The Fourier law in a momentum-conserving chain

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Abstract. We introduce a family of models for heat conduction with and without momentum conservation. They are analytically solvable in the high temperature limit and can also be efficiently simulated. In all cases the Fourier law is verified in one dimension.

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Contents

1. Introduction

When there is a temperature difference between the boundaries of a material, heat is transported from the hottest to the coldest side. The phenomenological law governing this process has been known for a long time: the *Fourier law* $J = k\nabla T$ states the proportionality of the heat flux J (the amount of heat transported through the unit surface in unit time) to the thermal gradient ∇T (the spatial derivative of the temperature field). The proportionality constant k is called the *thermal conductivity coefficient*. Almost two centuries after Fourier's law was discovered, its microscopic derivation is still an open problem from a fundamental point of view. At stake is not only a question of mathematical rigour: spatial constraints in certain experimental systems can significantly alter the transport properties in ways that are not yet fully understood. Systems with dimension $d \leq 2$ can have a thermal conductivity that can even become anomalous (i.e. diverging in the thermodynamical limit), implying a breakdown of the usual Fourier law. In the last few years such systems became experimentally realizable, and this has spurred a renewed interest in the theoretical basis among the physics community (for recent reviews see [1, 2]).

An important family of models which has been extensively studied consist of regular periodic d-dimensional lattices of $N = L^d$ point-like atoms interacting with their neighbours through *non-linear* forces, as in the Fermi–Pasta–Ulam (FPU) chain. For

the linear chain ($d = 1$) of oscillators it was rigorously established in the 1960s [3] that the heat conductivity diverges in the thermodynamic limit like $k \sim L$. This result was later generalized to the higher dimensional case in [4].

Indeed, the dynamics of such a system can be decomposed into the evolution of non-interacting waves (normal modes) which do not exchange energy amongst themselves, thus giving rise to ballistic transport. It is nowadays clear that in order to have a finite thermal coefficient the model must possess an efficient mechanism of scattering between phonons. However, numerical studies indicate that also in the presence of anharmonicity heat conductivity is still anomalous, with a power law divergence $k \sim L^{\alpha}$, where $\alpha \sim 0.37$ [5] for a linear chain. In recent years, an increasingly large amount of (very often conflicting) numerical results have appeared in the literature. Although some progress has been achieved, many puzzles remain. At present, the picture we have for 1D is as follows:

- *Anomalous conductivity* occurs in cases in which momentum is conserved, i.e. at least one acoustic phonon branch is present in the harmonic limit [5]–[10]. The reason for the anomalous behaviour has been traced back to the low frequency Fourier modes, which are only weakly damped by the interaction with other modes so they behave as very efficient energy carriers for the system. The condition of momentum conservation is however not sufficient: the 'coupled rotor model' seems to have normal conductivity [11, 12], the reason being phase jumps between barriers of the periodic potential which act as scatterers even for the long wavelength modes.

  Here a short discussion is in order: if a system is composed of free particles, momentum conservation is associated with the symmetry with respect to simultaneous translation of all particles. In a system such as the FPU or the coupled rotator system, we have particles with coordinates x_i—a deviation from the lattice position in the former, and an angle in the latter case. By translation invariance we may mean the symmetry 'in the coordinates' $i \to i + 1$, or the symmetry 'in the fields' $x_i \to x_i + \delta$. The issue is somewhat mixed up by the fact that in the FPU system we tend to picture the x_i along the line joining the baths, while for the coupled rotors we think of the x_i as being transverse. In fact, as already pointed out in [33], the difference between 'longitudinal' and 'transverse' only arises if the thermal baths interact with all the particles which reach a certain position (so that there is contact with the bath or not depending on the actual value of x_i), while it is irrelevant whether the bath is connected to some fixed particles at the end, whatever their positions x_i might be. One could conjecture that the transverse nature of the x_i in the rotor case was responsible for the finite conductivity, although this would suggest that the FPU chain with baths coupled to fixed particles at the ends should have normal conductivity too, contrary to observation.

