k_o = 0$, we recover the RLL result [25]:

$$J^{RLL} = \frac{kk_B(T_L - T_R)}{2\gamma}\Big[1 + \frac{\nu}{2} - \frac{\nu}{2}\sqrt{1 + \frac{4}{\nu}}\ \Big] \text{ where } \nu = \frac{mk}{\gamma^2}\ . \tag{73}$$

In the other case of free ends, *i.e.* $k' = 0$, one gets the Nakazawa result [26]:

$$J^N = \frac{k\gamma k_B(T_L - T_R)}{2(mk + \gamma^2)}\Big[1 + \frac{\lambda}{2} - \frac{\lambda}{2}\sqrt{1 + \frac{4}{\lambda}}\ \Big] \text{ where } \lambda = \frac{k_o\gamma^2}{k(mk + \gamma^2)}\ . \tag{74}$$

In the quantum case, in the linear response regime, Eq. (65) and similar manipulations made above for the $N \to \infty$ limit leads to the following final expression

for current:

$$J = \frac{\gamma k^2 \hbar^2 (T_L - T_R)}{4\pi k_B m T^2} \int_0^\pi dq \frac{\sin^2 q}{\Lambda - \Omega \cos q} \; \omega_q^2 \; \mathrm{cosech}^2\Big(\frac{\hbar\omega_q}{2k_B T}\Big), \quad (75)$$

where $\omega_q^2 = [k_o + 2k(1 - \cos q)]/m$.

While one cannot perform this integral exactly, numerically it is easy to obtain the integral for given parameter values. It is interesting to examine the temperature dependence of the conductance $J/\Delta T$. In the classical case this is independent of temperature while one finds that at low temperatures the quantum result is completely different. For three different cases one finds, in the low temperature ($T << \hbar(k/m)^{1/2}/k_B$) regime, the following behaviour:

$$J \sim \begin{cases} T^3 \quad \text{for} \quad k' = k, k_o = 0 \\ \sim T \quad \text{for} \quad k' = 0, k_o = 0 \\ \sim \frac{e^{-\hbar\omega_o/(k_B T)}}{T^{1/2}} \quad \text{for} \quad k' = 0, k_o \neq 0 \ , \end{cases} \quad (76)$$

where $\omega_o = (k_o/m)^{1/2}$. In studies trying to understand experimental work on nanosystems [see sec. (8)] , the temperature dependence of the conductance is usually derived from the Landauer formula, which corresponds to the Rubin model of bath. The temperature dependence will then be different from the above results.

3.3.2. Higher dimensions

As shown by Nakazawa [26] the problem of heat conduction in ordered harmonic lattices in more than one dimension can be reduced to an effectively one-dimensional problem. We will briefly give the arguments here and also give the quantum generalization.

Let us consider a d-dimensional hypercubic lattice with lattice sites labeled by the vector $\mathbf{n} = \{n_\alpha\}, \alpha = 1, 2...d$, where each n_α takes values from 1 to L_α. The total number of lattice sites is thus $N = L_1 L_2 ... L_d$. We assume that heat conduction takes place in the $\alpha = d$ direction. Periodic boundary conditions are imposed in the remaining $d - 1$ transverse directions. The Hamiltonian is described by a scalar displacement $X_{\mathbf{n}}$ and, as in the $1D$ case, we consider nearest neighbour harmonic interactions with a spring constant k and harmonic onsite pinning at all sites with spring constant k_o. All boundary particles at $n_d = 1$ and $n_d = L_d$ are additionally pinned by harmonic springs with stiffness k' and follow Langevin dynamics corresponding to baths at temperatures T_L and T_R respectively.

Let us write $\mathbf{n} = (\mathbf{n}_t, n_d)$ where $\mathbf{n}_t = (n_1, n_2 ... n_{d-1})$. Also let $\mathbf{q} = (q_1, q_2 ... q_{d-1})$ with $q_\alpha = 2\pi s/L_\alpha$ where s goes from 1 to L_α. Then defining variables

$$X_{n_d}(\mathbf{q}) = \frac{1}{L_1^{1/2} L_2^{1/2} ... L_{d-1}^{1/2}} \sum_{\mathbf{n}_t} X_{\mathbf{n}_t, n_d} e^{i\mathbf{q}.\mathbf{n}_t} \ , \quad (77)$$

one finds that, for each fixed $\mathbf{q}$, $X_{n_d}(\mathbf{q})$ ($n_d = 1, 2 ... L_d$) satisfy Langevin equations corresponding to the 1D Hamiltonian in Eq. (68) with the onsite spring constant k_o replaced by

$$\lambda(\mathbf{q}) = k_o + 2 \; k \; [\; d - 1 - \sum_{\alpha = 1, d-1} \cos(q_\alpha) \;] \ . \quad (78)$$

For $L_d \to \infty$, the heat current $J(\mathbf{q})$ for each mode with given $\mathbf{q}$ is then simply

given by Eq. (72) with k_o replaced by $\lambda_{\mathbf{q}}$. In the quantum mechanical case we use Eq. (75). The heat current per bond is then given by:

$$J = \frac{1}{L_1 L_2 .... L_{d-1}} \sum_{\mathbf{q}} J(\mathbf{q}) \ . \tag{79}$$

Note that the result holds for finite lengths in the transverse direction. For infinite transverse lengths we get $J = \int ... \int_0^{2\pi} d\mathbf{q} J(\mathbf{q})/(2\pi)^{d-1}$.

3.4. *Disordered harmonic lattices*

From the previous section we see that the heat current in an ordered harmonic lattice is independent of system size (for large systems) and hence transport is ballistic. Of course this is expected since there is no mechanism for scattering of the heat carriers, namely the phonons. Two ways of introducing scattering of phonons are by introducing disorder in the system, or by including anharmonicity which would cause phonon-phonon interactions. In this section we consider the effect of disorder on heat conduction in a harmonic system.

Disorder can be introduced in various ways, for example by making the masses of the particles random as would be the case in a isotopically disordered solid, or by making the spring constants random. Here we will discuss the case of mass-disorder only since the most important features do not seem to vary much with the type of disorder one is considering. Specifically, we will consider harmonic systems where the mass of each particle is an independent random variable chosen from some fixed distribution.

It can be expected that heat conduction in disordered harmonic systems will be strongly affected by the physics of Anderson localization. In fact the problem of finding the normal modes of the harmonic lattice can be directly mapped to that of finding the eigenstates of an electron in a disordered potential (in a tight-binding model, for example) and so we expect the same kind of physics as in electron localization. In the electron case the effect of localization is strongest in one dimensions where it can be proved rigorously that all eigenstates are exponentially localized, hence the current decays exponentially with system size and the system is an insulator. This is believed to be true in two dimensions also. In the phonon case the picture is much the same except that, in the absence of an external potential, the translational invariance of the problem leads to the fact that *low frequency modes are not localized and are effective in transporting energy.* Another important difference between the electron and phonon problems is that *electron transport is dominated by electrons near the Fermi level while in the case of phonons, all frequencies participate in transport.* These two differences lead to the fact that the disordered harmonic crystal in one and two dimensions is not a heat insulator, unlike its electronic counterpart. Here we will present results using the LEGF approach to determine the system size dependence of the current in one dimensional mass-disordered chains. We note that basically this same approach (NEGF) is also popular in the electron case and is widely used in mesoscopic physics. Also earlier treatments by, for example, Rubin and Greer [28] and by Casher and Lebowitz [29] of the disordered harmonic chain, can be viewed as special examples of the LEGF approach. We will also discuss results of simulations for the two-dimensional case.

Our main conclusions here will be that Fourier's law is not valid in a disordered harmonic crystal in one and two dimensions, the current decays as a power law with system size and the exponent α is sensitive to boundary conditions (BC) and spectral properties of the heat baths.

3.4.1. One dimensional disordered lattice

We first briefly review earlier work on this problem [2]. The thermal conductivity of disordered harmonic lattices was first investigated by Allen and Ford [13] who, using the Kubo formalism, obtained an exact expression for the thermal conductivity of a finite chain attached to infinite reservoirs. From this expression they concluded, erroneously as we now know, that the thermal conductivity remains finite in the limit of infinite system size. Simulations of the disordered lattice connected to white noise reservoirs were carried out by Payton et al. [153]. They were restricted to small system sizes ($N \sim 400$) and also obtained a finite thermal conductivity.

Possibly the first paper to notice anomalous transport was that by Matsuda and Ishii (MI) [27]. In an important work on the localization of normal modes in the disordered harmonic chain, MI showed that all high frequency modes were exponentially localized. However, for small ω the localization length in an infinite sample was shown to vary as ω^{-2}, hence normal modes with frequency $\omega \lesssim \omega_d$ have localization length greater than N, and cannot be considered as localized. For a harmonic chain of length N, given the average mass $m = \langle m_l \rangle$, the variance $\sigma^2 = \langle (m_l - m)^2 \rangle$ and interparticle spring constant k, it was shown that

$$\omega_d \sim \left(\frac{km}{N\sigma^2} \right)^{1/2} \tag{80}$$

They also evaluated expressions for thermal conductivity of a finite disordered chain connected to two different bath models, namely:

- model(a): white noise baths and
- model(b): baths modeled by semi-infinite ordered harmonic chains (Rubin's model of bath).

In the following we will also consider these two models of baths. For model(a) MI used fixed BC (boundary particles in external potential) and the limit of weak coupling to baths, while for case (b) they considered free BC (boundary particles not pinned) and this was treated using the Green-Kubo formalism given by Allen and Ford [13]. They found $\alpha = 1/2$ in both cases, a conclusion which we will see is incorrect. The other two important theoretical papers on heat conduction in the disordered chain were those by Rubin and Greer [28] who considered model(b) and of Casher and Lebowitz [29] who used model(a) for baths. A lower bound $[J] \geq 1/N^{1/2}$ was obtained for the disorder averaged current $[J]$ in refn. [28] who also gave numerical evidence for an exponent $\alpha = 1/2$. This was later proved rigorously by Verheggen [31]. On the other hand, for model(a), [29] found a rigorous bound $[J] \geq 1/N^{3/2}$ and simulations by Rich and Visscher [65] with the same baths supported the corresponding exponent $\alpha = -1/2$. The work in [32] gave a unified treatment of the problem of heat conduction in disordered harmonic chains connected to baths modeled by generalized Langevin equations and showed that models(a,b) were two special cases. An efficient numerical scheme was proposed and used to obtain the exponent α and it was established that $\alpha = -1/2$ for model(a) (with fixed BC) and $\alpha = 1/2$ for model(b) (with free BC). It was also pointed out that in general, α *depended on the spectral properties of the baths*. We will briefly describe this formulation [33] here and see how one can understand the effect of boundary conditions on heat transport in the disordered chain. We will consider both the white noise [model(a)] and Rubin baths [model(b)]. One of the main conclusions will be that the difference in exponents obtained for these two cases arises from use of different boundary conditions, rather than because of differences in spectral properties of the baths.

The Hamiltonian of the mass-disordered chain is given by

$$H = \sum_{l=1}^{N} \frac{p_l^2}{2m_l} + \sum_{l=1}^{N-1} \frac{1}{2}k(x_{l+1} - x_l)^2 + \frac{1}{2}k'(x_1^2 + x_N^2) \ . \tag{81}$$

The random masses $\{m_l\}$ are chosen from, say, a uniform distribution between $(m - \Delta)$ to $(m + \Delta)$. The strength of onsite potentials at the boundaries is k'. The particles at two ends are connected to heat baths, at temperature T_L and T_R, and modelled by generalized Langevin equations. The steady state classical heat current through the chain is given by:

$$J = \frac{k_B(T_L - T_R)}{4\pi} \int_{-\infty}^{\infty} d\omega \mathcal{T}_N(\omega), \tag{82}$$
$$\text{where } \ \mathcal{T}_N(\omega) = 4\Gamma^2(\omega)|\hat{G}_{1N}(\omega)|^2, \ \hat{G}(\omega) = \hat{Z}^{-1}/k$$
$$\text{and } \ \hat{Z} = [-\omega^2\hat{M} + \hat{\Phi} - \hat{\Sigma}(\omega)]/k \ ,$$

where $\hat{M}$ and $\hat{\Phi}$ are respectively the mass and force matrices corresponding to Eq. (81). As shown in [32], the non-zero elements of the diagonal matrix $\hat{\Sigma}(\omega)$ for models(a,b) are $\Sigma_{11}(\omega) = \Sigma_{NN}(\omega) = \Sigma(\omega)$ and given by

$$\Sigma(\omega) = -i\gamma\omega \quad \text{model(a)}$$
$$\Sigma(\omega) = k\{1 - m\omega^2/2k - i\omega(m/k)^{1/2}[1 - m\omega^2/(4k)]^{1/2}\} \quad \text{model(b)} \ , \tag{83}$$

where γ is the coupling strength with the white noise baths, while in case of Rubin's baths it has been assumed that the Rubin bath has spring constant k and equal masses m. As noted above, $\mathcal{T}_N(\omega)$ is the transmission coefficient of phonons through the disordered chain. To extract the asymptotic N dependence of the disorder averaged current $[J]$ one needs to determine the Green's function element $G_{1N}(\omega)$. It is convenient to write the matrix elements $Z_{11} = -m_1\omega^2/k + 1 + k'/k - \Sigma/k = -m_1\omega^2/k + 2 - \Sigma'$ where $\Sigma' = \Sigma/k - k'/k + 1$ and similarly $Z_{NN} = -m_N\omega^2/k + 2 - \Sigma'$. Following the techniques used in [29, 32] one gets:

$$|G_{1N}(\omega)|^2 = k^{-2}|\Delta_N(\omega)|^{-2} \ \text{ with} \tag{84}$$
$$\Delta_N(\omega) = D_{1,N} - \Sigma'(D_{2,N} + D_{1,N-1}) + \Sigma'^2 D_{2,N-1}$$

where $\Delta_N(\omega)$ is the determinant of $\hat{Z}$ and the matrix elements $D_{l,m}$ are given by the following product of (2×2) random matrices $\hat{T}_l$:

$$\hat{D} = \begin{pmatrix} D_{1,N} & -D_{1,N-1} \\ D_{2,N} & -D_{2,N-1} \end{pmatrix} = \hat{T}_1\hat{T}_2....\hat{T}_N \tag{85}$$
$$\text{where} \quad \hat{T}_l = \begin{pmatrix} 2 - m_l\omega^2/k & -1 \\ 1 & 0 \end{pmatrix}$$

We note that the information about bath properties and boundary conditions are now contained entirely in $\Sigma'(\omega)$ while $\hat{D}$ contains the system properties. It is known that $|D_{l,m}| \sim e^{cN\omega^2}$ [27], where c is a constant, and so we need to look only at the low frequency ($\omega \lesssim 1/N^{1/2}$) form of Σ' . Let us now discuss the various cases. For model(a) free BC correspond to $k' = 0$ and so $\Sigma' = 1 - i\gamma\omega/k$ while for

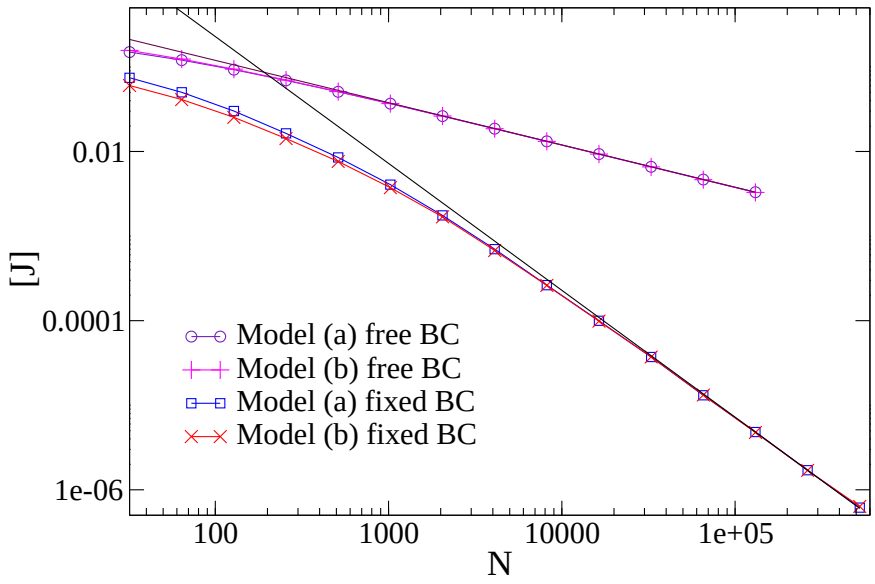

Figure 1. Plot of $[J]$ versus N for free and fixed boundary conditions. Results are given for both models(a,b) of baths. The two straight lines correspond to the asymptotic expressions given in Eqs. (87,88) and have slopes $-1/2$ and $-3/2$. Parameters used were $m = 1,\ \Delta = 0.5,\ k = 1,\ \gamma = 1,$ $T_L = 2$, $T_R = 1$ and $k_o = 1$ (from [33]).

model(b) free boundaries corresponds to $k' = k$ and this gives, at low frequencies, $\Sigma' = 1 - i(m/k)^{1/2}\omega$. Other choices of k' correspond to pinned boundary sites with an onsite potential $k_o x^2/2$ where $k_o = k'$ for model(a) and $k_o = k' - k$ for model(b). The main difference, from the unpinned case, is that now $Re[\Sigma'] \neq 1$. The arguments of [32] then immediately give $\alpha = 1/2$ for free BC and $\alpha = -1/2$ for fixed BC for both bath models. In fact for the choice of parameters $\gamma = (mk)^{1/2}$, the imaginary part of Σ' is the same for both baths and hence we expect, for large system sizes, the actual values of the current to be the same for both bath models. This can be seen in Fig. (1) where the system size dependence of the current for the various cases is shown. The current was evaluated numerically using Eq. (82) and averaging over many realizations. Note that for free BC, the exponent $\alpha = 1/2$ settles to its asymptotic value at relatively small values ($N \sim 10^3$) while, with pinning, one needs to examine much longer chains ($N \sim 10^5$).

These results clearly show that, for both models(a,b) of baths, the exponent α is the same and is controlled by the presence or absence of pinning at the boundaries. The reason that both models give the same exponents is that the imaginary part of their self energies, given by Eq. (83), have the same small ω dependence. If the imaginary part of the self energy, *i.e.* $\Gamma(\omega)$, has a different ω dependence, then one can get different exponents for the same boundary conditions [32].

For the present case, some more specific predictions can also be obtained. As mentioned before only modes $\omega \lesssim \omega_d$ are involved in conduction. An observation made in [106] was that *in this low frequency regime one can approximate* $[\mathcal{T}_N(\omega)]$ *by the transmission coefficient of the ordered chain* $\mathcal{T}_N^O(\omega)$. One can then write:

$$[J] \sim (T_L - T_R) \int_0^{\omega_d} \mathcal{T}_N^O(\omega) d\omega \ . \tag{86}$$

By looking at the $N \to \infty$ limit results for the ordered lattice, the following results

are obtained for the two different boundary conditions [33]:

$$[J]_{Fr} = A\ c\ \frac{k_B(T_L - T_R)}{\pi}\Big(\frac{km}{N\sigma^2}\Big)^{1/2} \tag{87}$$

$$[J]_{Fi} = A'\ c'\ \frac{k_B(T_L - T_R)}{\pi}\Big(\frac{km}{N\sigma^2}\Big)^{3/2}\ , \tag{88}$$

where $c = 2\gamma(mk)^{1/2}/(\gamma^2 + mk)$, 1 for model(a), model(b) respectively. For fixed boundaries we have $c' = \gamma(mk)^{1/2}/{k_o}^2$, $mk/{k_o}^2$ for model(a), model(b) respectively. A, A' are constant numbers, taken to be fitting parameters. For model(b) this agrees with an exact expression for $[J]_{Fr}$ due to Papanicolau (apart from a factor of 2π) and with $A = \pi^{3/2}\int_0^\infty dt\ [t\sinh(\pi t)]/[(t^2 + 1/4)^{1/2}\cosh^2(\pi t)] \approx 1.08417$ (see [[31]]).

In the case where all sites of the chain are pinned (*i.e.* in the presence of a substrate potential) it was been noted in [32, 34] that the current decays exponentially with N and this was proved in [156]. Another interesting result obtained in [33] is the case with a finite number n of pinned sites. It was shown, using heuristic arguments and numerics, that $\alpha = 3/2 - n$ for $2 \leq n << N$.

A question that has been discussed in the literature is that of uniqueness of the steady state. This depends on the choice of heat baths as well as the system studied. For models(a,b) of baths, the uniqueness of the steady state of a chain has been discussed in [28] and [29]. For baths consisting of harmonic oscillators one obvious necessary condition for uniqueness is that the bath spectrum should include the modes of the system (see for example [35]).

The quantum mechanical disordered chain has been discussed in [42] where it was argued that the asymptotic system size dependence of the current should remain unchanged from the classical case (unlike the low temperature behaviour for ordered case). The temperature profile in a quantum mechanical disordered chain and quantum aspects such as entanglement have been numerically studied in [36].

3.4.2. Two dimensional disordered harmonic lattice

So far there has not been much progress in understanding heat conduction in higher dimensional disordered lattices. The LEGF theory is still applicable and provides a general expression for the steady state current, Eq. (64), in terms of the phonon Green's function of the harmonic lattice. However in one dimension one could make progress by writing the transmission coefficient in terms of a product of random matrices as in Eqs. (84,85). This enables one to use some known mathematical theorems from which some analytic results could be obtained. Also this representation makes it possible to evaluate the current by very efficient numerical procedures. However in two and higher dimensions things become more complicated and it has not been possible to make much analytic progress. This state of things is also reflected in the fact that while in one dimension it can be proved exactly that all finite frequency states are localized, there is no such proof in two dimensions, although this is the general belief. As far as phonon localization is concerned a renormalization group study by John et al. [58] found that things are very similar to electronic localization. The important difference is again at low frequencies where one gets extended states. Their study indicates the following: in $1D$, all modes with $\omega > 1/L^{1/2}$ are localized; in $2D$, all modes with $\omega > [\log(L)]^{-1/2}$ are localized; in $3D$, there is a finite band of frequencies of non-localized states. However this study was unable to extract the system size dependence of heat current in a disordered lattice in any dimension.

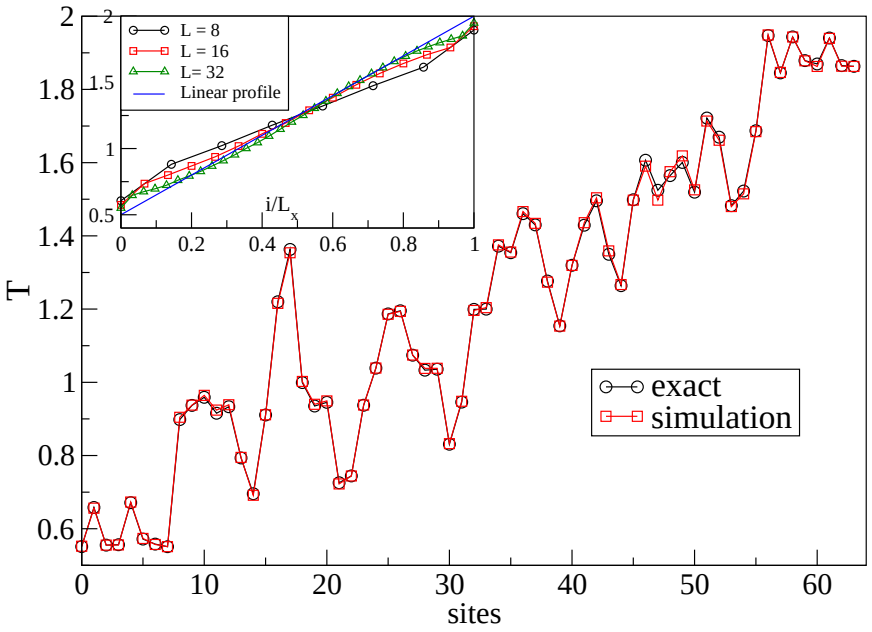

Figure 2. Temperature at all the sites of a 8×8 fully disordered lattice, from simulations and from the exact solution. Inset shows the disorder-averaged temperature profiles (averaged over the transverse direction) for different system sizes and seems to approach a linear form (from [63]).

There have been a few simulation studies on the $2D$ disordered harmonic lattice. Lei Yang [59] considered a lattice with bond-missing defects and looked at the system size dependence of conductivity at various defect densities. The first observation that was made was that disorder gives rise to a temperature gradient across the system, unlike the flat profile for the ordered case. Also it was found that at small densities, the conductivity diverged logarithmically, while at larger densities, a finite heat conductivity was obtained. However this conclusion is probably incorrect since the paper uses Nose-Hoover thermostats and it is known that, for harmonic systems, these have equilibration problems [37, 38, 60, 61, 62, 155].

The most detailed study of the $2D$ disordered harmonic lattice is by Lee and Dhar [63]. They considered stochastic heat baths and looked at the case of mass disorder. In their model, the masses of exactly half the particles on randomly chosen sites of a $L \times L$ square lattice were set to one and the remaining to two. To see the effect of spectral properties of baths, two kinds of baths were studied: one with uncorrelated Gaussian noise and the other with exponentially correlated Gaussian noise. Simulations in disordered systems have to be done with care since one can have slow equilibration. In [63] the authors first checked their simulation results by comparing them with results obtained from an exact numerical solution of the general RLL matrix equations Eq. (45) for a 8×8 lattice. The comparision, for the temperature at various lattice points, obtained by the two methods is shown in Fig. (2) and one can see excellent agreement between the exact results and simulation. Also shown in the inset are the disorder-averaged temperature profiles across the system for different sizes. One can see approach to a linear profile. To find the system size dependence of the current, lattices with sizes upto $L = 256$ were studied. In Fig. (3) we show the data for the disorder averaged current for different system sizes and for the two different bath models. From this data the exponents $\alpha \approx 0.41$ for white noise baths and $\alpha \approx 0.49$ for the correlated bath was obtained. A special case of correlated disorder, first discussed in [30], was also studied. Here the lattice was disordered in the conducting direction, but ordered in

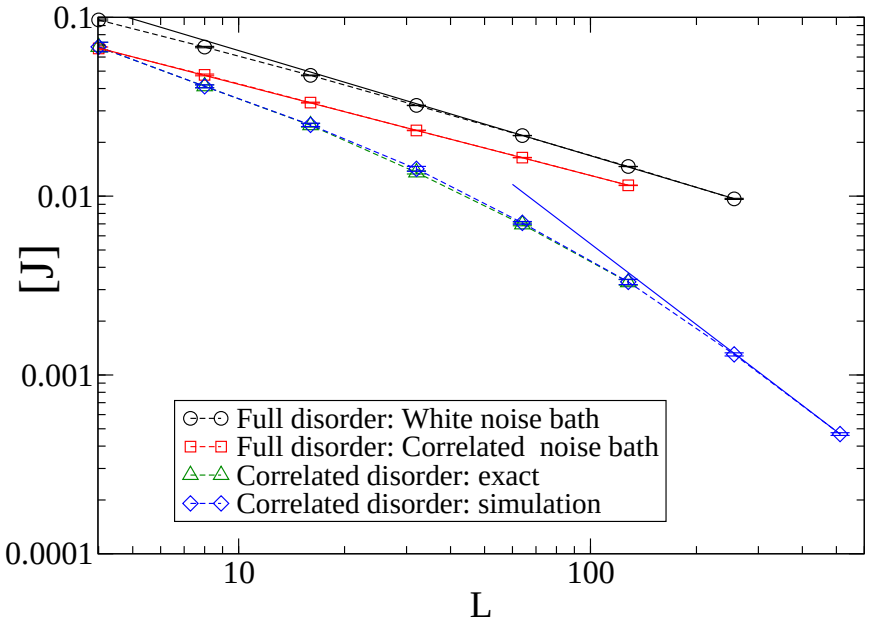

Figure 3. Plot of disorder-averaged-current versus system size for a $L \times L$ lattice two different heat baths. The case of correlated disorder with white noise is also shown. For the full disorder cases, the solid lines are fits to the last three points and have slopes -0.59 and -0.51. For the case of correlated disorder, the slope from exact numerics (and also simulations) is compared to -1.5 which is what one expects analytically (from [63]).

the transverse direction. Using the same methods as discussed in sec. (3.3.2), one can transform this into an effectively $1D$ problem and then use the numerical techniques for evaluating the heat current as in the $1D$ case. In [63], the current was evaluated numerically (upto $L = 512$) as well as from simulations (upto $L = 128$ and with white noise baths). Excellent agreement between the two confirmed the accuracy of the simulations. From the transformation to an effective $1D$ problem it is possible to argue for an exponent $\alpha = -1/2$ for the correlated disorder case and this could be already verified at the system size $L = 512$. This is somewhat surprising considering the fact that in the $1D$ case, one has to go to sizes $\sim 10^5$ to see this exponent [see Fig. (1)]. This result gives some confidence that the results obtained, for the fully disordered cases, are also close to the asymptotic values. An interesting observation in [63] is that equilibration times for local temperatures is typically much larger than that for the current. This is expected since the temperature gets contributions from all modes including the localized ones which are weakly coupled to the reservoirs. On the other hand the current is mainly carried by low frequency extended modes. This point was also noted for the disordered $1D$ chain in [34].

3.5. *Harmonic lattices with self-consistent reservoirs*

As another application of the LEGF formalism we consider the problem of heat transport in a harmonic chain with each site connected to self-consistent heat reservoirs. The classical version of this model was first studied by Bolsteri, Rich and Visscher [64, 65], who introduced the self-consistent reservoirs as a simple scattering mechanism for phonons which might ensure local equilibration and the validity of Fourier's law. The extra reservoirs connected to the system can roughly be thought of as other degrees of freedom with which the lattice interacts. It is interesting to note that the self-consistent reservoirs are very similar to the Buttiker probes [68, 69] which have been used to model inelastic scattering and phase decoherence

in electron transport. In the electron case they lead to Ohm's law being satisfied just as in the harmonic chain the introduction of self-consistent reservoirs leads to Fourier's law being satisfied. In fact it has recently been shown how one can obtain both Ohm's law and Fourier's law in an electron model by using self-consistent reservoirs represented microscopically by noninteracting electron baths [70].

The ordered harmonic lattice with self-consistent reservoirs was solved exactly by Bonetto et al [67], in arbitrary dimensions, who proved local equilibration and validity of Fourier's law, and obtained an expression for the thermal conductivity of the system. They also showed that the temperature profile in the wire was linear. The quantum version of the problem was also studied by Visscher and Rich [66] who analyzed the limiting case of weak coupling to the self-consistent reservoirs. We will here follow the LEGF approach as given in [44] to obtain results in the quantum-mechanical case. The classical results of Bonetto et al are obtained as the high temperature limit while the quantum mechanical results of Vischer and Rich are obtained in the weak coupling limit. We will consider only the one-dimensional case. A generalization to higher dimensions can be easily achieved, as in Sec. (3.3).

Consider the quantum-mechanical Hamiltonian:

$$H = \sum_{l=1}^{N} \; [\; \frac{p_l^2}{2m} + \frac{\omega_0^2 x_l^2}{2} \;] + \sum_{l=1}^{N+1} \frac{m\omega_c^2}{2}(x_l - x_{l-1})^2 \;, \tag{89}$$

where we have chosen the boundary conditions $x_0 = x_{N+1} = 0$. All the particles are connected to heat reservoirs which are taken to be Ohmic. The coupling strength to the reservoirs is controlled by the dissipation constant γ. The temperatures of the first and last reservoirs are fixed and taken to be $T_1 = T_L$ and $T_N = T_R$. For other particles, *i.e* , $l = 2, 3...(N-1)$, the temperature of the attached reservoir T_l is fixed self-consistently in such a way that the net current flowing into any of these reservoirs vanishes. The Langevin equations of motion for the particles on the wire are:

$$m\ddot{x}_l = -m\omega_c^2(2x_l - x_{l-1} - x_{l+1}) - m\omega_0^2 x_l - \gamma\dot{x}_l + \eta_l \quad l = 1, 2...N \;, \tag{90}$$

where the noise-noise correlation, from Eq. (62) and with $\Gamma(\omega) = \gamma\omega$ for Ohmic baths, is given by:

$$\frac{1}{2}\langle\; \eta_l(\omega)\eta_m(\omega') + \eta_l(\omega')\eta_m(\omega) \;\rangle = \frac{\gamma\hbar\omega}{2\pi}\coth(\frac{\hbar\omega}{2k_BT_l})\;\delta(\omega+\omega')\;\delta_{lm}\;. \tag{91}$$

From the equations of motion it is clear that the l^{th} particle is connected to a bath with a self energy matrix $\hat{\Sigma}_l^+(\omega)$ whose only non vanishing element is $(\Sigma_l^+)_{ll} = i\gamma\omega$. Generalizing Eq. (64) to the case of multiple baths, one finds that the heat current from the l^{th} reservoir into the wire is given by:

$$J_l = \sum_{m=1}^{N} \int_{-\infty}^{\infty} d\omega\; \mathcal{T}_{lm}\frac{\hbar\omega}{4\pi}\;[f(\omega,T_l) - f(\omega,T_m)]\;, \tag{92}$$

$$\text{where} \quad \mathcal{T}_{lm} = 4\;Tr[\;\hat{G}^+(\omega)\;\hat{\Gamma}_l(\omega)\hat{G}^-(\omega)\;\hat{\Gamma}_m(\omega)]$$

$$\text{and} \quad \hat{G}^+ = [\; -\omega^2\;\hat{M} + \hat{\Phi} - \sum_l \hat{\Sigma}_l^+(\omega)\;]^{-1}\;, \quad \hat{\Gamma}_l = Im[\hat{\Sigma}_l^+]\;.$$

Here $\mathcal{T}_{lm}$ is the transmission coefficient of phonons from the l^{th} to the m^{th} reservoir.

Using the form of $\hat{\Gamma}_l$ one gets, in the linear response regime:

$$J_l = \gamma^2 \int_{-\infty}^{\infty} d\omega \ \frac{\hbar\omega^3}{\pi} \frac{\partial f(\omega,T)}{\partial T} \sum_{m=1}^{N} \ | \ [\hat{G}^+(\omega)]_{lm} \ |^2 \ \ (T_l - T_m) \ . \tag{93}$$

For a long wire ($N >> 1$), for points far from the boundaries of the wire ($l = yN$ where $y = O(1),\ 1-y = O(1)$), one can explicitly evaluate the Green's function and show that:

$$G^+_{lm} = \frac{e^{-\alpha|l-m|}}{2m\omega_c^2 \sinh\alpha} \ , \tag{94}$$

where $e^\alpha = z/2 \pm [(z/2)^2 - 1]^{1/2}$ with $z = 2 + \omega_0^2/\omega_c^2 - \omega^2/\omega_c^2 - i\gamma\omega/(m\omega_c)^2$, and we choose the root α such that $Re[\alpha] > 0$. Using this form of G^+_{lm} and assuming a linear temperature profile given by

$$T_l = T_L + \frac{l-1}{N-1}(T_R - T_L) \ , \tag{95}$$

one can see at once that, for any point l in the bulk of the wire, the zero-current condition $J_l = 0$ is satisfied since $\sum_{m=-\infty}^{\infty}(l-m)|e^{-\alpha|l-m|}|^2 = 0$. For points which are within distance $O(1)$ from the boundaries the temperature profile deviates from the linear form. Knowing the form of the temperature profile T_l and the form of G^+_{lm}, one can proceed to find the net current in the wire. It is easiest to evaluate the following quantity giving current $J_{l,l+1}$ on the bond connecting sites l and $(l+1)$:

$$J_{l,\ l+1} = m\omega_c^2 \ \langle x_l \dot{x}_{l+1} \rangle = -\frac{m\omega_c^2\gamma}{\pi} \int_{-\infty}^{\infty} d\omega \ \omega \ \left(\frac{\hbar\omega}{2k_BT}\right)^2 \mathrm{cosech}^2(\frac{\hbar\omega}{2k_BT})$$
$$\times \sum_{m=1}^{N} k_BT_m \ Im\{[\hat{G}^+(\omega)]_{lm}[\hat{G}^+(\omega)]^*_{l+1\ m}\} \ .$$

Using Eqs. (94,95) one finally gets the following expression for the thermal conductivity $\kappa = JN/\Delta T$ (obtained in the large N limit):

$$\kappa = \frac{\gamma k_B}{16 m\omega_c^2 \pi i} \int_{-\infty}^{\infty} d\omega \ \frac{\omega}{\sinh^2\alpha_R} \left(\frac{\hbar\omega}{2k_BT}\right)^2 \mathrm{cosech}^2(\frac{\hbar\omega}{2k_BT}) \ \left(\frac{1}{\sinh\alpha} - \frac{1}{\sinh\alpha^*}\right), \tag{96}$$

where $\alpha_R(\omega) = Re[\alpha]$, $\alpha_I(\omega) = Im[\alpha]$. In the high temperature limit $(\hbar\omega/2k_BT)^2\mathrm{cosech}^2(\hbar\omega/2k_BT) \ \rightarrow \ 1$, this gives, after a change of variables from ω to α_I, the following result for the classical thermal conductivity:

$$\kappa_{cl} = \frac{2k_Bm\omega_c^2(2+\nu^2)}{\gamma\pi} \int_0^{\pi/2} d\alpha_I \ \frac{\sin^2(\alpha_I)}{(2+\nu^2)^2 - 4\cos^2(\alpha_I)}$$
$$= \frac{k_Bm\omega_c^2}{\gamma \ (2+\nu^2+[\nu^2(4+\nu^2)]^{1/2})} \ , \tag{97}$$

where $\nu = \omega_0/\omega_c$. This agrees with the result obtained in refn. [67]. Another interesting limiting case is the case of weak coupling to the reservoirs ($\gamma \rightarrow 0$). In this

case Eq. (96) gives:

$$\kappa_{wc} = \left(\frac{\hbar\omega_c^2}{k_B T}\right)^2 \frac{m k_B}{4\gamma\pi} \int_0^\pi d\alpha_I \ \sin^2\alpha_I \ \mathrm{cosech}^2(\frac{\hbar\omega_\alpha}{2k_B T}) \ , \tag{98}$$

$$\text{where} \quad \omega_\alpha^2 = \omega_0^2 + 2\omega_c^2[1-\cos(\alpha_I)] \ .$$

This agrees with the result obtained in [66]. In the low temperature limit, Eq. (98) gives $\kappa_{wc} \sim e^{-\hbar\omega_0/k_B T}/T^{1/2}$ for $\omega_0 \neq 0$ and $\kappa_{wc} \sim T$ for $\omega_0 = 0$. As noted in [66] the expression for thermal conductivity (in the weak scattering limit) is consistent with a simple relaxation-time form for the thermal conductivity. The temperature dependence of κ_{wc} then simply follows the temperature dependence of the specific heat of the $1D$ chain.

In the general case where the coupling constant has a finite value, the low-temperature behaviour again depends on whether or not there is an onsite potential. The form of the low-temperature behaviour is very different from the case of weak coupling. For small T it is easy to pull out the temperature dependence of the integral in Eq. (96) and one finds that $\kappa \sim T^3$ for $\nu \neq 0$ and $\kappa \sim T^{1/2}$ for $\nu = 0$.

A nice extension of the above problem has been done by Roy [71] who considered the case where the coupling of the bulk lattice points to reservoirs (γ') was taken to be different from that of the boundary points to the end reservoirs (γ). The quantum mechanical case with Ohmic reservoirs and the linear response regime were studied. For small values of γ' the transition from ballistic to diffusive transport could be seen with increasing system size. It was shown that the current, for any system size, could be written in the form

$$J = \frac{\kappa(T)\Delta T}{N+\ell} \ , \tag{99}$$

where ℓ was an effective mean free path for phonons which depended on γ'. Thus for $N << \ell$ one gets ballistic transport while for $N >> \ell$ one gets diffusive transport. In Fig. (4) the temperature profiles for different system sizes is shown and one can see the transition, from a relatively flat (in the ballistic regime), to a linear profile (in the diffusive regime).

4. Interacting systems in one dimension

In the case of systems with interactions there are few analytic results, for one-dimensional interacting particle systems, and these are all based on use of the Green-Kubo formula. All these theories aim at calculating the equilibrium current-current correlation function $C(t) = \langle \mathcal{J}(0)\mathcal{J}(t)\rangle$. Mainly there are three different theoretical approaches: renormalization group theory of hydrodynamic equations, mode coupling theory and the Peierls-Boltzmann kinetic theory approach. We will discuss these in Sec. (4.1). We will also discuss some exact results, which have been obtained for certain models for which the dynamics is not completely deterministic but includes some stochastic component. All the analytic approaches predict that momentum conserving systems in $1D$ exhibit anomalous transport with conductivity diverging as a power law $\kappa \sim N^\alpha$. However there is disagreement on the precise value of α and the number of universality classes. We will present the results of simulations for various momentum conserving models in Sec. (4.2.1). In general one finds anomalous transport with $\kappa \sim N^\alpha$ and again there is disagreement in

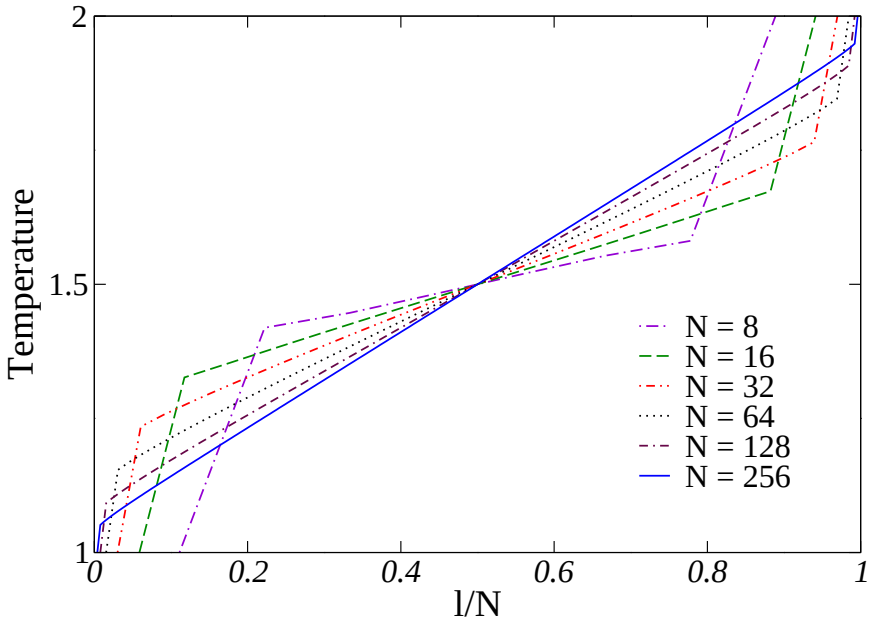

Figure 4. Plot of the temperature profile $\{T_l\}$ as a function of scaled length l/N for different N with $\gamma = 1.0$ and $\gamma' = 0.1$. Here mean free path $\ell \sim 30$ (from [71]).

the value of α obtained in simulations by different groups. However, the evidence seems strong that there is a single universality class with $\alpha = 1/3$.