- *Finite thermal conductivity* has been obtained for special models with interaction with a substrate which violates momentum conservation (the so-called ding-a-ling [13] and ding-dong [14] models or various Klein–Gordon chains [15, 16]).

- A Hamiltonian system for which a macroscopic transport law has been rigorously derived is a *gas of non-interacting particles* moving among a fixed array of periodic convex scatterers (the periodic Lorentz gas or Sinai billiard) [17]–[19]. More recently, a modified Lorentz gas with fixed freely rotating circular scatterers has also been considered [20]. In a further development, Eckmann and Young [30] introduced a

related model (having also normal heat conduction) that can be solved analytically in a limit.

- The consequences of the underlying *microscopic dynamics* are very controversial: while it was believed for a long time that dynamical chaos and full hyperbolicity are necessary and sufficient conditions for having finite conductivity, recent examples show that: (i) deterministic diffusion and normal heat transport can take place in systems with linear instability [21]–[23]; (ii) there are systems with positive Lyapunov exponents (FPU model) where the heat conduction does not obey the Fourier law.

- The role of *disorder* (in the form of random masses of the atoms) has also been considered. For the linear oscillators it has been rigorously shown that disorder is not enough to reproduce correctly the Fourier law (in fact one finds $k \sim L^{1/2}$ [24]–[26]). For non-linear oscillators the anomalous behaviour has been confirmed numerically [27].

- *Stochastic models* have also been studied [28, 29] and a finite thermal conductivity has been found. The large deviation properties of such models have also been investigated recently [31]. While these models can be useful for obtaining exact results under the assumption of suitable Markovian dynamics, one would like to obtain an explanation of the Fourier law starting from a pure deterministic description.

In the presence of anomalous heat conductivity there exist two main general theoretical predictions:

- A self-consistent 'mode-coupling' theory which predicts an exponent $\alpha = 2/5$ [32, 2].
- Renormalization group analysis of a set of hydrodynamic equations for a 1D fluid which yields $\alpha = 1/3$ [33].

It has been suggested that a crossover might exist between these two behaviours; see [34]. Both of them apply to momentum-conserving systems. It is worth mentioning that present numerical simulations are not fully in agreement with either mode-coupling or liquid theory predictions. Some authors suggested that the discrepancy might arise because intermediate sizes and timescales currently available in simulations are not able to probe the real behaviour in the thermodynamic limit. In this respect, the problem must be admittedly seen as an open question. The situation is even less clear for 2D lattices. Theoretical arguments support a weak logarithmic divergence for the thermal conductivity. On the other hand numerical simulations gave very conflicting results: logarithmic divergence [35], power law anomalous behaviour [36] and even finite thermal conductivity [37].

To understand some of the basic features of the energy transport in 1D systems, we develop in this paper a simple model, which can be cast also in the form of a set of discrete coupled maps such that in a limit the continuum version is reobtained. It can be solved analytically for high energies, and it is suitable at all energies for numerical simulations because it is much less demanding as regards computer time compared to a continuous flux. Because the approach to the high energy value of the conductivity can be seen in the simulations, the discussion is not plagued with doubts as to whether the results are preasymptotic. We have found no differences between the case in which momentum is conserved and the case in which it is not.

2. Hamiltonian model

We consider a chain of particles for simplicity in a one-dimensional lattice. In its most general form, the model is described by the following Hamiltonian:

$$H(x, p) = \sum_{i=1}^{N} \tfrac{1}{2}(p_i + A_i)^2 \tag{1}$$

where $A = (A_1(x), A_2(x), \ldots, A_N(x))$ is a generalized 'vector' potential in $\mathbb{R}^N$ and $x = (x_1, x_2, \ldots, x_N)$, $p = (p_1, p_2, \ldots, p_N)$ denote the particle position and momentum respectively. The Hamiltonian equations of motion read

$$\begin{aligned}
\frac{\mathrm{d}x_i}{\mathrm{d}t} &= p_i + A_i \\
\frac{\mathrm{d}p_i}{\mathrm{d}t} &= -\sum_{j=1}^{N} (p_j + A_j)\frac{\partial A_j}{\partial x_i}.
\end{aligned} \tag{2}$$

They are more transparent in the Newtonian formulation

$$\begin{aligned}
\frac{\mathrm{d}x_i}{\mathrm{d}t} &= v_i \\
\frac{\mathrm{d}v_i}{\mathrm{d}t} &= \sum_{j=1}^{N} B_{ij} v_j + \frac{\partial A_i}{\partial t}
\end{aligned} \tag{3}$$

where

$$B_{ij}(x) = \frac{\partial A_i(x)}{\partial x_j} - \frac{\partial A_j(x)}{\partial x_i} \tag{4}$$

is an *antisymmetric* matrix containing in the entries the 'magnetic fields' acting on the particles.

2.1. Conservation laws

2.1.1. Conservation of energy. Even if the forces depend on velocities and positions, the model always conserves the total (kinetic) energy if the fields are time independent due to the antisymmetry of the matrix B:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_i \frac{1}{2}v_i^2\right) = \sum_{i,j=1}^{N} B_{ij} v_i v_j = 0. \tag{5}$$

2.1.2. Conservation of momentum. Additional conserved quantities can be imposed by a suitable choice of the magnetic fields. For example, if we choose the $A_i(x)$ such that they are left invariant by the simultaneous translations $x_i \to x_i + \delta$, then the quantity $\sum_i p_i$ is conserved. If in addition we require that $\sum_i A_i(x) = 0 \;\; \forall x$, then this also implies the conservation of $\sum_i \dot{x}_i$.

3. Time-independent Hamiltonian, continuous time

The simplest way to realize this is the following: for a system with only energy conservation, we may put $A_i = f_i(x_i, x_{i+1})$ for some functions f_i. For periodic boundary conditions, one identifies the sites modulo N. Then, the matrix B takes the nearest-neighbour form

$$\mathbf{B} = \begin{pmatrix} 0 & B_1 & 0 & \ddots & 0 & -B_N \\ -B_1 & 0 & B_2 & 0 & \ddots & 0 \\ 0 & -B_2 & 0 & B_3 & 0 & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \ddots & \ddots & -B_{N-3} & 0 & B_{N-2} & 0 \\ 0 & \ddots & 0 & -B_{N-2} & 0 & B_{N-1} \\ B_N & 0 & \ddots & 0 & -B_{N-1} & 0 \end{pmatrix}. \tag{6}$$

An open chain is obtained putting $B_N = 0$. A momentum-conserving model with next-to-nearest-neighbour interaction can be obtained with

$$\begin{aligned} A_i &= C_{i+1} - C_i \\ C_i &= f_i(x_{i+1} - x_i) \end{aligned} \tag{7}$$

for any functions f_i. Again, one can take periodic boundary conditions (and then the indices are interpreted as modulo N), or consider an open chain, in which case one has to make $C_1 = 0$.

In both cases the end sites may be coupled to Langevin baths by modifying the equations of motion of p_1 and p_N by adding a noise and a friction term, satisfying the fluctuation-dissipation relations for temperatures T_1 and T_N, respectively.

4. Discrete time

One can also consider discrete time versions of these models, yielding a system of coupled maps. These have the advantage of being particularly easy to simulate, and, more importantly, they are analytically solvable in the high energy limit. As we shall see, the price we shall pay is that the map will not be symplectic[3], but it does preserve the phase-space volume and the Gibbs measure.

We first describe a version without momentum conservation in detail, and then describe more briefly the momentum-conserving case. We consider impulsive magnetic fields which act periodically and are of the form

$$B_{i,j}(x,t) = B_{ij}^{\text{even}}(x)K^{\text{even}}(t) + B_{i,j}^{\text{odd}}(x)K^{\text{odd}}(t) \tag{8}$$

---

[3] The same situation arises in [20, 30], where the rotation of the velocity vector is brought about by the impact on a 'rough' cylinder.

where

$$K^{\text{even}}(t) = \sum_{n=-\infty}^{+\infty} \Delta(t - n\tau)$$
$$K^{\text{odd}}(t) = \sum_{n=-\infty}^{+\infty} \Delta(t - (n+1/2)\tau)$$