For momentum non-conserving interacting systems the prediction of theory is that Fourier's law is valid. Simulations also show [Sec. (4.2.2)] that the presence of interactions (nonintegrable) and an external substrate potential are sufficient conditions to give rise to a finite thermal conductivity. Note that momentum non-conserving models are a bit unphysical in the context of heat transport by molecular motion except when one is considering wires and thin films attached to substrates. In the case of electron transport the background ionic lattice naturally provides an external potential for the electron and so momentum non-conservation makes physical sense. We will also briefly discuss a class of rotor models that have been studied in simulations which show Fourier behaviour inspite of absence of an external potential [135, 136]. These models are somewhat special, in the sense that it is more natural to think of the phase space degrees of freedom as local angle variables and thus these models should probably be thought of as angular-momentum conserving rather than linear-momentum conserving models.

4.1. *Analytic results*

4.1.1. Hydrodynamic equations and renormalization group theory

This approach was first proposed by Narayan and Ramaswamy [72]. Here one first notes that a one dimensional ($1D$) system of interacting particles will, at sufficiently large length scales, behave like a fluid. Suppose that the only conserved quantities in the system are the total number of particles, the total momentum and total energy. One can then write hydrodynamic equations to describe the variation, in time and space, of the density fields corresponding to these conserved quantities. Namely we have $\rho(x,t)$, $g(x,t) = \rho(x,t)v(x,t)$, and $\epsilon(x,t)$ for number, momentum and energy densities respectively and where $v(x,t)$ is the local average velocity field. This basically gives the Navier-Stokes equations for a $1D$ fluid. After adding noise terms to account for thermal fluctuations in the system the equations are

given by [72, 73]:

$$\begin{aligned}\partial_t\rho + \partial_x(\rho v) &= 0,\\ \partial_t(\rho v) + \partial_x(\rho v^2) &= -\partial_x p + \zeta\partial_x^2 v + \eta_v,\\ \partial_t\epsilon + \partial_x[(\epsilon+p)v] &= \kappa\partial_x^2 T + \zeta[(\partial_x v)^2 + v\partial_x^2 v] + \eta_\epsilon\ ,\end{aligned} \tag{100}$$

where the noise terms satisfy $\langle\eta_v(x_1,t_1)\eta_v(x_1',t_1')\rangle \propto -k_BT\delta(x_1-x_1')\delta(t_1-t_1')$ and similarly for η_ϵ. The local temperature $T(x,t)$ and pressure $p(x,t)$ are implicit functions of ρ and ϵ. There are two transport coefficients, the viscosity ζ and the thermal conductivity κ. The above equations can be solved in the linear approximation and this gives $C(t) \sim t^{-1/2}$ which in turn implies a divergence of the conductivity. However this divergence also means that the linear approximation is not good and one needs to take into account the nonlinear terms in the Navier-Stokes equations in order to get the correct long time behaviour of various correlation functions. In general this would require a RG analysis but it is argued in [72] that the exponents can be obtained from symmetry considerations. Using the Galilean invariance of the system and the fact that equal time correlations obey equilibrium statistical mechanics they finally obtain:

$$C(t) \sim t^{-2/3}\ . \tag{101}$$

For a finite size system, using the arguments in Sec. (2.1), one puts a upper cut-off $t_N \sim N$ in the Green-Kubo integral and this then gives $\kappa \sim N^{1/3}$. Thus $\alpha = 1/3$. Note that in this treatment, the details of the form of the Hamiltonian are unimportant. The only requirements are the presence of the three conservation laws and also, the interactions should be such that the nonequilibrium state satisfies local thermal equilibrium and should be describable by coarse grained hydrodynamic equations. We note that the possibility of breakdown of hydrodynamic equations in a one-dimensional fluid system has recently been pointed out [74].

An interesting question that arises in the context of the hydrodynamic theory is the behaviour of the other transport coefficient in the equations, *i.e.* , the bulk viscosity ζ. This has not been investigated much except in the work in refn. [75] who, somewhat surprisingly, find that this transport coefficient is finite.

4.1.2. Mode coupling theory

This approach was first applied in the context of heat conduction by Lepri, Livi and Politi [82] and has subsequently been used by several other authors [82, 83, 84, 85, 86, 87, 88, 89]. We will here outline the main steps as described in refn. [87]. Mode coupling theory (MCT) again begins with the realization that the divergence of conductivity is a result of the long time tails of the current-current correlation function which in turn can be attributed to the slow relaxation of spontaneous fluctuations of long-wavelength modes in low dimensional systems. For a $1D$ oscillator chain with periodic boundary conditions one considers the normal mode coordinates of the harmonic lattice which are given by:

$$Q(q) = \frac{1}{\sqrt{N}}\sum_{n=1}^{N}\ x_n\ \exp(-iqn)\ , \tag{102}$$

where the wavenumber $q = 2\pi k/N$ with $k = -N/2+1, -N/2+2, ...N/2$ (for even N). The evolution of a fluctuation at wavenumber q excited at $t = 0$ is described

by the following correlation function:

$$G(q,t) = \frac{\langle Q^*(q,t)Q(q,0)\rangle}{\langle |Q(q)|^2 \rangle} \ . \tag{103}$$

The long time decay rate of this quantity at small q is the main object of interest and MCT is one approach to obtain this. Basically one writes a set of approximate equations for $G(q,t)$ and this is then solved self-consistently. Formally one can in fact write an exact equation for the time evolution of $G(q,t)$. Using the Mori-Zwanzig projection methods [90] one gets the following equation:

$$\ddot{G}(q,t) + \varepsilon \int_0^t \Gamma(q,t-s)\dot{G}(q,s)\, ds + \omega^2(q)G(q,t) = 0 \quad , \tag{104}$$

where the memory kernel $\Gamma(q,t)$ is proportional to $\langle \mathcal{F}(q,t)\mathcal{F}(q,0)\rangle$, with $\mathcal{F}(q)$ being the nonlinear part of the fluctuating force between particles. The coupling constant ϵ and the frequency $\omega(q)$ are temperature dependent input parameters which have to be computed independently. Equations (104) must be solved with the initial conditions $G(q,0) = 1$ and $\dot{G}(q,0) = 0$. The mode-coupling approach proceeds by replacing the exact memory function $\Gamma(q,t)$ with an approximate one, where higher order correlators are written in terms of $G(q,t)$. Consider now the FPU interaction potential $U(x) = k_2x^2/2 + k_3x^3/3 + k_4x^4/4$. In the generic case, in which k_3 is different from zero, the lowest-order mode coupling approximation of the memory kernel gives:

$$\Gamma(q,t) = \omega^2(q)\,\frac{2\pi}{N} \sum_{p+p'-q=0,\pm\pi} G(p,t)G(p',t) \quad . \tag{105}$$

On the other hand for the case $k_3 = 0$, $k_4 \neq 0$, one gets:

$$\Gamma(q,t) = \omega^2(q)\left(\frac{2\pi}{N}\right)^2 \sum_{p+p'+p''-q=0,\pm\pi} G(p,t)G(p',t)G(p'',t) \quad . \tag{106}$$

Here $p\ , p', p''$ range over the whole Brillouin zone $(-\pi,\pi)$. Using either of Eq.(105) or Eq. (106) in Eq. (104) gives a closed system of nonlinear integro-differential equations. The coupling constant ε and the frequency $\omega(q)$ are taken as parameters which can be obtained from the harmonic approximation. The solution of these equations again involves making a number of other approximations and the final result one obtains for $G(q,t)$ at small values of q is the following form:

$$\begin{aligned} G(q,t) &= A(q,t)e^{i\omega(q)t} + c.c \\ \text{where} \quad A(q,t) &= \begin{cases} g(\varepsilon^{1/2}tq^{3/2}) & \text{for } k_3 \neq 0 \\ g(\varepsilon^{1/2}tq^2) & \text{for } k_3 = 0, k_4 \neq 0. \end{cases} \end{aligned} \tag{107}$$

Finally one can relate the current-current correlation function $C(t)$ to the correlator $G(q,t)$. Again making the same approximation of retaining only the lowest order correlation functions one gets:

$$C(t) \propto \sum_q G^2(q,t) \ , \tag{108}$$

and plugging into this the result from Eq. (107), one finally obtains:

$$C(t) \sim \begin{cases} t^{-2/3} & \text{for } k_3 \neq 0 \\ t^{-1/2} & \text{for } k_3 = 0, k_4 \neq 0 \ . \end{cases} \tag{109}$$

Inserting this into the Green-Kubo formula (with a cut-off proportional to N) then gives us $\kappa \sim N^{1/3}$ for the odd potential and $\kappa \sim N^{1/2}$ for the even potential.

Another recent MCT study is by Wang and Li [88, 89] who look at the effect of transverse degrees of freedom on the value of α. They consider a one dimensional chain where the particle positions are now two-dimensional vectors instead of being scalar variables. The Hamiltonian they consider corresponds to a polymer with bending rigidity and is given by:

$$H = \sum_l \frac{\mathbf{p}_l^2}{2m} + \frac{K_r}{2}(|\mathbf{r}_{l+1} - \mathbf{r}_l| - a)^2 + K_\phi \cos(\phi_l) \ , \tag{110}$$

where $\{\mathbf{r}_l, \mathbf{p}_l\}$, for $l = 1, 2...N$ denote two dimensional vectors and $\cos(\phi_l) = -\mathbf{n}_{l-1}.\mathbf{n}_l$ with $\mathbf{n}_l = \Delta\mathbf{r}_l/|\Delta\mathbf{r}_l|$ and $\Delta\mathbf{r}_l = \mathbf{r}_{l+1} - \mathbf{r}_l$. Based on their MCT analysis they suggest that the generic effect of including transverse degrees is to give $\alpha = 1/3$, while for the purely longitudinal model one has $\alpha = 2/5$.

For momentum non-conserving systems MCT predicts a finite conductivity.

4.1.3. Kinetic and Peierls-Boltzmann theory

In the kinetic theory picture, one thinks of a gas of weakly interacting particles, which are the heat carriers. These heat carriers could be molcules in a gas, electrons in a metal or phonons in a crystal. Using the idea that the heat carriers are experiencing random collisions, and hence moving diffusively, one can do a simple minded calculation. This gives us a simple expression for the thermal conductivity, namely $\kappa \sim cv\ell$, where c is the specific heat capacity per unit volume, v the typical particle velocity and ℓ the mean free path of the particles between collisions.

The Boltzmann equation approach gives a more systematic derivation of the results of kinetic theory, and was first developed for the case of molecular gases. In this theory, one writes an equation of motion for the distribution function $f(\mathbf{x}, \mathbf{p}, t)$, where $f(\mathbf{x}, \mathbf{p}, t)d^3xd^3p$ (in $3D$) gives the number of particles in the volume d^3xd^3p. The presence of collisions makes the Boltzmann equation equation nonlinear, and then one has to solve the equation under various approximations. The final result is quite often in the form of the kinetic theory answer, with an explicit expression for the mean free path ℓ. For phonons, the Boltzmann theory of conductivity was developed by Peierls [91]. He wrote the Boltzmann transport equation for the phonon gas and pointed out the importance of lattice momentum non-conserving processes (Umpklapp processes) in giving rise to finite conductivity. Solving the Boltzmann equation in the relaxation time approximation gives a simple kinetic theory like expression for the thermal conductivity, $\kappa \sim \int d\mathbf{q} c_\mathbf{q} v_\mathbf{q}^2 \tau_\mathbf{q}$, where $\tau_\mathbf{q}$ is the time between collisions, and $\mathbf{q}$ refers to different phonon modes of the crystal. The relaxation time $\tau_\mathbf{q}$ can get contributions from various sources, such as phonon-phonon interactions and impurity scattering, and its calculation from first principles is one of the main tasks. In three dimensional solids, the Peierls-Boltzmann theory is well-developed [92, 93] and probably quite accurate. One worry here is that the meaning of the distribution $f(\mathbf{x}, \mathbf{q}, t)$ for phonons is not really clear, since phonons are extended objects. The recent work of Spohn [94] tries to give a rigorous basis for the phonon Boltzmann equation for a crystal with a weakly anharmonic onsite potential. We note that, as far as making definite predictions (starting from a given

Hamiltonian) on the actual conductivity of a system and properties such as the temperature dependence of the conductivity, the kinetic theory approach probably has more chance of success than the other two approaches described before.

Let us now consider the application of the kinetic theory approach to the one dimensional case. If we look at the result $\kappa \sim \int dq c_q v_q^2 \tau_q$, we see that a divergence with system size can arise because the relaxation time τ_q, and correspondingly the mean free path $\ell_q = v_q \tau_q$, becomes large at small q. Let us assume that c_q, v_q are constants, and that τ_q has the power-law dependence $\tau_q \sim q^{-a}$. Then all modes with $q < q_m \sim L^{-1/a}$ travel ballistically and this immediately gives $\kappa \sim L^{1-1/a}$, and for $a > 1$ one would get a diverging conductivity.

In a way the kinetic approach is similar to the MCT method. Here too, one tries to calculate the rate of decay of long-wavelength fluctuations at small q, but now using a different approximation scheme. The current-current correlation function is then related to this decay constant. The Kinetic theory approach for the FPU chain was first considered by Pereverzev [95] who studied the model with $k_3 = 0$ and a small non-zero value for k_4. It was noted that the approximate time evolution of a fluctuation in the average energy ϵ_q of a mode with wavenumber q is given by the homogeneous classical linearized Peierls equation. This equation is then brought to the following form, corresponding to the relaxation time approximation:

$$\frac{d\langle \epsilon_q(t) \rangle}{dt} = -\frac{1}{\tau_q}(\langle \epsilon_q \rangle - k_B T) \ , \tag{111}$$

where one has an explicit form for τ_q. For small q, making some more approximations enables one to evaluate τ_q and one finds $\tau_q \sim q^{-5/3}$. Finally using the same set of approximations and in the limit $N \to \infty$ one can show that:

$$C(t) = \frac{2k_B^2 T^2}{\pi} \int_0^\pi dq e^{-t/\tau_q} v_q^2 \ , \tag{112}$$

where v_q is the phonon group velocity. At small q the phonon velocity $v_q \sim$ const and the above equation gives:

$$C(t) \sim t^{-3/5} \ . \tag{113}$$

This then implies $\kappa \sim N^{2/5}$. In fact, the arguments given at the beginning of this paragraph directly give this (putting $a = 5/3$), and one does not need to find $C(t)$.

The kinetic theory approach has been made more rigorous by the work of Lukkarinen and Spohn [96]. They also work with the linearized collision operator and make the relaxation time approximation, and for the quartic FPU chain they confirm the result in [95], namely $C(t) \sim t^{-3/5}$. However they point out the possibility that the kinetic theory approach may not be able to predict the correct long-time decay of the correlation function. Another paper using the linearized Peierls-Boltzmann equation for the quartic Hamiltonian also finds $\kappa \sim N^{2/5}$ [97]. Finally a quantum calculation of the phonon relaxation rate at small q has been carried out in [98, 99]. They studied both the cubic and quartic FPU chain and obtained relaxation times $\tau_q \sim q^{-3/2}, \ q^{-5/3}$ for the two cases respectively.

For the case of momentum non-conserving systems, Lefevere and Schenkel [130] and later Aoki et al. [131] have used the kinetic theory approach for the case of weak anharmonicity and obtained a finite conductivity.

4.1.4. Exactly solvable model

A harmonic chain with a energy conserving stochastic dynamics was considered by Kipnis et al. [76] who could prove exactly that the model satisfied Fourier's law. The dynamics was momentum non-conserving and completely stochastic so it is not surprising that Fourier's law was obtained. Models with self-consistent reservoirs can also be viewed as stochastic models (but with Hamiltonian components in the dynamics) where energy is conserved on average, while momentum is not and again Fourier's law is satisfied.

Recently a similar stochastic model, but in which total momentum conservation was also enforced, was introduced by Basile et al. [77, 78]. In their lattice model the dynamics consisted of two parts. Apart from a deterministic Hamiltonian dynamics the system was subjected to a stochastic dynamics which conserved both total energy and momentum exactly. The stochastic dynamics consisted of a random exchange of momentum between three neighboring particles (in $1D$) while conserving both energy and momentum. Thus a triplet of particles with momenta (p_{l-1}, p_l, p_{l+1}) is chosen and this set performs a diffusive motion on the curve given by:

$$p_{l-1} + p_l + p_{l+1} = \text{const.}$$
$$\frac{p_{l-1}^2}{2m} + \frac{p_l^2}{2m} + \frac{p_{l+1}^2}{2m} = \text{const.}$$

The Hamiltonian of the system was taken to be that of a harmonic system. A Fokker-Planck equation for the probability density $P(\mathbf{x}, \mathbf{p}, t)$ could be written, which in $1D$ is given by:

$$\frac{\partial P}{\partial t} = (\hat{L}^H + \gamma \hat{S})\ P\ , \tag{114}$$

where $\hat{L}^H$ is the usual Liouville operator for the given Hamiltonian and $\hat{S}$, the generator of the stochastic perturbation of strength γ, has the form

$$\hat{S} = \frac{1}{6} \sum_l \hat{Y}_l^2,$$
$$\text{with}\ \ \hat{Y}_l = (p_l - p_{l+1})\partial_{p_{l-1}} + (p_{l+1} - p_{l-1})\partial_{p_l} + (p_{l-1} - p_l)\partial_{p_{l+1}}\ .$$

The authors were able to compute exactly an explicit form for the current-current correlation function $C(t)$, for system size $N \to \infty$, and from this they found the following asymptotic long-time behaviour:

$$C(t) \sim \begin{cases} t^{-1/2} & \text{for no pinning} \\ t^{-3/2} & \text{with pinning.} \end{cases} \tag{115}$$

Plugging this into the Green-Kubo formula one gets $\alpha = 1/2$ in the unpinned case, while for the pinned case a finite conductivity is obtained. One can argue that the stochastic dynamics in a way mimics anharmonicity and the problem considered corresponds to an even interaction potential. The latest prediction from MCT also gives $\alpha = 1/2$, which agrees with the result from this model. However all simulation results of momentum conserving interacting Hamiltonian models give exponents quite far from this value (between $0.3 - 0.4$). The exponent $\alpha = 1/2$ then comes as quite a surprise. One possibility is that the choice of a harmonic Hamiltonian makes

the model special, and thus solvable, and at the same time makes it a non-generic case.

Some simulations with a dynamics which is roughly similar to the above stochastic dynamics were recently done with FPU type anharmonic terms included in the Hamiltonian [79]. These are equilibrium simulations using the Green-Kubo formula. The authors have argued that their results support the two-universality class scenario. It will be interesting to understand in more details the role of the Hamiltonian part of the dynamics in determining the exponent α in this model.

More recently, a similar one-dimensional stochastic model with random two particle momentum exchanges has been numerically [80] and analytically [81] studied, for the nonequilibrium case with Langevin heat baths attached at the two ends. Apart from confirming the exponent $\alpha = 1/2$, these studies have also looked at the temperature profiles. An analytic expression for the temperature profile was obtained and it was noted that the profiles were very similar to those obtained for FPU chains.

4.2. *Results from simulation*

4.2.1. Momentum conserving models

Gas of elastically colliding particles of two masses: One of the simplest model of interacting particles that one can consider is a gas of elastically colliding point particles where the boundary particles interact with thermal reservoirs, usually modeled by Maxwell boundary conditions. If all the particles have equal masses then this model, without reservoirs, is the so-called Jepsen model [100]. As far as heat conduction properties are concerned the model is somewhat trivial. This is because at each collision the particles simply exchange momentum and so the net heat transfer can be calculated by considering a single particle that is bouncing between the hot and a cold walls. One finds a system- size independent heat current $J = k_B^{3/2}(2m/\pi)^{1/2}\rho(T_L^2T_R - T_R^2T_L)/(T_L^{1/2}T_R + T_R^{1/2}T_L)$, where ρ is the particle density, and a flat temperature profile given by $T = (T_LT_R)^{1/2}$. Thus this model is somewhat like the ordered harmonic chain. However the model becomes interesting and non-trivial if one considers a dimerized model where alternate particles have different masses say m_1 and m_2. In this case one finds a current which decays with system size, and a slowly varying temperature profile.