(9)

where $\Delta(u)$ is a square pulse of intensity k and duration $1/k$, and we consider $k \to \infty$. During the short time when the fields are acting, the particles move a negligible amount, but their velocities rotate under their action. In contrast, between kicks the velocities are constant and the motion is uniform. Without loss of generality we can set $\tau = 1$ because changing the time interval between kicks amounts to rescaling the velocities. In the spirit of references [28]–[30], we consider a chain with even N and choose the B_{ij}^{even} and B_{ij}^{odd} such that the impulsive fields couple sites pairwise as follows:

- B_{ij}^{odd} is of the form (6) with $B_2 = B_4 = B_6 = \cdots = 0$ and $B_1 = G(x_1, x_2)$, $B_3 = G(x_3, x_4), \ldots$.
- B_{ij}^{even} is of the form (6) with $B_1 = B_3 = B_5 = \cdots = 0$ and $B_2 = G(x_2, x_3)$, $B_4 = G(x_4, x_5), \ldots$.

A periodic chain might be used, or, as we shall do later, one can connect the end sites to thermal baths during a half-cycle between kicks. The definition is completed by saying that whenever a site is connected to a heat bath during half a cycle, the interaction is so strong as to completely equilibrate the site at the bath's temperature.

As we mentioned above, the map as we define it is not symplectic, even though it might seem like the composition of Hamiltonian steps. The reason for this is subtle: just before the end of the period during which the magnetic field is on, the velocity is $v_i = p_i + A_i$, and just after it is turned off it is $v_i' = p_i$. If we wish to impose that $v_i = v_i'$ (which we need for energy conservation), we see that this implies a jump in the momenta of magnitude $A_i(x)$. This is a transformation that is *not* symplectic unless $\partial A_i / \partial q_j = \partial A_j / \partial q_i$, as is easy to check. An alternative way to see this is to consider the map as resulting from a time-dependent field, and then adding a (non-conservative!) force that exactly cancels $\partial A_i / \partial t$ in (3), so that energy is conserved. Note, however, that the map conserves the volume for all trajectories, and leaves the Gibbs measure invariant, even if there is a potential $V(q)$ acting during the intervals between kicks.

Because in this time-dependent version we have given up symplecticity, we might just as well give up the requirement that the $B_{ij} = B_{ji}$ derive from a 'vector potential' A_i. This will alter neither the equilibrium nor the volume conservation properties of the map, but gives us the freedom to use simpler functional forms for the B_{ij}. We tried different possibilities for the dependence on x of the magnetic field acting on each couple of sites, obtaining similar results. We present here those corresponding to the choice

$$G(x_i, x_{i+1}) = K[(x_i + x_{i+1}) - 2\pi].$$

(10)

With this choice the magnetic fields take values in the interval $[-2K\pi, 2K\pi]$, where K is a constant parameter.

By integrating the equations of motion (3) between two successive kicks, and having imposed the condition of continuity of the velocities described above, we arrive at the following discrete time dynamics: denote by $R_i(t)$ the 2×2 rotation matrix

$$R_i(t) = \begin{pmatrix} c(B_i) & s(B_i) \\ -s(B_i) & c(B_i) \end{pmatrix} \tag{11}$$

where

$$\begin{aligned} c(B_i) &= \cos(B_i(t)) \\ s(B_i) &= \sin(B_i(t)) \end{aligned} \tag{12}$$

and consider the matrices $C(t)$ and $D(t)$ composed of a series of two-by-two blocks:

$$C(t) = \begin{pmatrix} R_1 & \begin{matrix}0 & 0\\0 & 0\end{matrix} & \begin{matrix}0 & 0\\0 & 0\end{matrix} & \cdots & \begin{matrix}0 & 0\\0 & 0\end{matrix} & \begin{matrix}0 & 0\\0 & 0\end{matrix} \\ \begin{matrix}0 & 0\\0 & 0\end{matrix} & R_3 & & & & \begin{matrix}0 & 0\\0 & 0\end{matrix} \\ \begin{matrix}0 & 0\\0 & 0\end{matrix} & & R_5 & & & \begin{matrix}0 & 0\\0 & 0\end{matrix} \\ \vdots & & & \ddots & & \vdots \\ \begin{matrix}0 & 0\\0 & 0\end{matrix} & & & & R_{N-3} & \begin{matrix}0 & 0\\0 & 0\end{matrix} \\ \begin{matrix}0 & 0\\0 & 0\end{matrix} & \begin{matrix}0 & 0\\0 & 0\end{matrix} & \begin{matrix}0 & 0\\0 & 0\end{matrix} & \cdots & \begin{matrix}0 & 0\\0 & 0\end{matrix} & R_{N-1} \end{pmatrix} \tag{13}$$

$$D(t) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ \begin{matrix}0\\0\end{matrix} & R_2 & & & & & & & \begin{matrix}0\\0\end{matrix} \\ \begin{matrix}0\\0\end{matrix} & & R_4 & & & & & & \begin{matrix}0\\0\end{matrix} \\ \vdots & & & \ddots & & & & & \vdots \\ \begin{matrix}0\\0\end{matrix} & & & & R_{N-4} & & & & \begin{matrix}0\\0\end{matrix} \\ \begin{matrix}0\\0\end{matrix} & & & & & R_{N-2} & & & \begin{matrix}0\\0\end{matrix} \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{14}$$

Given $x(t), v(t)$, the position–velocity vector at time t, its evolution will be

$$\begin{aligned} x(t+1/2) &= x(t) + v(t) \\ v(t+1/2) &= C(t) \cdot v(t) \end{aligned} \tag{15}$$

$$\begin{aligned} x(t+1) &= x(t+1/2) + v(t+1/2) \\ v(t+1) &= D(t) \cdot v(t+1/2) + \xi(t) \end{aligned} \tag{16}$$

where $\xi(t)$ is a N-dimensional vector which is introduced to model interaction with heat baths:

$$\xi(t) = \begin{pmatrix} \xi_1(t) \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \xi_N(t) \end{pmatrix}. \tag{17}$$

At each time the non-zero components $\xi_1(t)$ and $\xi_N(t)$ are i.i.d. random variables with Gaussian distribution

$$P(y) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-y^2/2\sigma^2} \tag{18}$$

where the variances of $\xi_1(t)$ and $\xi_N(t)$ are respectively T_1 and T_N.

All odd sites interact with the site to their right during half a cycle, and with the site to their left during the other half-cycle. The sites at the ends interact with the baths during the corresponding half-cycles, and during that time they completely thermalize. In order to keep things simple we restrict the configuration space of each particle to the torus ($x \in [0, 2\pi]$), so that all the $x_i(t)$ are understood modulo 2π.

As usual with these maps, if we consider the limit of small velocities and weak kicks, we recover a continuous evolution.

4.1. Chaoticity properties of the map

In order to see what chaoticity properties to expect from a chain, we begin in this section with the study of the dynamical properties of the elementary map with only two sites $(x_1, x_2) \equiv (x, y)$. This a particle moving in the x–y plane (actually we restrict ourselves to the torus $\mathbb{T}^2$) under the action of an impulsive field along the z direction whose amplitude depends on the particle's position itself. Between kicks the motion is free; at each kick the velocity vector is rotated by an angle which is exactly given by the magnetic field, evaluated at the point where the kick takes place. Since the dynamics conserves the energy the accessible phase space is a three-dimensional one. Denoting by v the modulus of the velocity ($v = \sqrt{v_x^2 + v_y^2}$) and by β its angle w.r.t. the x direction in the plane, we have

$$\begin{aligned} x(t+1) &= \{x(t) + v\cos(\beta(t))\} \bmod(2\pi) \\ y(t+1) &= \{y(t) + v\sin(\beta(t))\} \bmod(2\pi) \\ \beta(t+1) &= \beta(t) + K[(x(t+1) + y(t+1)) - 2\pi]. \end{aligned} \tag{19}$$