The diatomic hard particle gas model was first studied by Casati [101] but the numerical results were not sufficient to draw any definite conclusions. This model, along with the diatomic Toda lattice, were later studied by Hatano [102]. Using nonequilibrium simulations and system sizes upto $N = 5000$, an exponent $\alpha \approx 0.35$ was obtained for both these models. The current-current correlation function was also evaluated for a periodic closed system and it was found that $C(t) \sim N^{-0.65}$ consistent with the nonequilibrium results. Subsequently, a number of further studies were made using both nonequilibrium simulations, and also the Kubo formalism and using much larger system sizes. Unfortunately there is not much agreement on the numerically obtained value of the exponent. The various reported values include: Garrido et al. ($\alpha = 0$ implying Fourier behavior) [103, 104, 105], Dhar ($\alpha \approx 0.2$) [106], Grassberger et al. ($\alpha \approx 0.33$) [108], Savin et al. ($\alpha \approx 0.2$) [107] and Casati et al. ($\alpha \approx 0.25$) [109]. However, based on the theoretical predictions, there seems reason to believe that the value obtained by Grassberger et al. is the correct one and here we will discuss their results in some detail. We also mention here the work of Cipriani et al. [110] who performed zero-temperature studies on diffusion of localized pulses and using a Levy walk

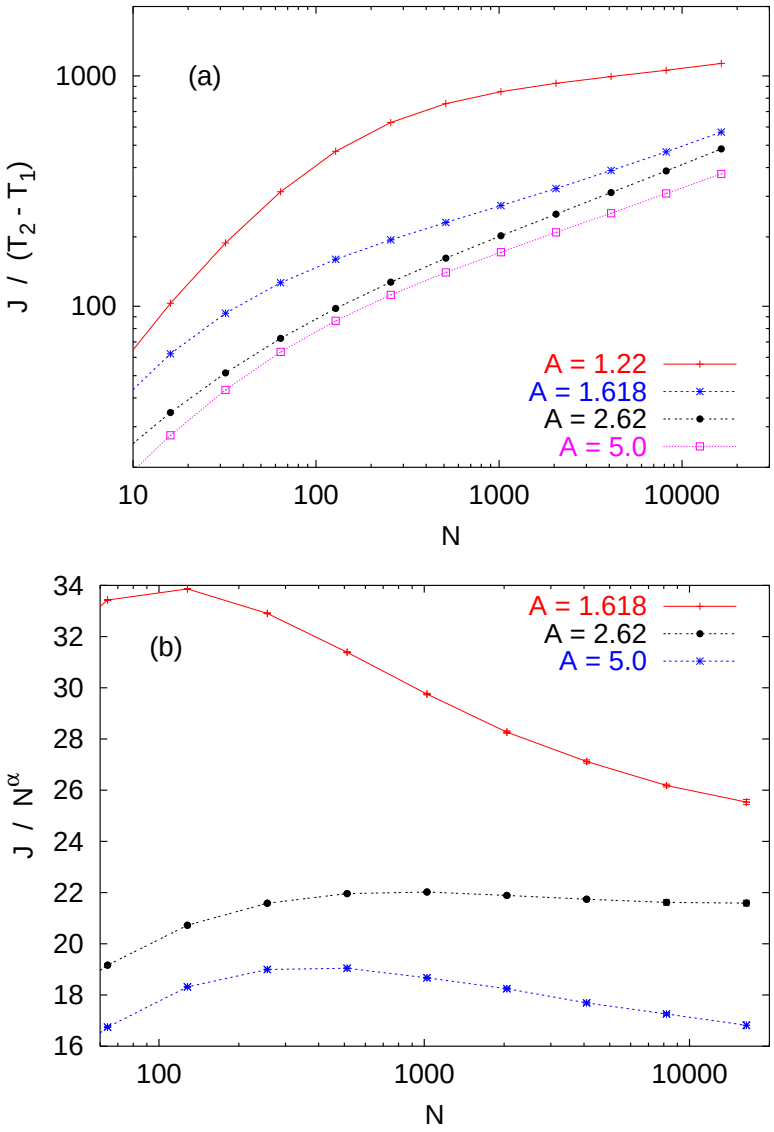

Figure 5. (a): Log-log plot of $J/(T_2 - T_1)$ versus N for four values of the mass ratio A. (b): Part of the same data divided by N^α with $\alpha = 0.32$, so the y-axis is much expanded (from [108]).

interpretation concluded that $\alpha = 0.333 \pm 0.004$.

We now present some of the results obtained by Grassberger et al. [108]. Apart from looking at much larger system sizes (upto $N = 16384$), they made the observation that the asymptotic behaviour is easier to observe at some optimal value of the mass ratio $A = m_2/m_1$. It was argued that $A = 1$ and $A = \infty$ were special integrable limits where one would clearly get ballistic and non-typical behavior. If the value of A was too close to 1 or too large then one would have to go to very large system sizes to see the correct asymptotic form. However by choosing an appropriate value of A, one can reach asymptotic behaviour much faster. This feature can be seen in Fig. (5) where the system size dependence of the current for different values of A is given. One can see that for $A = 2.62$, asymptotics is reached faster than for $A = 1.618$ and $A = 5.0$. The value of the exponent obtained from this data was $\alpha = 0.32^{+0.03}_{-0.01}$. Equilibrium simulations were also performed and in Fig. (6) results are shown for the current-current autocorrelation function obtained for a periodic system. For large system sizes one can see a $t^{-0.66}$ decay with a cutoff at $t \propto N$. This again gives $\alpha = 0.34$ in agreement with the value obtained from

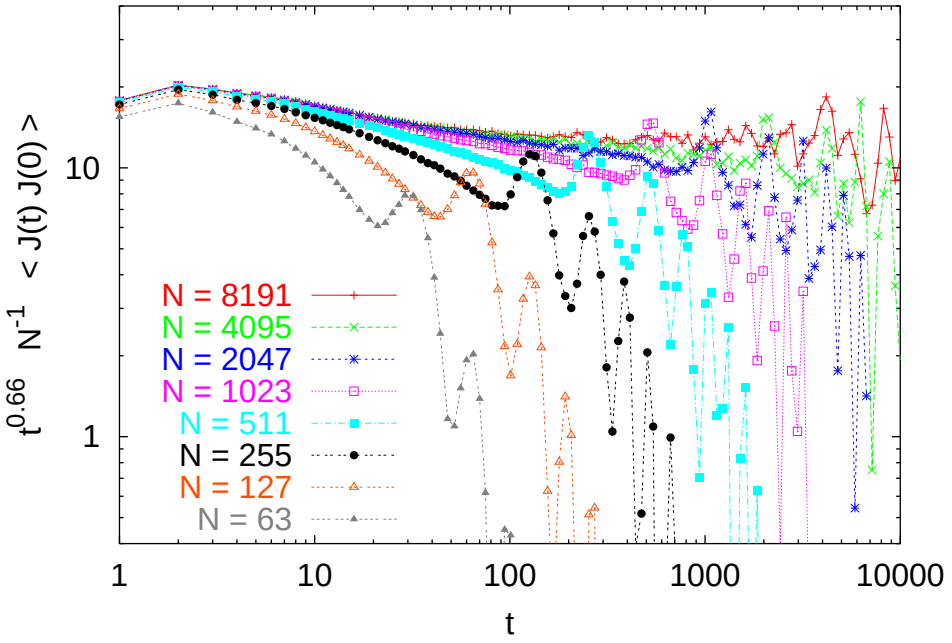

Figure 6. Total heat current autocorrelation, $t^{0.66}N^{-1}\ \langle J(t)J(0)\rangle$ for $A = 2.2$ and $T = 2$. Total momentum is $P = 0$ (from [108]).

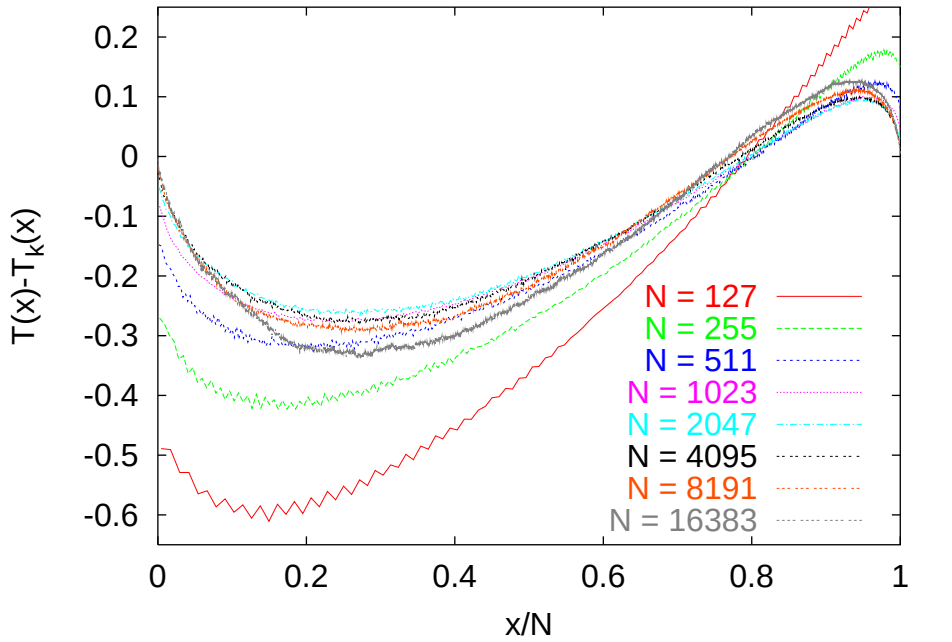

Figure 7. $T(x) - T_k(x)$ against x/N for $A = 1.618$. This shows non-convergence of the steady state temperature profile to the profile expected from the $\kappa \sim T^{1/2}$ result of kinetic theory (from [108]).

the nonequilibrium simulation.

Some interesting features were seen in the temperature profiles also and we now discuss these. Simple kinetic theory predicts that the thermal conductivity of a hard particle gas should have a temperature dependence $\kappa \sim T^{1/2}$ (this can also be obtained from the Green-Kubo formula). Now if we plug this in Fourier's law then, with specified boundary temperatures, one easily obtains the following nonlinear

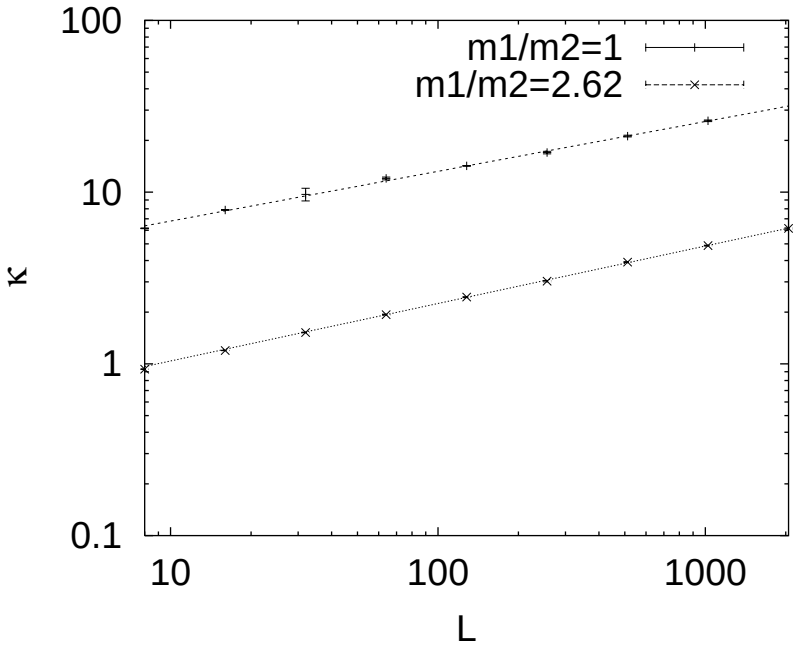

Figure 8. Log-log plot of the conductivity as a function of the number of particles for the random collision model introduced in [111]. The upper plot is for all the particles with mass ratio $A = 1$, while the lower plot is for $A = 2.62$. The slopes for the two plots are 0.29 ± 0.01 and 0.335 ± 0.01 (from [111]).

temperature profile:

$$T_k(x) = [T_L^{3/2}(1 - x/N) + T_R^{3/2} x/N]^{2/3}. \tag{116}$$

In refn. [106], it was noted that a convergence, of the actual nonequilibrium temperature profile $T(x)$, to the kinetic theory prediction $T_k(x)$ given above, seemed to take place. However the study in [108] found that this apparent convergence stops as one looks at larger systems and in fact one finds $T(x) - T_k(x)$ attains a non-zero profile for $N \to \infty$. This is shown in Fig. (7). This result indicates that there is a problem in writing Fourier's law in the form $J = -\kappa_N \nabla T$, with κ_N defined as a length dependent conductivity. We will see similar problems with other $1D$ models.

Random collision model: In studies on heat conduction, one often finds that a faster convergence to the asymptotic system size limit can be obtained by particular choices of model and parameter values. In this context one should mention a stochastic model introduced by Deutsch and Narayan [111]. They consider a binary mass gas of hard point particles where any particle's motion is strictly confined to one dimensions while its momentum is a two dimensional vector (p_x, p_y). During a collision between two particles their momenta gets changed randomly while conserving total energy and both components of total momentum. Physically one can think of this model as approximating a system of small particles with rough surfaces, moving in a narrow tube. The results of nonequilibrium simulations for two different mass ratios is shown in Fig. (8). For the case $m_1/m_2 = 2.62$, at system sizes as small as $N \sim 10^3$, one already gets $\alpha = 0.335 \pm 0.01$, which is close to the expected value $\alpha = 1/3$.

Fermi-Pasta-Ulam chain: The Fermi-Pasta-Ulam (FPU) model consists of an oscillator chain with harmonic as well as anharmonic nearest neighbour interparticle interactions. This model was first studied by the authors in a landmark paper [112] where they wanted to verify the common assumption of statistical mechanics that anharmonic interactions should lead to equilibration and equipartition.

Surprisingly the numerical experiments on the FPU chain gave a negative result, *i.e.* the chain *failed to equilibrate*. Understanding the FPU results led to the development of new areas and concepts in physics [113]. It is probably fair to state that a complete understanding of the problem is still lacking. For example it is believed that for high enough energy densities and large system sizes one may achieve equilibration but there are details which are not yet understood precisely [114].

What about heat transport across the FPU chain ? Clearly this is the simplest model to study in order to see the effect of anharmonicity on heat transport. One might suspect that the equilibration problem of the FPU chain is likely to show up in some way when one looks at transport properties, especially so when one thinks in terms of the Green-Kubo formula. It turns out that a FPU chain connected to heat reservoirs is better-behaved. It can in fact be proved rigorously that a FPU chain connected to equal temperature Langevin heat baths at its two ends will always equilibrate. At long times it will converge uniquely to the appropriate Boltzmann-Gibbs distribution. Also it can be shown that even with unequal temperature baths (stochastic or Hamiltonian) the system reaches a unique nonequilibrium steady state [115] and this is very reassuring when one begins to consider heat transport studies in the FPU chain.

The first study of heat conduction in the FPU chain was by Lepri et al. [116] who considered an interparticle potential of the form $U(x) = k_2x^2/2 + k_4x^4/4$ and performed nonequilibrium simulations with Nose-Hoover baths. Looking at system sizes upto $N = 400$ they obtained $\alpha = 0.55 \pm 0.05$. In a subsequent paper [82], by studying systems upto $N = 2048$, they obtained $\alpha \approx 0.37$. They also found a highly *nonlinear and singular* temperature profile and noted that this was true even for relatively small temperature differences applied to the ends. We will comment more on the temperature profile of the FPU chain later in this section.

Since the important work of [116], a large amount of numerical and analytical work has been carried out on heat conduction in the FPU chain. We first summarize the various analytic results discussed in Sec. (4.1). We assume that the interparticle interaction is of the general FPU form $U(x) = k_2x^2/2 + k_3x^3/3 + k_4x^4/4$. The predictions from theory are then:

(i) Renormalization group theory of hydrodynamic equations: This predicts that there is only one universality class with $\alpha = 1/3$.

(ii) Mode-coupling theory: This predicts that there are two universality classes depending on the parity of the leading nonlinearity in the Hamiltonian. For the case where the leading nonlinearity is cubic, *i.e.* $k_3 \neq 0$, the prediction is $\alpha = 1/3$ while for $k_3 = 0, k_4 \neq 0$, the prediction is $\alpha = 1/2$.

(iii) Kinetic theory and the Peierls-Boltzmann equation approach: This gives $\alpha = 2/5$ for the quartic case.

Results of simulations: As we have seen in the last section simulations of hard particle gases [108, 110, 111] seem to indicate a value $\alpha = 1/3$ for the heat conduction exponent, though even here the issue is not completely settled [107, 109]. On the other hand, numerical simulations of oscillator chains, including FPU chains, give various exponents [2, 82, 84, 88, 116] for different systems, often slightly higher than 1/3. This seems consistent with early results from mode-coupling theory (MCT), which predicted $\alpha = 2/5$. The most recent MCT analysis [86, 87] predicts that $\alpha = 1/2$ for potentials $U(x)$ with quartic leading nonlinearity while for potentials with cubic nonlinearity, there seems to be agreement between different theories about $\alpha = 1/3$. Here we will focus on simulations for the even potential only. We will discuss the results of the most recent simulations by Mai et al. [118] of the even potential FPU model and another simulation by Dhar and Saito [157] of the alternate mass FPU chain.

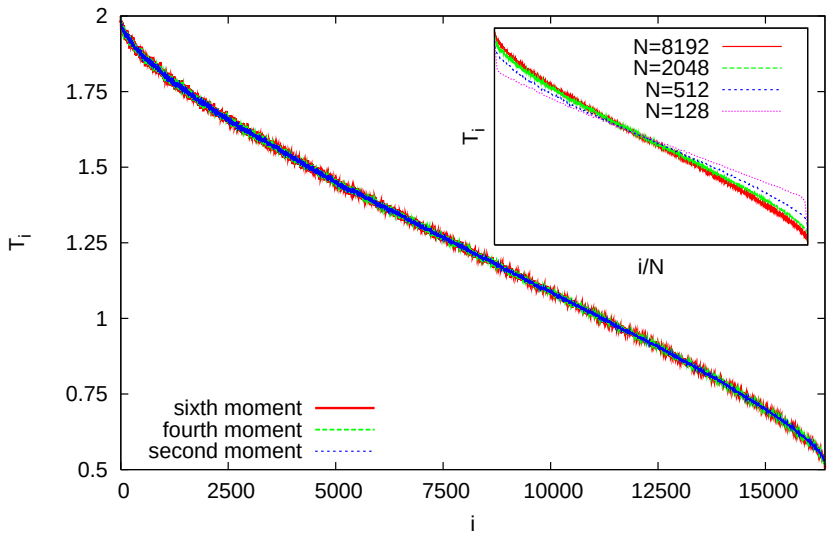

Figure 9. Kinetic temperature profile for a FPU-β chain with $N = 16384$, $T_L = 2.0$, $T_R = 0.5$ and $\gamma = 2.0$. The temperature evaluated from the first three even moments of the velocity are shown; their agreement indicates a Gaussian velocity distribution. (Inset) Normalized temperature profiles for different N (from [118]).

An important aspect addressed in the simulations by Mai et al. was the effect of boundary conditions. It is well known [2] that the of coupling of a system to thermal reservoirs leads to so-called contact resistances. These show up, for example, in the jumps that one observes in the temperature profile in such a system. It is only for sufficiently large system sizes, when the resistance of the system is much larger than the contact resistance, that one can neglect the contact resistance. In simulations where one is interested in determining the precise dependence of current on system size, it is important to ensure that one has reached the required system size where contact resistances are negligible compared to the actual system resistance. This point has been discussed in some detail by Aoki and Kusnezov [117]. The study by Mai et al. ensured this by performing simulations with two different baths, namely, stochastic white noise baths and the deterministic Nose-Hoover bath. Further they did simulations for different coupling strengths of the system to reservoir. It was found that for small system sizes the current values were significantly different (for the same applied temperature difference). This is expected since the contact resistance, which is different for the different boundary conditions, dominates the transport current. However at large system sizes, the actual values of the currents for all the different cases tend to converge. In this system-size regime one is thus assured that boundary effects have been eliminated and one can then extract the correct exponent.

The simulation in [118] was done for parameter values $k_2 = 1, k_3 = 0, k_4 = 1$ and $m = 1$. The temperature at the two ends were fixed at $T_L = 2.0$ and $T_R = 0.5$. Both white noise baths with coupling parameter γ and Nose-Hoover baths, with coupling parameter θ were studied. The white noise simulations were done using a velocity-Verlet type algorithm [119], while the Nose-Hoover simulations were implemented using a fourth order Runga-Kutta integrator. Time steps of order $dt = 0.0025 - 0.005$ were used and, for the largest system size ($N = 65536$), upto 10^9 equilibration steps and an equal number of data-collecting steps were used.