The two-site map has two control parameters: the modulus of the velocity v (a constant of motion) and the amplitude of the field K. To illustrate the effect of varying them we have studied the Poincaré section. In figure 1 we plot the surface section obtained by using the plane $y = 0$ for $K = 1$ and several initial conditions. We see that as v tends to zero the trajectories are regular. As v increases, a smooth transition to a chaotic behaviour is observed. If one considers a chain of more than two sites of coupled maps of this kind, one can expect the property of chaoticity to be stronger for larger system sizes.
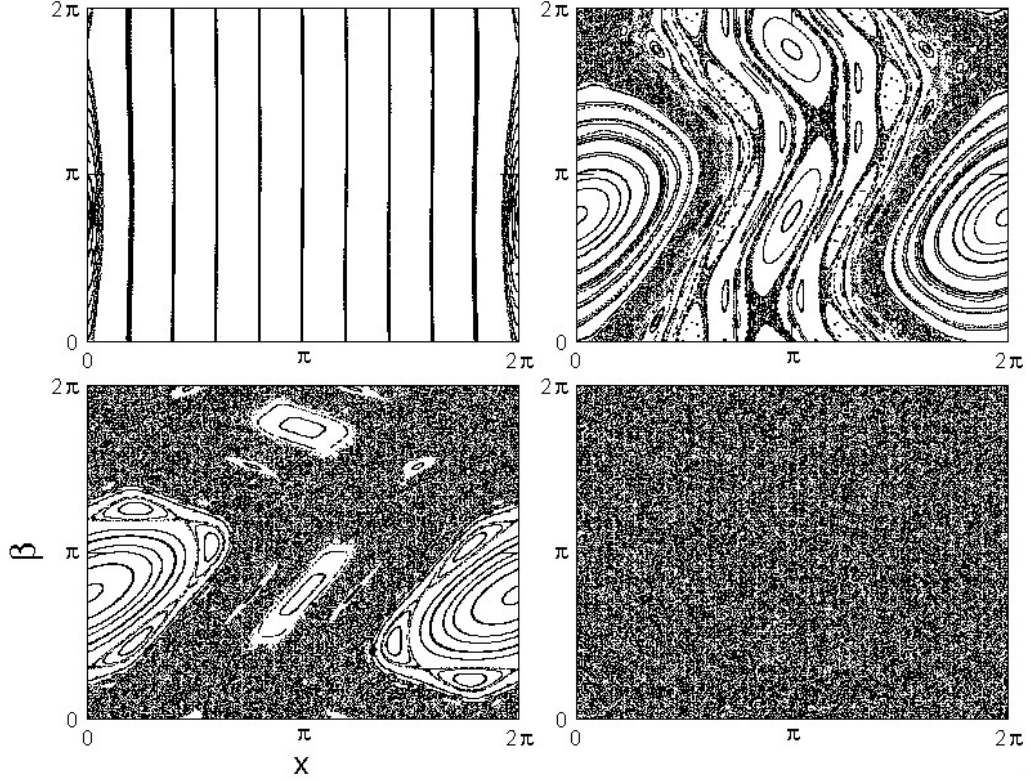
Figure 1. Poincaré sections for the map (19). Here $K = 1$ and $v = 0.01$ (top left), $v = 0.6$ (top right), $v = 1$ (bottom left), $v = 5$ (bottom right).

4.2. Numerical analysis of the Fourier law

To compute the heat conductivity one has two possible procedures: the first is the direct non-equilibrium measure with two reservoirs at different temperatures, taking the ratio between the time averaged flux and the temperature gradient. If a linear response regime is applicable, one can also use the Green–Kubo formula, which enables one to calculate transport coefficients as integrals of the autocorrelation function in equilibrium states. The thermal conductivity is then given by

$$k(T) = \frac{N}{T^2} \sum_{t=0}^{\infty} \langle J(t)J(0) \rangle_{\text{GB}} \left(1 - \frac{\delta_{t,0}}{2} \right) \tag{20}$$

where $J(t)$ is the flux per particle

$$J(t) = \frac{1}{N} \sum_{i=1}^{N} J_i(t). \tag{21}$$

The local heat flux $J_i(t)$ is given by the change in energy for the couple $(i, i + 1)$ before and after a kick. The angular brackets denote here an equilibrium average and the factor with the Kronecker delta function arises from the discreteness of time.