The temperature profile for a chain of size $N = 16384$ is shown in Fig. (9). The temperature is defined through the first three even moments of the velocity

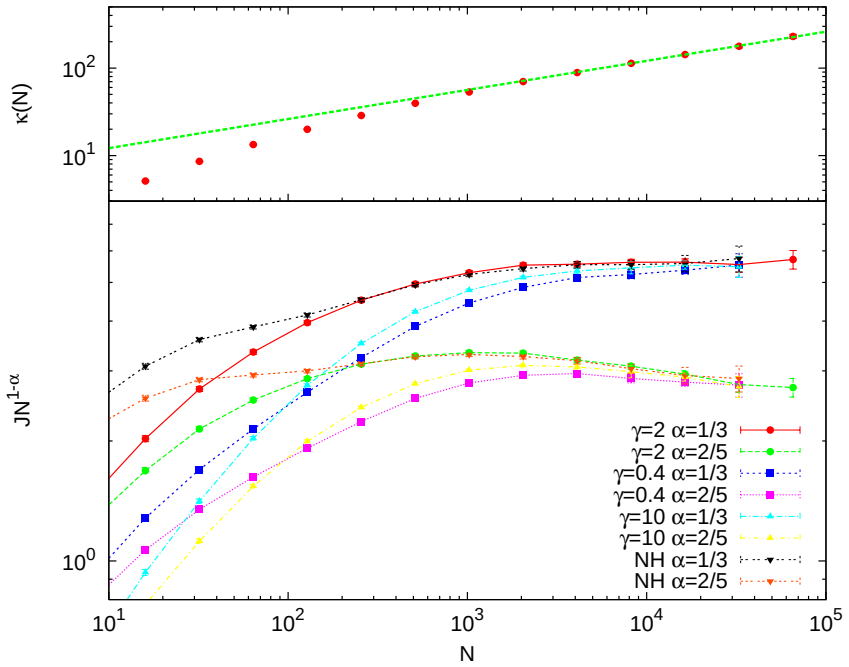

Figure 10. (Top) Conductivity versus N. The last five points fit to a slope of $\alpha = 0.333 \pm 0.004$. (Bottom) $JN^{1-\alpha}$ versus N for $\alpha = 1/3$ and $\alpha = 2/5$. In the large N regime, α is definitely less than 2/5 and appears to agree quite well with the 1/3 prediction for all data sets. Langevin baths with $\gamma = 0.4, 2$ and 10, and one data set with Nose-Hoover baths, are shown (from [118]).

as $T_l = \langle v_l^2 \rangle$, $T_l = (\langle v_l^4 \rangle/3)^{1/2}$ and $T_l = (\langle v_l^4 \rangle/2 - \langle v_l^6 \rangle/30)^{1/3}$ respectively. Their agreement indicates that local thermal equilibrium has been achieved and the local velocity distribution is close to Gaussian. Also we notice that the boundary jumps are almost absent for this system size. The inset shows smaller system sizes where the boundary jumps, arising from the contact resistance, can be clearly seen. As noted and discussed earlier by Lepri et al.[2] the temperature profile is nonlinear and this feature seems to be *present even for small temperature differences* and is another indication of anomalous transport. As for the hard particle case this also indicates that one cannot find the temperature profile using a temperature (and system size) dependent conductivity in Fourier's law.

In Fig. (10) (upper figure), the conductivity defined as $\kappa(N) = JN/\Delta T$ is plotted against system size. This data gives

$$\alpha = 0.333 \pm 0.004 \ . \tag{117}$$

The results of various simulation runs with Langevin baths with different damping constants $\gamma = 0.4, 2$, and 10 as well as the deterministic Nose-Hoover thermostat is shown (lower figure) in Fig.(10). This compares the RG prediction ($\alpha = 1/3$) and the old MCT prediction ($\alpha = 2/5$) for systems with these different baths and bath parameters. As can be seen in the figure, an asymptotic exponent of 1/3 is attained for *all* these systems, whereas the apparent exponents for smaller N depend on system parameters. It is possible to understand the deviation of the apparent exponent from 1/3 for small system sizes. As shown in refn. [2], if the damping constant for the Langevin baths is very large or small, there is a large 'contact resistance' at the boundaries of the chain. The current only depends weakly on N, resulting in an apparent $\alpha > 1/3$ (similar considerations apply to

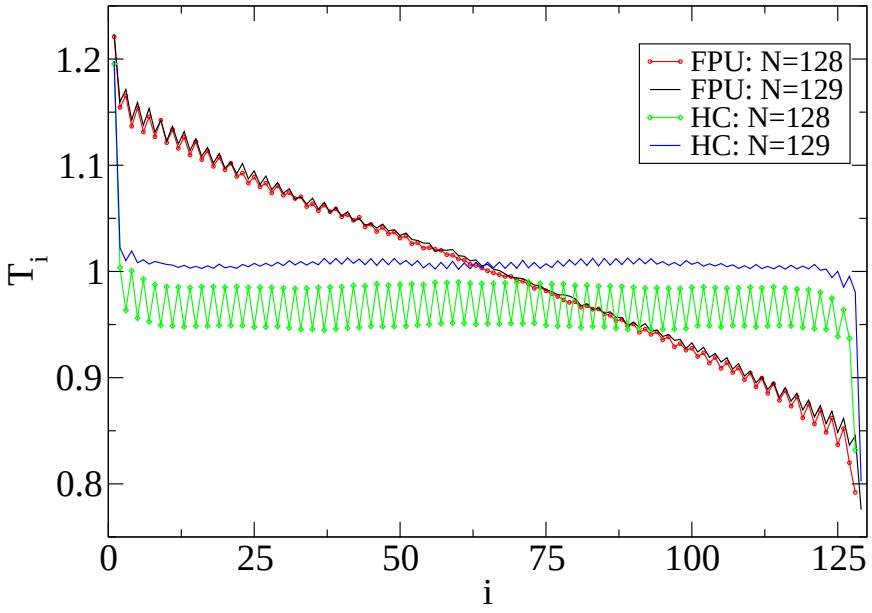

Figure 11. Temperature profiles for alternate mass chains with FPU interactions ($k_2 = 1, k_4 = 1$) compared to those with purely harmonic interactions ($k_2 = 1$). Results for chains of even ($N = 128$) and odd lengths ($N = 129$) are shown.

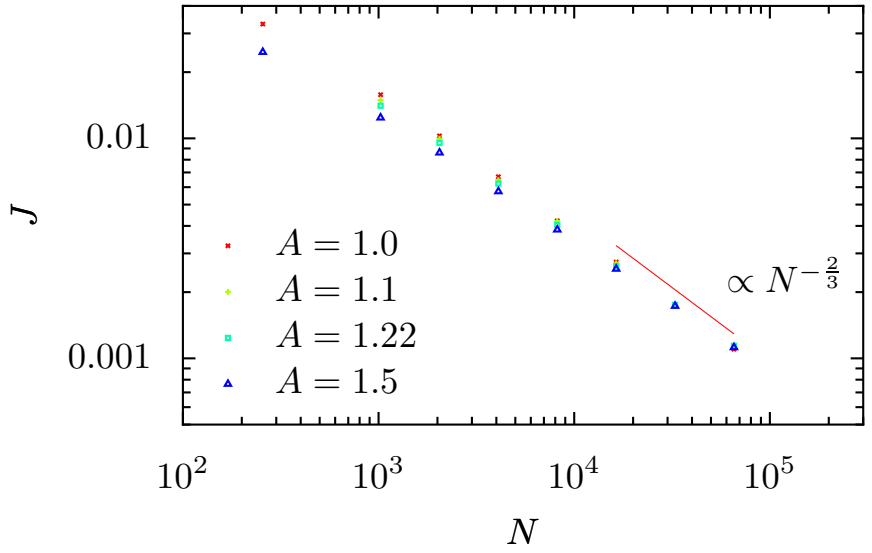

Figure 12. Plot of the heat current J versus system size in the alternate mass FPU chain for different values of the mass ratio $A = 1.0, 1.1, 1.22$ and 1.5 (from [157]).

Nose-Hoover baths). This is confirmed by the plots in the figures: the plot for $\gamma = 2$ reaches the asymptotic limit fastest, whereas $\gamma = 0.4, 10$ have apparent exponents closer to 0.4 for small N.

Thus the simulations of Mai et al. seem to give good evidence for $\alpha = 1/3$ in the quartic FPU model and hence gives support for the idea of a single universality class. A discussion on these results is contained in refns. [120, 121]. We note that the new prediction of $\alpha = 1/2$ from MCT appears to be even harder to verify from simulations.

Alternate mass FPU chain: Further support for the value $\alpha = 1/3$ in the FPU system and its universality comes from recent simulations of an alternate mass FPU chain [157]. In this model one considers a chain with masses of particles

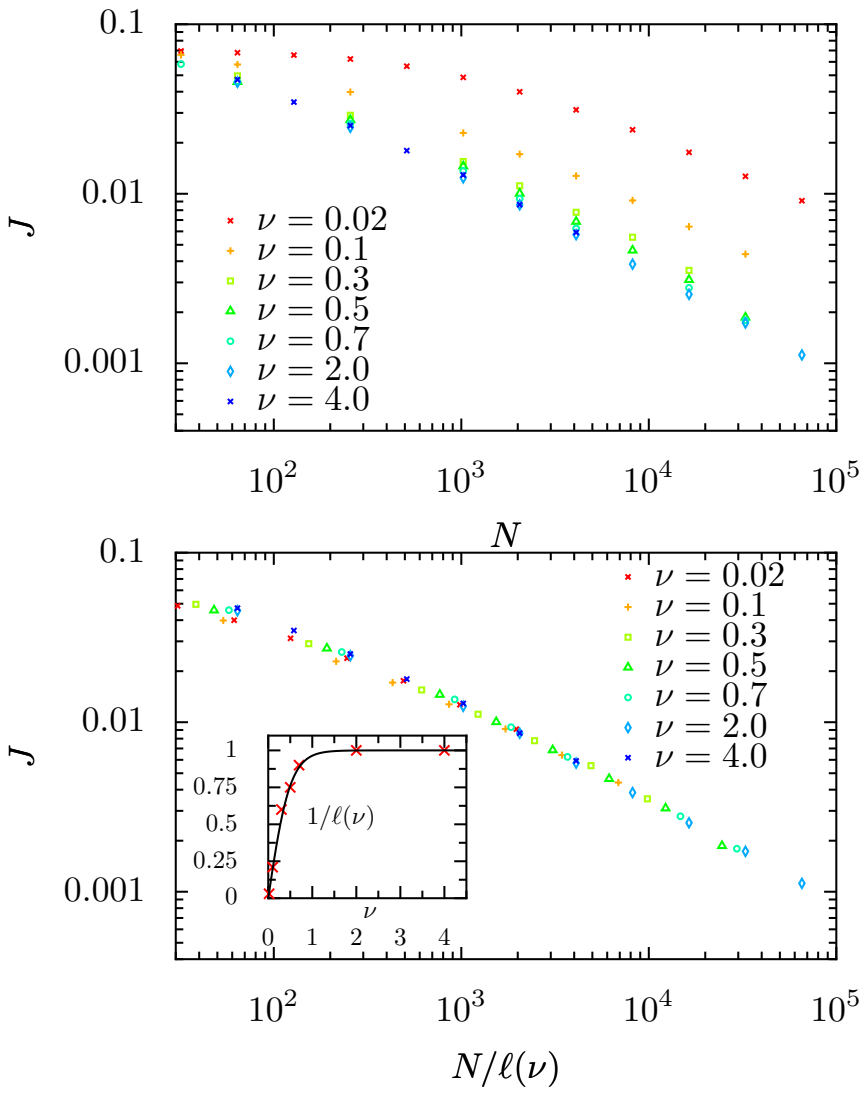

Figure 13. Plot of the heat current J versus system size for the alternate mass FPU chain, for different values of $\nu \equiv k_4$ and with the mass ratio $A = 1.5$ (a). Fig (b) shows the same data plotted with a scaled x-axis (from [157]).

at all even numbered sites being m_1 and at odd numbered sites being m_2 with their ratio being $A = m_1/m_2$. This system was first studied in [118] where it was noticed that the temperature profile showed peculiar oscillations whose amplitude seemed to decay as $N^{-1/2}$ with system size and scale linearly with the applied temperature difference. This can be seen in Fig. (11). At the hotter end the lighter particles have a higher kinetic temperature, while at the colder end, the heavier particles are hotter. It was pointed out in refn. [118] that the temperature oscillations make it difficult to define a local equilibrium temperature even at a coarse grained level. Temperature oscillations can in fact be seen even in an ordered binary mass harmonic chain but there seem to be some significant differences. In the harmonic case, there is a big difference between the case where N is even and that where N is odd. This can be seen in Fig. (11) where we plot the temperature profiles for chains of length $N = 128$ and $N = 129$ for both the FPU chain and the harmonic chain with $m_1 = 0.8$ and $m_2 = 1.2$. For the harmonic case the oscillations for even

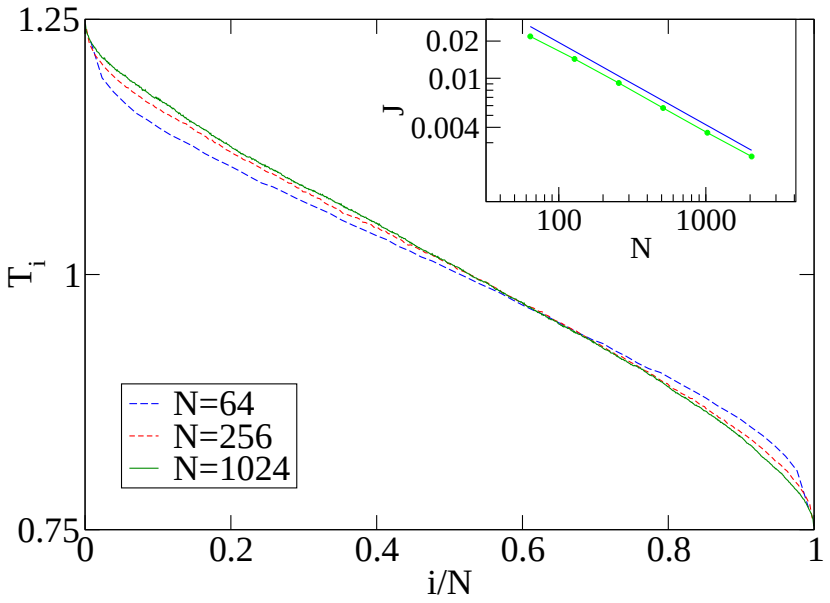

Figure 14. Plot of the temperature profile in the double-well potential model for different system sizes. The inset shows the system size dependence of the current and the straight line drawn has slope $-2/3$. Error bars are much smaller than symbol sizes. The parameter values for the figure are $k_2 = -1, k_4 = 1, T_L = 1.25, T_R = 0.75$ and bath coupling $\gamma = 1$.

N are large and do not decrease with system size while those for odd N decrease with system size. In the FPU case there is not much difference between a chain with odd or even number of particles. Also for the harmonic case, in the bulk, the heavier particles are always hotter.

However, even though there appears to be a problem in defining a local temperature, one can still measure the system size dependence of the current in this system and this was done in refn. [157]. They studied the size dependence of the current for different values of the mass ratio A, keeping the average mass $(m_1 + m_2)/2$ constant. Remarkably it was found that at large enough system sizes the currents for different A all tend to converge to the same value. This can be seen in Fig. (12) where one can see that the exponent is again as that at $A = 1$, *i.e.* $\alpha \approx 0.33$. In this paper the authors next took a fixed value of $A = 1.5$ and studied the effect of changing the interparticle interaction strength (denoted as $\nu = k_4$ in the paper). These results for current for different system sizes are shown in Fig. (13). For small system sizes, one sees a flat region which is expected since for system sizes much smaller than the phonon-phonon scattering length scale, the system will behave like a harmonic chain. The scattering length should be larger for smaller ν and this can be seen in the plot. At larger system sizes, all the curves tend to show the same decay coefficient with $\alpha \approx 0.33$. A nice collapse of the data was obtained by scaling the system size by a length factor $\ell(\nu)$ and this is shown in Fig. (13b). The ν-dependence of the length parameter seems to be given by $\ell(\nu) = 1/\tanh(2\nu)$. A surprising point is that for any fixed system size, the value of the current saturates to a constant non-zero value as $\nu \to \infty$.

Double-well potential: It is interesting to consider simulation results obtained for the FPU interaction potential $U(x) = k_2x^2/2 + k_4x^4/4$ with *negative* k_2 in which case we have a double-well potential. This case was first studied in [135] which had initially reported a finite conductivity for this model but later it was found to have a power law divergence [2]. Here we present some new simulation results for

this model which in fact show that this model exhibits a fast convergence to the asymptotic regime with exponent $\alpha = 1/3$. The parameter values $k_2 = -1, k_4 = 1$ and $T_L = 1.25, T_R = 0.75$ were considered. The temperature profiles in this system for different system sizes are shown in Fig. (14) and are similar to the FPU profiles [Fig. (9)] except that the boundary jumps are smaller. The inset of the figure shows a plot of J as a function of N. One can see that that by around $N = 512$ the curve has reached the expected asymptotic slope corresponding to $\alpha = 1/3$. Thus we again see evidence for $\alpha = 1/3$.

Discussion: In the absence of a rigorous proof it is fair to say that the question of universality of the heat conduction exponent and its precise value, in momentum conserving interacting systems in one dimensions, is still an open problem. This is especially more so since all the analytic methods and the exact result discussed in Sec.(4.1) rely on use of the Green-Kubo formula for a closed system. As pointed out in sec (2.2) the use of this formula and interpretation in systems with anomalous transport is not clear. The simulation results that we have presented in this review strongly suggest a single universality class, with $\alpha = 1/3$, for momentum conserving interacting systems in $1D$. However one should probably bear in mind that in simulations, one can never really be sure that the asymptotic system size limit has been reached. It is possible for exponents to change in unexpected ways when one goes to larger system sizes.

4.2.2. Momentum non-conserving models

We will now look at heat conduction in one dimensional chains where the particles experience, in addition to interparticle interactions, also external potentials which physically can be thought of as arising from interactions with a substrate. One of the first verification of Fourier's law in computer simulations was obtained by Casati et al. in the so-called ding-a-ling model [101, 122]. In this model one considers a system of equal mass hard point particles which interact through elastic collisions and where alternate particles are pinned by harmonic springs placed at fixed distances. The particles in between the pinned ones move freely. Clearly momentum is not conserved and the authors, by studying system sizes upto $N = 20$, found evidence for diffusive behaviour. They calculated the thermal conductivity using both nonequilibrium simulations as well as using the Kubo formula and found good agreement between the two. We note that the system sizes studied in this paper are clearly too small to arrive at definite conclusions. Larger system sizes with the same parameter values were studied later by Mimnagh and Ballentine [123]. They found that in fact the conductivity again started to increase as one went to larger sizes. Finally though, at system sizes $N \sim 400$, the conductivity again saturated at a new value which is much higher than that obtained in [122]. This example nicely demonstrates the need for caution in drawing conclusions from small size data (also see discussion in [2] on these results).

Since the work of Casati et al. , a number of papers have looked at heat conduction in various momentum non-conserving models in one dimension and have all found evidence for the validity of Fourier's law. A model similar to the ding-a-ling is the ding-dong model and has all particles connected to fixed harmonic springs. This was studied by Prosen and Robnik and also shows Fourier behaviour [124]. One of the first papers to recognize the fact that momentum non-conservation is a necessary condition to get finite heat conductivity in one-dimensional systems is that of Hu et al. [125]. From their simulations with various forms of Hamiltonians including, both a harmonic interparticle potential $U(x)$ and a periodic onsite potential of the Frenkel-Kontorva form [$V(x) \sim \cos(ax)$], they found that the presence of an external potential typically led to a finite conductivity. The Frenkel-Kontorva model was also studied in [126] who arrived at similar conclusions. A study of the

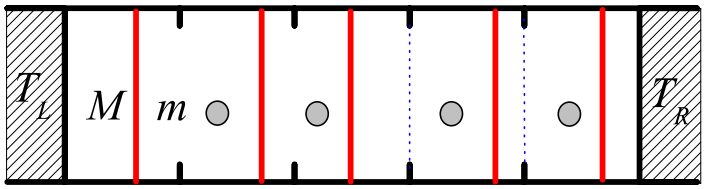

Figure 15. The geometry of the momentum-nonconserving, alternate-mass hardcore model, studied in [134]. The elementary cell (indicated by two dotted lines) has unit length $l = 1$. The bars have mass m_1, and the particles have mass m_2. The two heat baths at temperatures T_L and T_R are indicated.

ϕ^4 model [where $U(x) = k_2x^2/2,\ V(x) = \lambda x^4/4$] by Hu et al. [128], again led to the conclusion of a finite conductivity. This study also emphasized the following point. Nonlinear integrable models usually give a flat temperature profile and making them non-integrable leads to a temperature gradient. However this in itself is not a sufficient condition to give a finite conductivity.

Another nice simulation demonstrating the role of an external potential in giving rise to Fourier behaviour is that on the binary mass hard particle gas [134]. Momentum non-conservation is ensured by confining the motion of alternate particles inside finite cells while allowing them to interact, through elastic collisions with neighbors [shown in Fig. (15)]. The nonequilibrium simulations in this paper with Maxwell heat baths (with $N \sim 512$) convincingly shows the validity of Fourier's law and also the presence of local thermal equilibrium. Secondly, equilibrium simulations were also performed to compute current-current correlation functions, and, using the Green-Kubo formula a value of κ close to the nonequilibrium result was obtained. It is worth noting that this model has zero Lyapunov exponent and thus is non-chaotic. A related study is that in refn. [133] who studied heat conduction in a gas of hard rods placed in a periodic potential.

Results for the ϕ^4 model: We will describe in some more details work on the ϕ^4 model [$U(x) = k_2x^2/2,\ V(x) = \lambda x^4/4$] which appears to be one of the most well-studied of the momentum non-conserving models and where some analytic results have also been obtained. Heat conduction in the ϕ^4 model was first studied by Aoki and Kusnezov [127, 129] who performed both nonequilibrium measurements as well as Green-Kubo based equilibrium measurements. Studying system sizes upto $N = 8000$ they concluded that this system had a finite conductivity and Fourier's law was valid. The value of κ obtained from the nonequilibrium measurements and from the Green-Kubo formula were again shown to be in good agreement. The authors also numerically obtained the temperature dependence of κ and found $\kappa(T) \sim T^{-1.35}$. A number of other papers have performed simulations of the ϕ^4 model and studied various aspects such as the spreading of localized disturbances [128] and the dependence of thermal conductivity on temperature [132]. The model was studied analytically by Lefevere and Schenkel [130] and later by Aoki et al. [131] using a Peierls-Boltzmann kind of approach for the case of weak anharmonicity and they too obtained a finite conductivity. They however obtained a temperature dependence $\kappa \sim 1/T^2$ and this is probably the correct low temperature (corresponding to weak anharmonicity) behaviour, since kinetic theory is expected to be reliable in this regime. Direct nonequilibrium simulations in [131] infact found reasonable agreement with the predictions from kinetic theory, at low temperatures. The study in [132] however finds a somewhat different temperature dependence at low temperatures ($\kappa \sim 1/T^{1.56}$). We note that a scaling property of

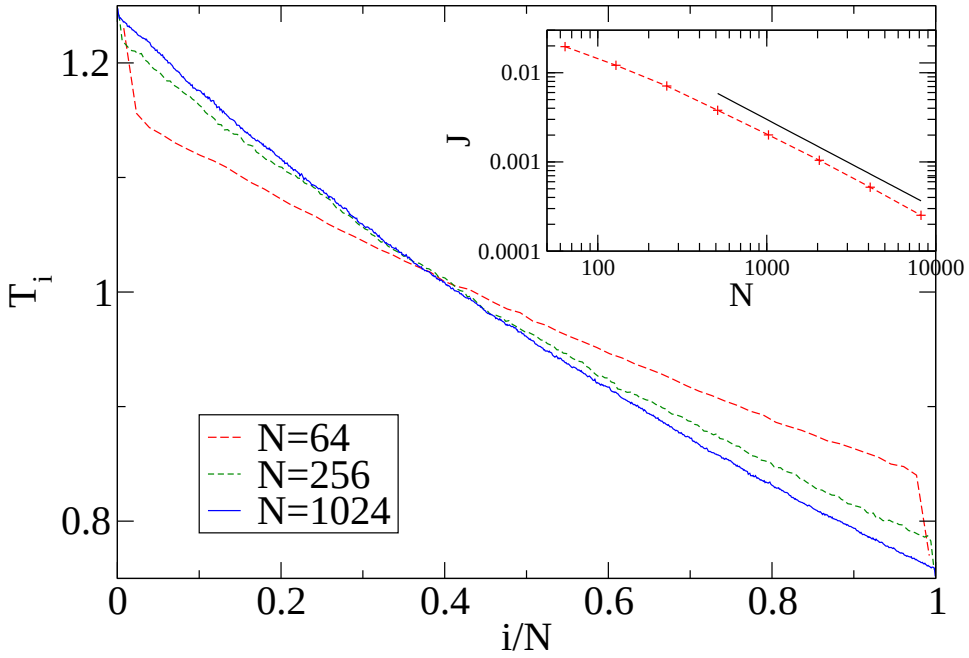

Figure 16. Plot of the temperature profile in the ϕ^4 model for different system sizes. The inset shows the system size dependence of the current and the straight line drawn has slope -1. Error bars are much smaller than symbol sizes. The parameter values for the figure are $k_2 = 1, \lambda = 1, T_L = 1.25, T_R = 0.75$ and bath coupling $\gamma = 1$.

$\kappa(T, \lambda)$, to be discussed later in Sec. (5), implies that $\kappa = \kappa(\lambda T)$.

In Fig. (16) we show typical plots of the temperature profile in the ϕ^4 chain. The inset in the figure shows the $1/N$ dependence for the current. These simulations were performed using white noise Langevin dynamics using the velocity-Verlet algorithm and for the largest system size ($N = 8192$) required $\sim 2 \times 10^9$ time steps with $\Delta t = 0.0025$, to equilibrate.

Before concluding this section we mention the results on a class of rotor models studied by Giardina et al. [135] and Gendelmann et al. [136]. These models were originally proposed as examples of momentum conserving systems which gave Fourier behaviour. The interparticle potential is taken to be $U(x) = 1 - \cos(x)$ and the onsite term $V(x) = 0$. Nonequilibrium and equilibrium (Green-Kubo based) simulations in [135, 136] both indicated that this model gave a finite conductivity. The paper by [136] also reports a phase transition from infinite to finite conductivity as a function of temperature. Given that these simulations are restricted to relatively small sizes (upto $N = 2400$), one suspects that this is probably a crossover effect. Simulations for larger systems in [137, 138, 158] indeed suggest that there may not be any true transitions and that, at all temperatures the asymptotic beaviour is Fourier-like. An analytic study of the rotor model using self-consistent reservoirs (with vanishingly small coupling to interior points) has also claimed a transition [139]. A similar claim of possible transitions from finite to diverging conductivity in other momentum non-conserving models such as the Frenkel-Kontorva and ϕ^4 model has been made in [140].

The fact that a momentum conserving model gives finite conductivity is at first surprising. However given the form of the interparticle potential in the rotor model it is probably more physical to think of this model as an angular momentum conserving model rather than linear momentum conserving one. Thus it seems

more natural to think of the position variables x_l as transverse angular degrees of freedom. In this case one expects different hydrodynamic equations (see for example [141]) and the Fourier behaviour observed is then not surprising. One can also think of the rotor model as the classical limit (large spin) of quantum lattice spin chain models which also are momentum-nonconserving.

Quantum mechanical models: The study of nonequilibrium steady states of interacting quantum systems by simulations is an important and difficult problem. There have been a few attempts at addressing this issue, and we will summarize these. The first set of papers were by Saito et al. [143, 144], who used the master equation approach to connect different temperature reservoirs to a quantum spin chain. One interesting result was that a temperature gradient was formed for the case where the model was non-integrable, while a flat profile was obtained for an integrable model. A study of the current-curent correlator yielded a power law decay $C(t) \sim t^{-1.5}$ implying a finite conductivity [144].

In another interesting work, Mejía-Monasterio et al. [145] have devised what they call a quantum stochastic reservoir. Using this they have performed nonequilibrium simulations, again of a quantum spin chain. They also observe a temperature gradient for the non-integrable model and a flat profile for the integrable model. Further they measured the nonequilibrium steady state current for different sytem sizes and found a $J \sim N^{-1}$ dependence for the non-integrable case and $J \sim N^0$ for the integrable case.

5. Systems with disorder and interactions

As discussed in sec. (3.4) localization of eigenfunctions or of normal modes strongly affects transport in materials containing random impurities. In electronic systems localization has its strongest effect in one dimensions where any finite disorder makes all eigenstates localized and one has an insulator. The presence of inelastic scattering, such as is caused by electron-phonon interactions, leads to hopping of electrons between localized states and gives rise to a finite conductivity. The question as to whether electron-electron interactions lead to a similar effect has attracted much attention recently but is still not fully understood [146, 147, 148, 149, 150, 151, 152]. The main interest is to understand the transition, from an insulating state governed by the physics of Anderson localization, to a conducting state as one increases interactions. One can ask the same question in the context of heat conduction by phonons and consider the effect that phonon-phonon interactions have on localization. Here we will mainly discuss the effect of anharmonicities on the steady state transport of heat through a chain of oscillators with random masses . The effect of interactions between phonons on localization caused by disorder has also been investigated by looking at the spreading of wave packets [151, 152, 159, 160] and we will briefly discuss these results at the end of this section.

An early work on steady state heat conduction in disordered anharmonic systems is that of Payton, Rich and Visscher [153] who studied mass-disordered lattices in the presence of cubic and quartic interparticle anharmonicities. They performed nonequilibrium simulations with stochastic baths in one and two dimensions. Their main conclusion was that in most cases interactions (interparticle anharmonicity) seemed to greatly enhance the conductivity of the system (except for the case of very weak disorder). We note that, at that time simulations were restricted to small sizes and it was wrongly assumed by the authors that the disordered harmonic lattices in one and two dimensions, as well as the anharmonic ones, had finite thermal conductivities. The system size dependence was not studied systematically.

Similarly a study by Poetzsch and Bottger [154] for a two dimensional lattice system found that, while quartic anharmonicity enhances the conductivity of the disordered system, cubic anharmonicity reduces it. Again this study was restricted to small system sizes and assumed that the conductivity is finite.

The first systematic study of the joint effects of anharmoncity and disorder on the system-size dependence of heat current was by Li et al. [155]. They studied the mass-disordered FPU chain using Nose-Hoover nonequilibrium simulations. Their conclusion was that this model showed a transition, from a Fourier like scaling $J \sim N^{-1}$ at low temperatures, to a pure FPU like behaviour with $J \sim N^{-0.57}$ at high temperatures. A more recent simulation of the same model by Dhar and Saito [157] suggests that this conclusion may be incorrect. What Li et al.observe is probably a cross-over effect and there is really no true transition in transport properties. It appears that *disorder becomes irrelevant* as far as the value of the exponent α is concerned. We will here present the latest simulation results of the disordered FPU chain as well as results from the study of the disordered ϕ^4 lattice, where similar conclusions are reached [156]. Temperature driven phase transitions in one dimensional heat conduction have also been reported in some other models. However as has been pointed out in refn. [158] these are probably cross-over effects and there is no true transition in these models.

The general form of the Hamiltonian that has been studied by various people is, in the one-dimensional case, given by:

$$H = \sum_{l=1,N} [\frac{p_l^2}{2m_l} + k_o\frac{x_l^2}{2} + \lambda\frac{x_l^4}{4}] + \sum_{l=1,N+1} [\ k\frac{(x_l - x_{l-1})^2}{2} + \nu\frac{(x_l - x_{l-1})^4}{4}\ ] \quad (118)$$

with fixed boundary conditions $x_0 = x_{N+1} = 0$. The masses $\{m_l\}$ are chosen independently from some distribution $p(m)$, *e.g.* one uniform in the interval $(\bar{m} - \Delta, \bar{m} + \Delta)$ or a binary distribution given by $P(m) = \delta[m - (\bar{m} - \Delta)]/2 + \delta[m - (\bar{m} + \Delta)]/2$. The chain is connected at its ends to two heat baths at temperatures T_L and T_R respectively. Here we will mostly consider white noise reservoirs, but will also give some results with Nose-Hoover baths. The equations of motion of the chain are then given by:

$$m_l\ddot{x}_l = -k_o x_l - l x_l^3 - k(2x_l - x_{l-1} - x_{l+1}) - \nu[(x_l - x_{l-1})^3 + (x_l - x_{l+1})^3] - \gamma_l\dot{x}_l + \eta_l\ , \quad (119)$$

with $\eta_l = \eta_L\delta_{l,1} + \eta_R\delta_{l,N}$, $\gamma_l = \gamma(\delta_{l,1} + \delta_{l,N})$, and where the Gaussian noise terms satisfy the fluctuation dissipation relations $\langle\eta_L(t)\eta_L(t')\rangle = 2\gamma k_B T_L\delta(t - t')$, $\langle\eta_R(t)\eta_R(t')\rangle = 2\gamma k_B T_R\delta(t - t')$.

Note that Eq.(119) is invariant under the transformation $T_{L,R} \to sT_{L,R}$, $\{x_l\} \to \{s^{1/2}x_l\}$ and $(l, \nu) \to (l, \nu)/s$. This implies the scaling relation $J(sT_L, sT_R, l, \nu)\rangle = sJ(T_L, T_R, sl, s\nu)$. For the conductivity κ this implies $\kappa = \kappa(\nu T, lT)$. Thus the effect of changing temperatures can be equivalently studied by changing anharmonicity. We will first discuss the unpinned (momentum conserving) case and then the pinned (momentum non-conserving) case.

Disordered FPU chain: This corresponds to taking $k_o = \lambda = 0$ in the Hamiltonian in Eq. (118), and is the case studied by [155] and in [157]. There are two important parameters in the problem, namely the disorder strength given by Δ and

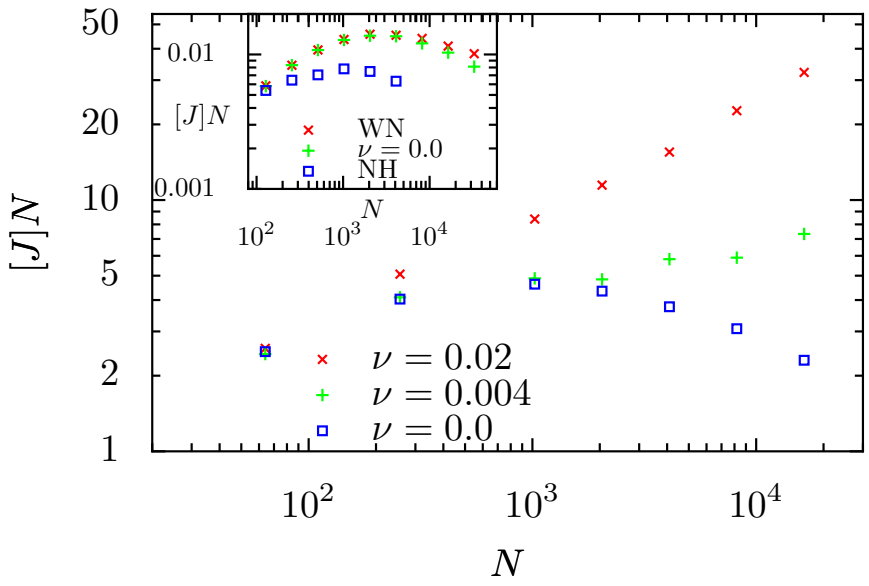

Figure 17. Plot of heat current versus system size, for the disordered FPU chain, for different values of ν. The data in the inset corresponds to parameters as in [155], namely $(T_L, T_R) = (0.001, 0.0005)$ with Gaussian white noise bath for $\nu = 1$ (WN) and $\nu = 0$, and Nose-Hoover bath (NH) for $\nu = 1$ (from [157]).

the anharmonicity given by ν. Let us consider the two limiting cases, of the disordered harmonic chain ($\nu = 0, \Delta \neq 0$), and of the ordered FPU chain ($\nu \neq 0, \Delta = 0$). For the former, with fixed boundary conditions it is expected that $\alpha = -1/2$, while for the ordered FPU chain one expects $\alpha = 1/3$. In the presence of both disorder and interactions a possible scenario is that for strong disorder one gets $\alpha = -1/2$ while with strong interactions, one gets $\alpha = 1/3$ and there is a phase transition between the two behaviours as we change parameters. The numerical results that we will discuss, suggest that there is no such transition. Note that in both the limiting cases, the low frequency long wavelength modes are believed to play an important role in transport.

The simulations in [157] looked at the case of binary mass distribution with $\bar{m} = 1, \Delta = 0.2$ and different values of the interaction strength $\nu = 0.004, 0.02, 0.1, 2.0$. Averages were taken over $50 - 100$ samples for $N < 1024$, 10 samples for $N = 1024 - 16384$, and 2 samples for $N = 32768$ and 65536. In Fig. (17) the results of simulations for the disorder averaged current $[J]$ for $\nu = 0.004$, 0.02 and $\nu = 0.0$ are shown. For small values of ν one sees that, at small system sizes the current value is close to the $\nu = 0$ value. As expected one has to go to large system sizes to see the effect of the weak anharmonicity. At sufficiently large N the same system size dependence of J is obtained as that for the ordered FPU chain, namely with $\alpha = 1/3$. The authors in [157] then show that by scaling the current by appropriate factors, the data for the disordered case can be made to collapse on to the binary-mass ordered case. This is shown in Fig. (18) (for $\nu = 0.02, 0.1, 2.0$). Thus these results show that the asymptotic power law dependence of the current is always dominated by anharmonicity and there seems to be no transition. Disorder only decreases the overall conductance of a sample.

The authors of [157] have also investigated the parameter range studied in [155] and explained the reasons which led to the erroneous conclusions in [155], of a transition in conducting properties at low temperatures (or equivalently small anharmonicity). In fact this can be understood even from the data for $[J]N$ in Fig. (17) for $\nu = 0.004$. We see that at around $N \sim 1000 - 2000$ the data seems to flatten and if one had just looked at data in this range, as was done by [155], one would

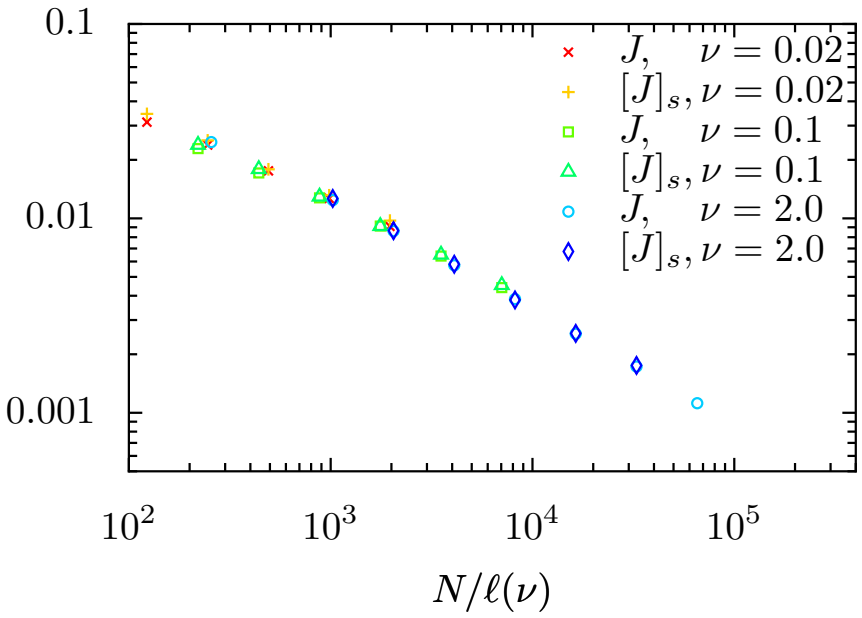

Figure 18. Plot of scaled heat current $[J]_s$ for the disordered FPU chain and the current J for the ordered chain, for different values of ν. The $x-$axis is scaled as in Fig. (13) (from [157]).

conclude that Fourier's law is valid. However the behaviour changes drastically when one looks at larger system sizes and one again gets the usual FPU behaviour. The inset of Fig. (17) shows results for parameters as in [155] but for much larger system sizes. This case corresponds to a much smaller value of ν and so it is expected that it will follow the $\nu = 0$ curve till very long length scales and this is clearly seen. However, at around $N = 16384$, there is a tendency for the curve to turn up and it can be expected that the same asymptotic behaviour to eventually show up. While a transition cannot be ruled out at even lower temperatures and with stronger disorder, this seems unlikely. Also, if there is such a transition, it should probably be to a disordered phase with $[J] \sim N^{-3/2}$.

It is interesting to consider the temperature dependence of conductivity in the disordered FPU chain. The scaling property of the current, mentioned earlier [after Eq. (119)], implies that the thermal conductivity has the form $\kappa = \kappa(\nu T)$. For small anharmonicity ($\nu << 1$), the earlier results for the ordered alternate mass FPU chain imply that at large system sizes $\kappa \sim N^{1/3}/\nu^{2/3}$ and from the scaling property this immediately gives $\kappa \sim 1/T^{2/3}$ at low temperatures. However at small system sizes [$N << \ell(\nu)$], we expect the system to behave like a harmonic system with $\kappa \sim T^0$. At high temperatures the conductivity will saturate to a constant value. Experimentally, the temperature dependence of the thermal conductivity may be easier to measure and one can verify if this is unaffected by disorder [see, for example sec. (8)].

Disordered ϕ^4 chain: Let us now look at the case where the particles are subjected to an external pinning potential in addition to nearest neighbor harmonic interactions. We will consider the anharmonicity to be an onsite quartic term (thus $\lambda > 0, \nu = 0$, also $k_o, k > 0$) in which case this corresponds to the discrete ϕ^4 model. Pinning greatly enhances the difference between heat transport in a random chain with and without anharmonicity and thus is a good testing ground for the effect of anharmonicity on localization. This model is also closer in spirit to charge transport by hopping in random media. Again let us look at the two limiting cases. In the case with a pinning potential at all sites the disordered case ($\lambda = 0, \Delta \neq 0$) gives $J \sim e^{-cN}$. For $\Delta = 0$ and $\lambda \neq 0$ we have seen from sec. (4.2.2) that one expects

Fourier's law to be valid and so $\alpha = 0$.

The case with parameters $k = k_o = 1, \lambda > 0$ and a uniform mass distribution with $\bar{m} = 1.0$ and $\Delta = 0.2$ was studied in [156]. In Fig. (19) the result of simulations for different values of anharmonicity $\lambda = 0.004 - 1.0$ is given. As can be seen from the data, there is a dramatic *increase* in the heat current on introduction of a small amount of anharmonicity and the system-size dependence goes from exponential decay to a $1/N$ dependence implying diffusive transport. For smaller λ the diffusive regime sets in at larger length scales but as in the FPU case, here too one finds that anharmonicity determines the system size scaling and no transition is observed. A measure of the relative strengths of anharmonicity and disorder is obtained by looking at the ratio of the energy scales $E_a = l\langle x^4\rangle/4$ and $E_d = T\Delta/m$. For the given parameters one finds $\epsilon = E_a/E_d \approx 0.008$ for $\lambda = 0.004$. Unlike the FPU case, in this model, it does not seem that any simple scaling of the data is possible.

Thus this study shows that introduction of a small amount of phonon-phonon interactions in the disordered harmonic chain leads to diffusive energy transfer, *i.e.*, the insulating chain becomes a normal heat conductor. How exactly this occurs is not clear. It is possible that anharmonicity gives rise to extended states or leads to hopping of energy between states which are now approximately localized (*i.e* they are no longer exact normal modes, but have a small rate of energy leakage to nearby modes) . There is no evidence of the existence of a finite critical value of anharmonicity required for this transition. For small values of anharmonicity it is necessary to go to larger system sizes to see the transition from insulating to diffusive. As in the FPU case, a transition to a localized phase at a very small value of anharmonicity is possible and would be difficult to observe in simulations, because equilibration times increase rapidly with decreasing λ.

An interesting question in this model is the limiting behavior of $\kappa(\lambda T)$ for $(\lambda T) \to 0$. It turns out that the temperature profiles for the disordered ϕ^4 chain are qualitatively different from the ordered chain and this means that the temperature dependence of conductivity is different for the two cases. For the ordered case, from kinetic theory one gets $\kappa \sim 1/(\lambda^2 T^2)$ for small λT [131], while for the disordered case [156] found $\kappa \approx (\lambda T)^{1/2}$. For the FPU chain on other hand, the ordered and disordered cases give similar temperature profiles [157].

There have been a number of studies on disordered anharmonic chains which have investigated the spreading of localized pulses of energy injected into a system at zero temperature. The study by Bourbonnais and Maynard [159] looked at FPU type of systems in one and two dimensions and observed that anharmonicity destabilizes the localized modes and the diffusion of pulses was found to be anomalous. This seems to be consistent with the heat conduction results on the disordered FPU chain. A similar zero temperature study of the mass disordered FPU system was carried out by Snyder and Kirkpatrick [160] who however found evidence for diffusive transport at sufficiently strong anharmonicity. In the case of the ϕ^4 and related models there have been some extensive recent numerical studies and here the conclusions are somewhat contradictory to the heat conduction results. The spreading of localized energy pulses has been reported to be sub-diffusive in [151] while [152] reports absence of diffusion. The study in refn. [152] offers a picture of spreading of an initially localized energy wavepacket to a limiting profile as taking place through nonlinearity induced coupling between the localized modes. All these studies suggests that the behaviour of a heat pulse at zero temperature and that at finite temperature can be very different. Indeed as pointed out nicely in [142], it is necessary to look at appropriate spatiotemporal correlation functions of closed systems at finite temperatures in order to understand diffusion in the open system. This of course is also what one effectively does in the Green-Kubo approach.

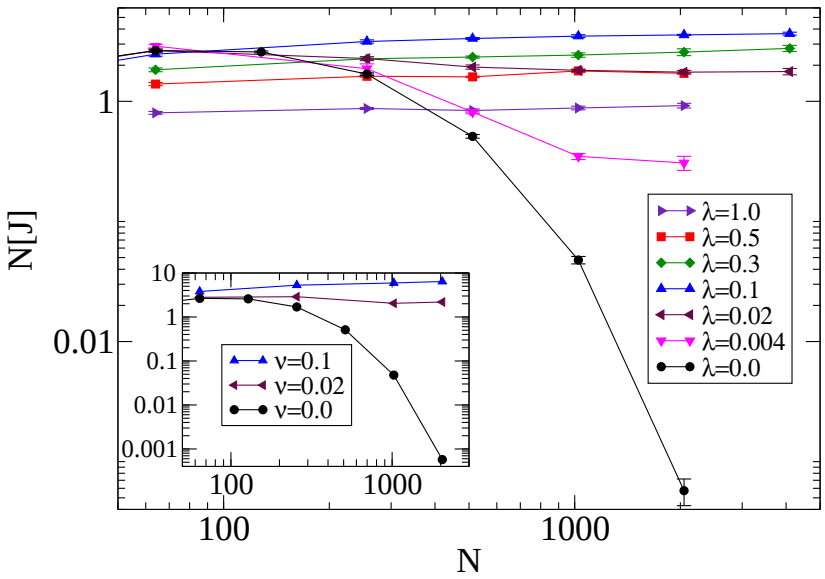

Figure 19. Plot of $[J]N$ versus N for the disordered ϕ^4 chain, for different values of λ. The inset shows results obtained for the case with interparticle anharmonicity and onsite harmonic pinning (from [156]).

Finally we note an interesting related problem that was studied by Rich and Visscher [65]. They considered heat conduction in a disordered Harmonic chain with self-consistent reservoirs. Since self-consistent reservoirs can be roughly though of as some sort of nonlinearity leading to incoherent scattering of phonons, this problem has some similarity with that considered in this section. Based on exact numerical calculations on small chains, their main conclusion was that the presence of self-consistent reservoirs leads to a finite conductivity for chains with both free and fixed boundary conditions (and no bulk pinning). The self-consistent reservoirs makes the model momentum non-conserving so this is consistent with the results of the disordered ϕ^4 chain presented here. A very interesting conjecture made in this paper is that a finite conductivity will be obtained if the limits $N \to \infty$ first, and then coupling to self-consistent reservoirs $\to 0$ are taken. A recent paper [161] has studied heat conduction in a disordered harmonic chain with an energy conserving stochastic dynamics and has obtained rigorous results which indicate a finite thermal conductivity of the system.

6. Interacting systems in two dimensions

We have seen that, in the one-dimensional case, it is usually quite difficult to obtain the asymptotic system size dependence of the current. In order to get the correct exponent requires one to go to large system sizes and at some point the sizes required are beyond current computational capabilities. Of course a combination of simulations and results from analytic work gives one some confidence about the results obtained so far. In the case of higher dimensional systems naturally one can expect the same computational difficulties and in fact here they become more pronounced since the number of particles is now L^d where L is the linear size and d the dimensionality. The good news is that there is general agreement on the system-size dependence of conductivity from different analytical methods. Both MCT [2] and the hydrodynamics approach [72] predict that for a momentum conserving system, the thermal conductivity diverges logarithmically with system size in $2D$ and is finite in $3D$. In the presence of pinning all theories predict a finite conductivity in all dimensions.

There are few simulation studies in higher dimensional systems and we summarize the main results obtained so far. Early studies of heat conduction were mainly interested in finding the temperature dependence of thermal conductivity and *assumed* that this was finite [153, 162, 164]. One of the first paper to study system size dependence was probably that by Jackson and Mistriotis [163]. They studied the diatomic Toda lattice and concluded that the thermal conductivity was finite for mass ratio greater than a critical value and diverged otherwise.

More extensive studies on the system size dependence were made by Lippi and Livi [165] for an oscillator system in two dimensions with vector displacements and interparticle interactions. They considered a $L_x \times L_y$ lattice with the following Hamiltonian:

$$H = \sum_{i=1}^{L_x} \sum_{j=1}^{L_y} \frac{|\mathbf{p}_{ij}|^2}{2m} + U(|\mathbf{x}_{i+1,j} - \mathbf{x}_{ij}|) + U(|\mathbf{x}_{i,j+1} - \mathbf{x}_{ij}|) \ , \tag{120}$$

where $\mathbf{x}_{ij}$ denotes the vector displacement (taken to be two-dimensional vectors) of a particle at lattice site (i, j) where $i = 1, 2..L_x$ and $j = 1, 2...L_y$ and $\mathbf{p}_{ij}$ denotes the corresponding momentum vector. Two kinds of interparticle potentials were studied, namely a FPU type potential given by $U(x) = x^2/2 + k_4 x^4/4$ and a Lennard-Jones potential given by $U(x) = A/x^{12} - B/x^6$. Both models gave similar results. Nonequilibrium simulations using Nose-Hoover baths, as well as equilibrium simulations based on the Kubo formula, were performed. Nonequilibrium simulations were first performed on strips of width L_y with aspect ratio $L_y/L_x < 1$ and with heat conduction in the x-direction. It was observed that for fixed L_x, as one increased L_y, the current seemed to saturate to a constant value for quite small values of L_y/L_x. Subsequently, to save on computational time, the authors considered the value $L_y/L_x = 1/2$ in all their simulations. Studying system sizes upto $L_x = 128$ they obtained a logarithmic divergence, with system size, of the conductivity *i.e.* $\kappa \sim \ln(L_x)$. The equilibrium simulations, performed over similar system sizes, and using a microcanonical ensemble gave a t^{-1} dependence for the current-current correlation function. Using the Green-Kubo formula this implies again a logarithmic divergence, with system size, of the conductivity.

The same Hamiltonian as in Eq. (120) with FPU interactions but with a scalar displacement field was studied later by Yang and Grassberger [166]. This paper looked at somewhat bigger system sizes than [165] but were unable to verify the logarithmic divergence and instead obtained a power law dependence with an exponent $\alpha \approx 0.22$. A careful investigation of the value of $r = L_x/L_y$, at which a dimensional cross-over from $1D$ to $2D$ behaviour occured was carried out. Their conclusion was that at large values of r, the conductivity κ diverged as a power law with $\alpha = 0.37 \pm 0.01$ while for small r they obtained $\alpha \approx 0.2$. The data for conductivity versus system size for different values of r is shown in Fig. (20). The conductivity plotted in the figure was defined as

$$\kappa_{center} = \frac{J}{(dT/dx)_{center}} \ , \tag{121}$$

where $(dT/dx)_{center}$ is the temperature gradient evaluated numerically at the center. This definition was used to take care of the boundary temperature jumps that are usually present for small system sizes [see Fig. (21)]. Based on the data in Fig. (20) the authors also made the interesting suggestion that the cross-over from $1D$ to $2D$ behaviour takes place at $r \to \infty$ in the limit $L_x \to \infty$. This has obvious implications for experimental tests on the dependence of conductivity on length,

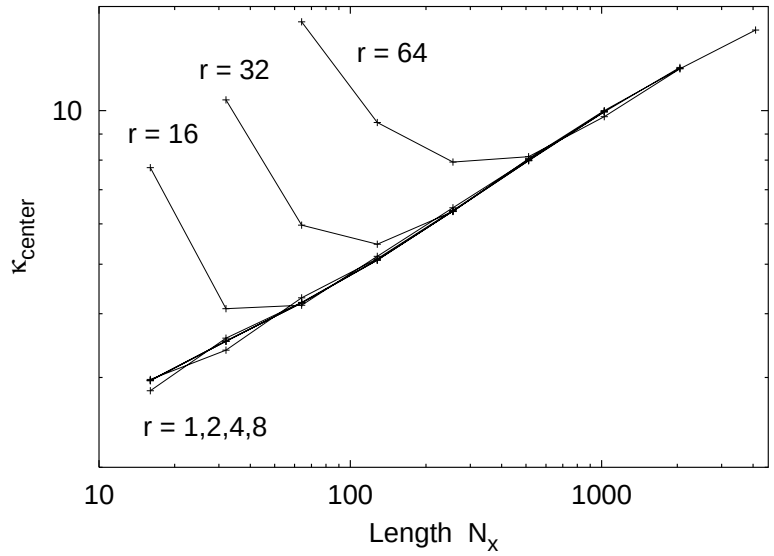

Figure 20. Plot of conductivity, defined by Eq. (121), versus system size L_x for $2D$ scalar FPU model. Curves for different aspect ratios $r = L_x/L_y$ are shown. The asymptotic slope was ≈ 0.22 (data from [166]).

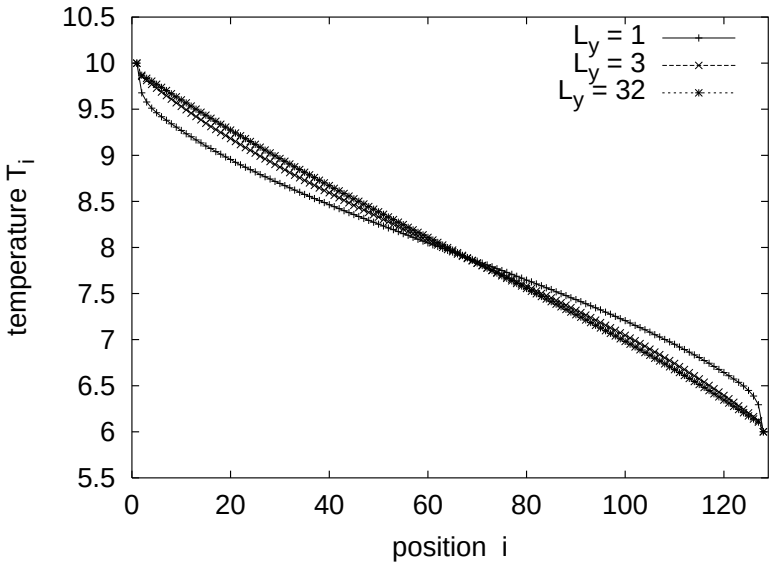

Figure 21. Temperature profiles for scalar $2D$ FPU lattices with $L_x = 128$ and $L_y = 1, 3$, and 32. The temperatures of the heat baths at both ends were fixed at $(T_L, T_R) = (10.0, 6.0)$ (data from [166]).

for systems such as nanotubes and nanowires. Another paper [167] again studying the vector model for even larger system sizes (upto 64×65536) has claimed observing a logarithmic divergence. However one of the authors of the paper has expressed doubts about whether convergence has been attained at these sizes [168] and this seems very likely to be the case.

The most recent simulations by Shiba and Ito [170] considered the same Hamiltonian as in Eq. (120) and used the same parameter set as [165], namely $k_4 = 0.1, T_L = 20, T_R = 10$. They performed nonequilibrium Nose-Hoover simulations and studied system sizes upto 384×768. Their data for conductivity versus system size is plotted in Fig. (22). The exponent $\alpha \approx 0.268$ obtained by them appears to be significantly different from logarithmic behaviour. We also show the temperature profiles for different system sizes [Fig. (23)] and it appears that the boundary jumps are quite negligible.

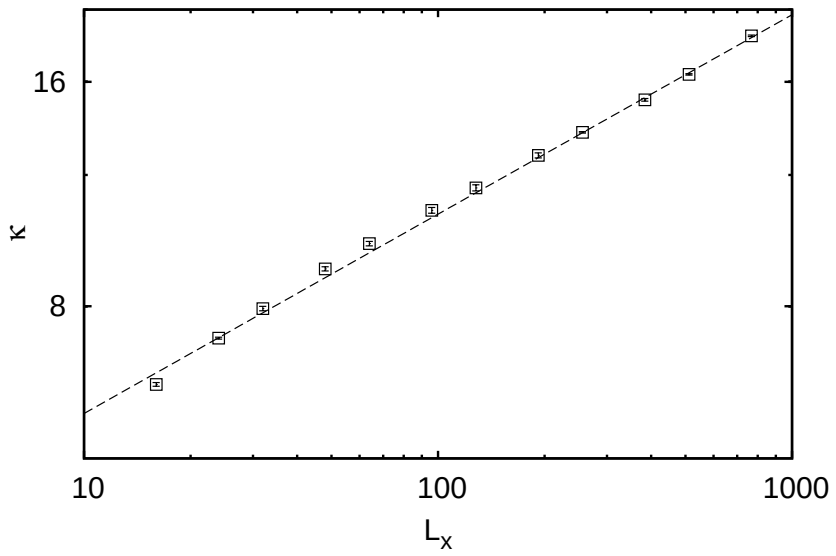

Figure 22. System size dependence of the thermal conductivity for 2D FPU lattice with $L_y : L_x = 1 : 2$, plotted on a $\log - \log$ scale. The dashed line represents the result of a power-law fitting in the region $L_x \geq 128$, yielding the result $\kappa(L_x) \sim L_x^{0.267(5)}$ (data from [170])

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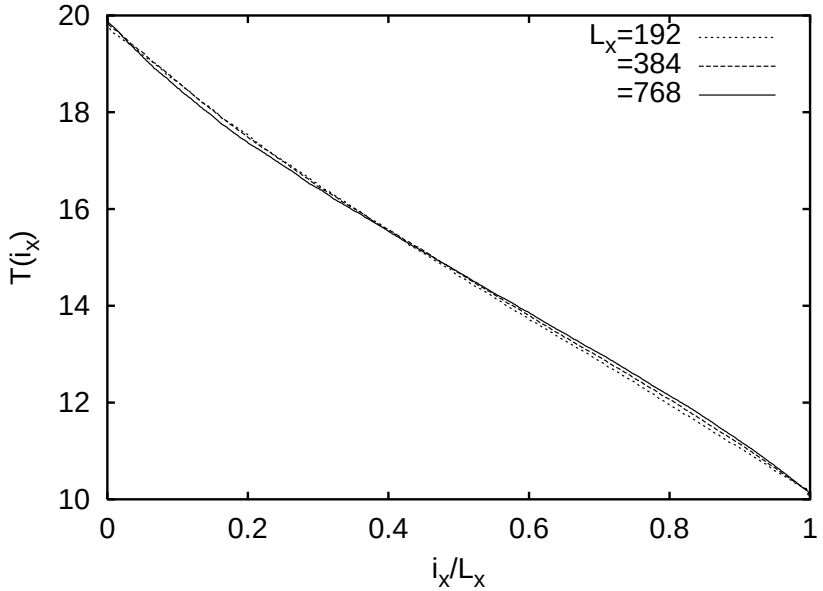

Figure 23. Temperature profiles for the 2D FPU lattice with $L_y : L_x = 1 : 2$. The sequences represent the results for the sizes $L_x = 192, 384$, and 768. The temperatures of the heat baths at both ends were fixed to $(T_L, T_R) = (20.0, 10.0)$. The horizontal axis represents the position in the x-direction, scaled by the system size L_x, and the vertical axis represents the local temperature (data from [170]).

Unlike in $1D$, where the hard particle gas has been intensely studied, there have been very few studies on hard disc systems. For a hard disk fluid system, Shimada et al. [169] reported α to be less than 0.2. Thus for momentum-conserving systems in $2D$ it is fair to say that simulations have not been able to unambiguously establish the logarithmic divergence of the conductivity predicted from theory. Further work is clearly needed here.

As far as momentum non-conserving interacting systems are concerned one would naturally expect Fourier behaviour, given that this is the case even in one dimen-

sion. In the next section we will discuss a number of momentum non-conserving models of *non-interacting* particle systems which can be shown (including some rigorously) to satisfy Fourier's law. In these models noninteracting particles are scattered from fixed scatterers. These models however suffer from the drawback that there is no mechanism for local thermal equilibration and so the meaning of temperature and Fourier's law is somewhat artificial. There have been a few papers which have introduced particle interactions in these kind (hard particle scattering) of models. Here we discuss two such models.

The first model, introduced by Mejía-Monasterio et al. [171, 172], is one in which noninteracting particles move among a periodic array of circular scatterers [see Fig. (24)]. The dynamics is specified as follows. Consider dimensionless units such that the mass of the moving particles is 1 and the moment of inertia of the scatterers is η. Then, if (v_n, v_t) are the normal and tangential components of velocity of the particle at the time of collision, and ω is the angular velocity of the discs, then after the collision they are transformed to (v_n', v_t', ω') which are given by the linear transformation:

$$\begin{aligned} v_n' &= -v_n, \\ v_t' &= v_t - \frac{2\eta}{1+\eta}(v_t - \omega), \\ \omega' &= \omega + \frac{2}{1+\eta}(v_t - \omega) \ . \end{aligned} \tag{122}$$

The dynamics conserves total energy $v_n^2/2 + v_t^2/2 + \eta\omega^2/2$ and angular momentum and is time-reversal invariant (however, the transformation is non-syplectic). This system was then connected to two reservoirs of both heat and particle and which are specified by temperature and chemical potentials (T_L, μ_L) and (T_R, μ_R) respectively. Thus both heat and particle currents were generated. Performing detailed simulations on this system, some of the main conclusions of the paper were: (i) the system satisfied local thermal equilibrium, (ii) both heat and particle currents satisfied usual linear response relations with finite transport coefficients, (iii) Onsager reciprocity relations were satisfied. The largest system studied had about 100 discs in the conducting direction (and two discs in the vertical direction). Note that in this model interactions between particles is introduced indirectly. Motivated by this model, refn. [173] studied an idealized model with noninteracting tracer particles moving between fixed energy storing centres and exchanging energy with these. Local thermal equilibration and temperature profiles were analytically studied in this work. Another model where an explicit verification, of linear response relations for heat and particle transport were obtained, as well as Onsager reciprocity relations, is a $1D$ electronic system with self-consistent reservoirs [70].

Another recent study by Gaspard and Gilbert [174, 175, 176] has considered a system where hard disc particles are confined within periodic array of cells formed by fixed scatterers. The model is explained in Fig. (25). The main idea of the authors has been to introduce a three time-scale mechanism in generating the heat conduction state: (i) a short time scale τ_{wall} corresponding to particles motion within a cell with negligible energy transfers, (ii) an intermediate time scale τ_{binary} corresponding to binary collisions which lead to local equilibrium and (iii) a long time scale τ_{macro} of the macroscopic relaxation of Fourier modes. Based on a master equation approach the authors are able to demonstrate the validity of Fourier's law and find an explicit expression for the thermal conductivity of the system. Note the similarity of the model with the one dimensional model described in Fig. (15), though the mechanism leading to Fourier behaviour there is possibly different.

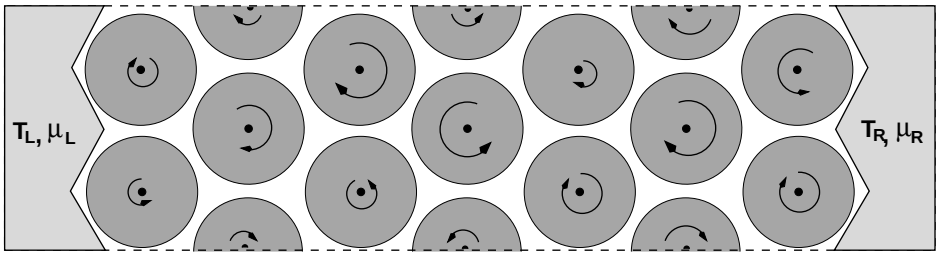

Figure 24. Schematic illustration of the model studied in [171]. The scatterers are on a triangular array arranged such as to avoid infinitely long trajectories. The scatterers can perform rotational motion after collisions with the moving point particles. Periodic boundary conditions are used in the vertical direction (from [171]).

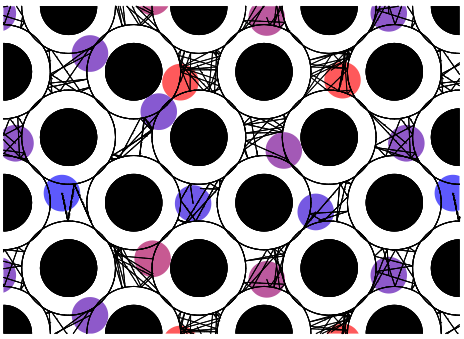

Figure 25. Model studied in [174]. The small colored discs move among a periodic array of fixed black discs. Each small disc is confined to move in a cell bounded by four fixed discs. Most of the time the small disc moves with constant energy and undergoing elastic collisions with the fixed discs. Once in a while there is a collision between particles in two neighboring cells and there is exchange of energy. The solid lines show the trajectories of the centers of the moving particles about their respective cells. The colors are coded according to the particles kinetic temperatures (from blue to red with increasing temperature) (from [174]).

As far as simulations of oscillator systems is concerned, a two dimensional momentum non-conserving lattice model was studied by Barik [177, 178] who studied a scalar displacement model with harmonic interparticle interactions and an onsite potential $V(x)$. Several different forms of $V(x)$ were studied. With a Frenkel-Kontorva interaction given by $V_a(x) = \cos(x)$ the author reports a power law divergence of the conductivity [177]. For two other models, of the form $V_b(x) = -\cos(x) - \sin(2x)/2$, a logarithmic divergence of the conductivity was found [178]. However the reason why a finite conductivity has not been obtained in these momentum non-conserving systems is probably because the system sizes studied are too small (upto 240×240). This is evident from the quite large boundary temperature jumps that can be seen in the temperature profiles reported in these papers [177, 178]. This means that the contact resistances are contributing significantly to the measured resistance. As we have discussed earlier in sec. (4.2.1) this will give a higher apparent divergence of the conductivity than is actually the case. In this case looking at κ_{center}, defined in Eq. (121), may be a good idea. Another point is that specific forms of interaction strengths also might lead to a faster convergence. Thus in [178] it can be seen that for the same applied temperature difference and same system size, the potential $V_a(x)$ gives a flat temperature profile while with $V_b(x)$ one gets a significant gradient. This feature has also been observed earlier in sec. (4.2.1) where we saw that the random collision model and the $1D$ double-well potential gave fast convergence to the asymptotic limit.

It appears that the simulation results in two dimensions are quite inconclusive for momentum conserving systems as regards the system size dependence of conductivity. More extensive studies with larger system sizes and different forms of

interaction potentials are needed to confirm the theoretical predictions. For momentum non-conserving lattice systems it is likely that simulations on larger system sizes will verify validity of Fourier's law.

7. Non-interacting non-integrable systems

Probably the first rigorous demonstration of Fourier-like dependence of the current in a Hamiltonian system was by Lebowitz and Spohn [179] in the Lorenz gas model. This model consists of a gas of classical point particles in dimension $d \geq 2$ which undergo elastic collisions with fixed randomly placed spherical scatterers. The authors studied this system with stochastic boundary conditions on two bounding walls corresponding to temperatures T_L and T_R. They could prove rigorously that in the Boltzmann-Grad limit of a large number of small scatterers, one gets $J \sim (T_L - T_R)/L$, where L is the length of the box.

A number of quasi-$1D$ Lorenz-gas-like systems have been numerically investigated recently and have provided some more insight. Alonso et al. [180] studied a channel with an array of periodically placed semicircular scatterers. From their nonequilibrium simulations with Maxwell baths, they verified Fourier's law and showed that the nonlinear temperature profile could be understood by a simple model of diffusing particles with an energy dependent diffusion constant $D(E) \sim E^{1/2}$.

The particle dynamics of the Lorenz-gas model with convex scatterers is known to be chaotic. Li et al.[181] explored the question as to whether a positive Lyapunov exponent, *i.e.* , a chaotic dynamics, is a necessary condition in order to get Fourier's law. They considered a system of non-interacting particles moving in a quasi $1D$ channel and suffering elastic collisions with fixed triangular shaped scatterers placed throughout the channel. The cases of a regular, and a random, array of scatterers was considered. It can be shown that in both these cases, the dynamics has zero Lyapunov exponent unlike the case with convex scatterers. The authors found from their nonequilibrium simulations that while the regular array gave a diverging thermal conductivity, the random array gave a finite conductivity. In both cases a temperature gradient was obtained, though they had very different forms, highly nonlinear in the periodic case and linear in the random case. Thus the random array of non-chaotic scatterers gave rise to normal Fourier heat transport in the channel. Correspondingly it was shown that the particle motion was superdiffusive for the periodic case and diffusive for the random case. Thus this simulation shows *that chaos is not a necessary condition for diffusive transport.* In other studies [182, 183] it has been seen that, even with a periodic array of triangular scatterers, one gets Fourier transport whenever the internal angles are irrational multiples of π. Finally Li and Wang [184] and Denisov et al. [185] have given analytic arguments to relate the diffusion exponent of the heat carriers to the conductivity exponent α. That chaos is not a necessary condition for normal transport was also seen earlier in sec. (4). There we saw that the interacting hard particle dimer gas (which is non-chaotic) gives normal transport in the presence of an external potential.

The validity of Fourier's law in Lorenz-gas models basically arises due to the diffusive motion of the heat carriers. However the absence of interactions makes these models somewhat ill-behaved from the thermodynamic point of view. As pointed out in [186] these models lack local thermal equilibrium and so the meaning of temperature and Fourier's law in these systems is somewhat different from that one usually has in nonequilibrium thermodynamics. The models studied in [171, 172, 174], and discussed in sec. (6), are examples of similar momentum non-

conserving models of particles with collisional dynamics where however the introduction of interactions leads to local thermal equilibrium.

8. Experiments

The experimental measurement of thermal conductivity of a system is much more difficult than, for example, its electrical conductivity. One realizes this from the simple fact that it is easy to construct an ammeter to measure electrical current but that is not so in the case for heat current. Thus measurements of thermal conductivity require special methods and often the interpretation of experimental data themselves require involved theoretical modeling. This is perhaps one reason as to why there has, until recently, not been much experimental studies which have addressed the precise question of the system size dependence of thermal conductivity and its expected divergence in low dimensional systems. The situation has changed recently with the advent of nanophysics. Understanding heat transfer in systems such as nanowires and nanotubes is not only a question of basic interest but of technological importance too. With amazing advances in nano-technology it has now become actually possible to measure the thermal conductivity of a nanotube suspended between two thermal reservoirs. Here we briefly discuss some of the experiments on nanowires and nanotubes. We will try to explain the present understanding and also try to emphasize the relevance, of the knowledge that has been obtained from studies of simple models discussed in this review. In all the experiments that we will describe here the heat current is believed to be mainly due to phonons.

The most common approach to understanding experimental data on heat conduction is perhaps through simple kinetic theory picture which says that the conductivity in a phonon system is proportional to $cv\ell$ where c is the specific heat per unit volume, v the sound speed and ℓ the phonon mean free path. For system sizes smaller than ℓ, one expects ballistic transport and roughly one can replace ℓ by L in the conductivity formula, and hence get $\kappa \sim L$. On the other hand for $\ell >> L$ it is normally expected that a finite conductivity will be obtained. However, from the results presented in the previous sections, it is clear that this picture cannot be correct. At sufficiently large length scales, for low dimensional systems such as nanowires and nanotubes, we expect the conductivity to diverge as a power law $\kappa \sim L^{\alpha}$.

In the ballistic limit (defined as one where anharmonicity can be neglected) one can use the Landauer or NEGF formula and here there are examples where good agreement between theory and experiments can be seen. For nanotubes and nanowires with low impurity level it turns out that phonon mean free paths can be quite long and so transport is ballistic over fairly long length scales.

Experiments on nanowires: One of the first measurements of phonon thermal conductance of a nanosystem was that by Tighe et al. [187]. In a beautiful experiment they measured the conductance of insulating GaAs wires of length $\approx 5.5\mu m$ and cross-section $\approx 200nm \times 300nm$. At low temperatures $(1.5-5K)$ they obtained conductances of order $\sim 10^{-9}W/K$. From their data and using kinetic theory arguments they estimated the phonon mean free path to be of order $\sim 1\mu m$. Now one can ask the question: what is the thermal conductance of a perfectly transmitting $1D$ wire? This can be easily obtained from Eq. (65) by setting $\mathcal{T}(\omega) = 1$ and one

gets:

$$G = \frac{J}{\Delta T} = \frac{k_B}{2\pi} \int_0^{\omega_m} d\omega \left(\frac{\hbar\omega}{k_B T}\right)^2 \frac{e^{\hbar\omega/(k_B T)}}{[e^{\hbar\omega/(k_B T)} - 1]^2} \ , \tag{123}$$

where we assume a phonon dispersion between $0 - \omega_m$. At temperatures $T << \hbar\omega/k_B$ this gives:

$$G_{th} = g_0 = \pi^2 k_B^2 T/(3h) \tag{124}$$

where $g_0 = (9.456 \times 10^{-13} W/K^2)T$ has been proposed as the quantum of thermal conductance [53, 188] and is the maximum value of energy transported per phonon mode. In a wire that is not strictly $1D$, as is the case of a wire of diameter $\sim 200nm$, other modes would contribute also to the current. In another nice and difficult experiment, Schwab et al. [188] were able to measure the quantum of thermal conductance. They used a silicon nitride wire which had four lowest massless modes and other massive modes corresponding to the finite width of the wire. By going to sufficiently low temperatures ($T < 1K$) they were able to suppress transport by the massive modes. Also one had to ensure very good contacts between the wires and reservoirs. The authors were able to verify that the resulting conductance corresponded to the value g_0. The agreement is in fact quite impressive. At high temperatures all modes would contribute and so it will be difficult to verify the classical $1D$ result with this system. Note that theoretically $\mathcal{T}(\omega) = 1$ can probably be achieved only with Rubin baths. For other baths (for example Ohmic) this cannot be obtained even for ordered chains and as a result, the temperature dependence of conductivity can be quite different [for example see sec.(3.3.1)] from the linear dependence in Eq. (124).

Another experiment [189] reported measurements of thermal conductivity of single crystalline Si nanowires with wires several microns long and with varying diameters between $22nm$ to $115nm$. They found that the thermal conductivity increased rapidly with diameter and was almost two orders of magnitude smaller ($\sim 20W/mK$) than the bulk value. These results have not been clearly understood. So far there has been no experiments measuring the dependence of conductivity on length in nanowires.

Experiments on nanotubes: Apart from nanowires, there have also been a number of measurements of heat current in nanotubes. One of the first measurements of conductance in individual samples was by Kim et al. [190], on a $2.4\mu m$ long and $14nm$ diameter multiwalled carbon nanotube (MWCNT). They found a very high thermal conductivity of $\approx 3000W/mK$ (at room temperature) and noted that this corresponded to a phonon mean free of $\sim 500nm$. Somewhat surprisingly this was close to a theoretically predicted value by Berber et al. [191] who had performed classical molecular dynamics simulations (using the Green-Kubo formula) for a $(10, 10)$ carbon nanotube. Using realistic potentials they reported a high thermal conductivity of $\approx 6000W/mK$, at room temperature. From our expectations of diverging conductivity we expect that these reported values, both in experiments and simulations, will increase with increasing length of the wire. In fact simulations by Maruyama [192], Zhang and Li [193], and by Yao et al. [195], again with realistic potentials, do find such a increase. A more recent simulation [196] however finds a converging conductivity.

As far as theoretical work on heat conduction in carbon nanotubes is concerned, we mention the insightful paper by Mingo and Broido [194], who point out that it is necessary to perform quantum mechanical calculations in order to understand the

experimental results and that classical calculations can be misleading. They mostly consider the ballistic conductance using the Landauer formula [Eq. (65)] and also the Boltzmann-Peierls equation at longer lengths. However they do not comment on the system size dependence of conductivity. It is likely that as far as the question of system size dependence of conductivity is concerned, the answer should probably be independent of whether one is doing a classical or a quantum calculation. Hence it will be useful to settle this issue through classical molecular dynamics simulations. From our experience with the difficulty in reaching asymptotic system sizes for $1D$ and $2D$ systems, it is clear that one has to be careful before coming to quick conclusions.

The experimental results of Fujii et al. [197] on individual MWCNT give some hints of anomalous behaviour. They also obtain large values of thermal conductivity but find that it decreases with the diameter of the tubes. At room temperatures the thermal conductivity of a $3.7\mu m$ long nanotube with diameter $\approx 10nm$ was about $2500W/mK$ while that of a $3.6\mu m$ long, diameter $\approx 30nm$ nanotube was about $500W/mK$. Note that the dependence of κ on diameter is opposite to that found for nanowires mentioned earlier.

Measurements on individual single-wall carbon nanotubes (SWCNT) also have now been done. Yu et al. [198] observed that the thermal conductance of a $2.76\mu m$ long suspended tube was very close to the calculated ballistic thermal conductance (calculated using the Landauer formula) of a $1nm$ diameter tube. In the temperature range of $100 - 300K$ they found increasing conductance and no signs of significant phonon-phonon scattering. Another measurement on a single-walled carbon nanotube by Pop et al. [199] measured the conductance to temperatures upto $800K$ and they found a $1/T$ decay at large temperatures. They also report measurements on various lengths, ranging from $0.5\mu m$ to $10\mu m$ and diameter $1.5nm$, and curiously, they found increasing conductance with length. This the authors explain can be understood to be a result of the large phonon mean free path $\sim 0.5\mu m$ and phonon boundary scattering.

An experimental proof of the divergence of thermal conductivity with system size is probably the dream of many theorists. There seems to be rapid progress in the direction of making this possible. The first indication of length dependence was reported by Wang et al. [200], for the case of a SWCNT placed on a silicon substrate. They measured samples of lengths between $0.5 - 7\mu m$ at room temperature and found a slow increase of the conductance. The most recent experiments by Chang et al. [201] makes a detailed investigation of the length dependence of conductivity in multiwalled nanotubes, of carbon and boron-nitride, and claim to have found convincing evidence for violation of Fourier's law. These room temperature measurements were on suspended tubes of effective length between $\approx 3.7 - 7\mu m$ and their estimate of phonon mean free path is $\sim 20 - 50nm$. From their measurements (over the rather limited length scale) the authors conclude that $\alpha \approx 0.6$ for the carbon nanotube $\alpha \approx 0.5$ for the boron nitride sample (which is isotopically disordered). It is interesting to note that the two samples in this experiment, approximately correspond to the ordered and disordered FPU models.

Experiments on suspended single layer graphene sheets have also been made recently [202] and so interesting experimental results from two dimensional systems can also be expected in the near future. It is of course too early to make definite conclusions from these experiments.

Finally we briefly discuss one other area, that of thermal rectifiers, where an experiment was motivated by theoretical work on simple models of heat conduction. In a paper by Terraneo et al. [203], an inhomogeneous nonlinear lattice model of heat conduction was proposed. This model had the interesting property that by

changing a single parameter on a part of the chain one could cause a transition from insulating to conducting behaviour. A related observation was that the absolute value of the heat current depended on the sign of $\Delta T = T_L - T_R$. Thus one basically had a model for a thermal rectifier. Note that it can be proved rigorously, for both harmonic systems (with inhomogeneity but without self-consistent reservoirs) as well as homogeneous anharmonic systems, that $J(\Delta T) = -J(-\Delta T)$ and so these systems cannot work as rectifiers. For harmonic systems this follows immediately from the general expression for current given in sec. (3.2). Clearly one needs both inhomogeneity as well as anharmonicity to get rectification and Terraneo et al. gave a simple explicit demonstration of how this could be achieved. Physically their results can be understood easily by thinking of the anharmonicity as giving rise to effective phonon bands which can be moved up and down by increasing or decreasing local temperatures. Phonon flow from the reservoirs into the system can thus be controlled.

Since the work in [203], a number of papers have observed this effect in a number of models [204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214]. Based on the model of thermal recifier, Yang and Li have proposed a design of a thermal logic gate [215]. An experimental observation of thermal rectification was made recently by Chang et al. [216, 217]. They made measurements of the heat current in a boron-nitride nanotube which was mass-loaded externally in an inhomogeneous way, and were able to obtain a small rectification.

We conclude this section with the note that the situation looks hopeful for vigorous interactions between theory and experiments.

9. Concluding remarks

The fact that Fourier's law is not valid in $1D$ and $2D$ systems is a surprising result and probably the most important knowledge gained from the large number of studies on heat conduction in low dimensional systems. Even in the limit of the system length being much larger than typical scattering lengths in a system, one finds that it is not possible to define a thermal conductivity as an intrinsic size-independent property of the system. This discovery is not only of academic interest but also important from the point of view of understanding real experiments. For example this tells us that it does not make sense to talk about the thermal conductivity of a carbon nanotube since this will keep changing with the length of the nanotube.

To summarize, the main conclusions of this review are:

(i) Fourier's law is not valid in momentum-conserving systems in one and two dimensions.

For disordered harmonic systems, $\kappa \sim N^{\alpha}$, where α depends on boundary conditions and spectral properties of heat baths.

For nonlinearly interacting systems without disorder, simulation results on a number of models indicate that in $1D$, $\alpha = 1/3$, and that there is only one universality class. There is disagreement between predictions from different theoretical approaches. In $2D$, the theoretical prediction of $\kappa \sim \log(N)$ has not been verified in the latest simulations.

(ii) Fourier's law, as far as the scaling $J \sim 1/N$ is concerned, is valid in momentum-non-conserving non-integrable systems in all dimensions. Both theory and most simulations agree on this.

(iii) In $1D$ oscillator systems with both disorder and anharmonicity, the asymptotic system size dependence of current is determined by anharmonicity alone, and localization becomes irrelevant.

(iii) Chaos is neither a necessary nor a sufficient condition for validity of Fourier's

law. This result follows from the observation that Fourier's law is valid in billiard-like systems with polygonal scatterers which have zero-Lyapunov coefficient and hence are non-chaotic. On the other hand Fourier's law is not valid for the FPU system in any parameter regime even though it has positive Lyapunov exponents.

(iv) For momentum-conserving $1D$ systems, it is not possible to write Fourier's law in the form $J = -\kappa_N \nabla T$ with κ_N defined as a size dependent conductivity. This follows from the anomalous steady state temperature profiles that seem to be invariably obtained in such systems.

(v) For harmonic lattice systems, the Langevin equation Green's function (LEGF) formalism provides a very useful theoretical framework for understanding heat transport, in both classical and quantum systems.

Some interesting problems that need to be addressed in the future are the following:

(a) Exact determination of the exponent α in any one dimensional momentum conserving model with purely Hamiltonian dynamics and without use of the usual Green-Kubo formula.

(b) Simulations on nonlinearly interacting systems in $1D$, $2D$ and $3D$ for larger system sizes and different models, in order to establish the exponents convincingly. It will be nice to have more results on systems such as hard discs and spheres.

We point out that the understanding of heat conduction even in three dimensional macroscopic systems is incomplete. A nice example of this can be seen from the discussion given in [218], in the context of understanding experimental results on heat conductivity of a highly purified single crystal diamond. A related point: in $3D$ it is a belief (see for example [93]) that at low temperatures, where Umpklapp processes become exponentially rare, normal processes along with impurity scattering lead to a finite conductivity for the system. Can this be given some more rigorous justification, or, verified in simulations ?

(c) Finding α for two and three dimensional disordered harmonic systems analytically. Further simulations are also necessary here. What are the connections with localization theory ?

(d) For disordered anharmonic systems, for disorder strength and anharmonicity strengths denoted by Δ and λ respectively, what is the phase diagram in the $\Delta - \lambda$ plane ?

(e) For open systems there is a rigorous derivation of a linear response result which is valid for finite systems. Is it possible to prove the equivalence of this with the usual Green-Kubo formula for closed systems, in some example ? This is probably true for systems with normal transport and probably *not true* for systems with anomalous transport.

(f) Proof of non-existence (or existence) of phase transitions in one dimensional models of heat conduction with short range interactions.

(g) One needs studies for quantum interacting systems since most experimental work seems to be in this domain. We have seen that the Green's function approach has been successful in understanding harmonic systems (*i.e.* ballistic transport). An extension of this approach to the anharmonic case would be very useful. Apart from the Green's function formalism, the approach used by Chen et al. [39] may be a useful method for this problem.

(h) How valid is the hydrodynamic description for systems with anomalous transport? If they are valid, what are the correct hydrodynamic equations? For example we have seen that one cannot use the equation $J = -\kappa_N(T)\nabla T$ to describe the steady state.

(i) Non steady state properties: most of the studies on heat conduction have been on measurement of current and temperature in the nonequilibrium steady state.

In general of course one is interested also in time dependent properties. In fact the diffusion equation following from Fourier's law is itself a time-dependent equation. Also many experiments make measurements in non-steady state conditions, such as by studying heat pulses and frequency dependent studies. Thus it is necessary to have more theoretical studies on heat flow in non steady state situations. Interesting questions can be asked here, *e.g.*, can one talk of a frequency dependent thermal conductivity [219] ?

(j) Scalar versus vector models: for lattice models one question is whether the dimensionality of the displacement vectors matters as far as exponents are concerned. While it is usually assumed that dimensionality does not matter, it will be nice to have a proof of this.

(k) Temperature dependence of conductivity or conductance: Apart from the system size dependence it will be useful to get more results on the temperature dependence of the linear response heat current, since this is one of the things that experimentalists are interested in.

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