We first performed the numerical simulation with two heat baths at temperatures $T_L = 0.08$ and $T_R = 0.12$. After a transient of 10^7 steps, we checked that a linear
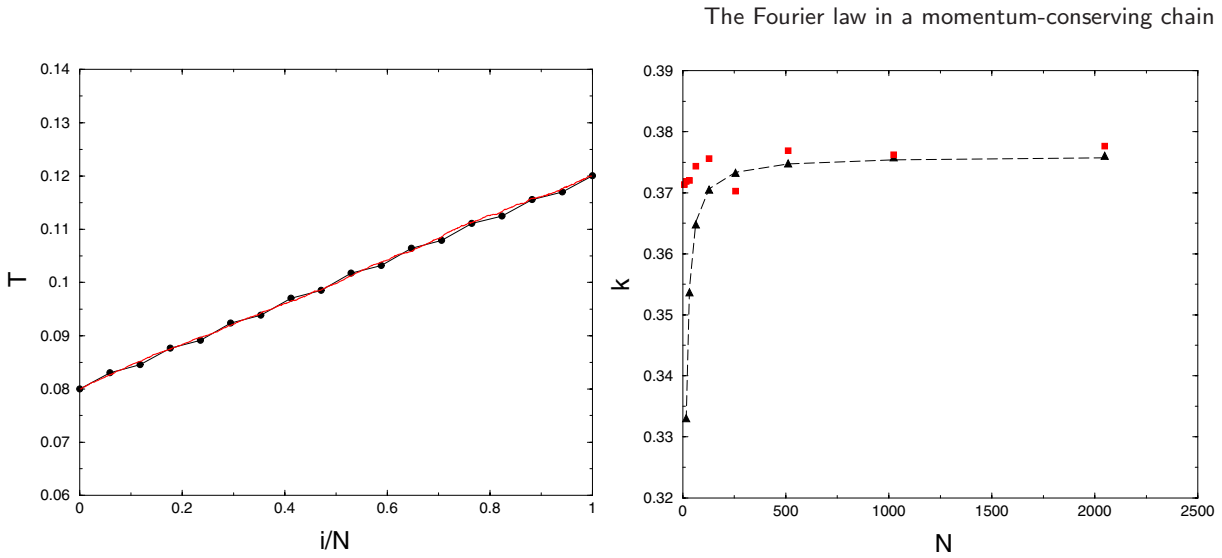
Figure 2. Results of simulations for $K = 1$. Left: temperature profile with two heat baths for $N = 16$ (circles) and $N = 2048$ (full line). Right: heat conductivity versus the chain length N obtained through non-equilibrium simulations (squares) and the GK formula (triangles). The continuous line represents the best fit with a function $k_\infty + a/N$.

temperature profile is established by measuring the temporal average of twice the kinetic energy at each site (see figure 2, left). We also kept track of the time averaged flux until it converged to its stationary value. We used at least 10^8 steps to check that fluctuations are less then a few per cent. The measured heat conductivity is reported in figure 2, right, for different chain lengths from $N = 8$ to 2048. One can see that the conductivity has some fluctuation in the interval $[0.37, 0.38]$ with an overall trend to stabilize, which suggests the approach to a finite value in the thermodynamic limit. We ran the dynamics for a large number of different initial random conditions (at least 10^3) and computed the heat conductivity using the Green–Kubo formula. We chose $e = E/N = 0.05$ which, according to the virial theorem, gives a kinetic temperature $T = 0.1$, the average of the temperatures of the two baths. The best fit of the data shows convincing evidence that finite size effects are of the form $\mathcal{O}(1/N)$ with an asymptotic value $k_\infty = 0.376$.

4.3. High temperature limit of the discrete model

In the high temperature limit the velocities $\dot{x}_i$ are large, so between two consecutive kicks new positions are translated by a large amount. Since the spatial coordinates are taken modulo 2π, the sequence of positions constitutes a (quasi-)random number generator. Hence, we assume that in this limit, the position of the particle when the fields are flashed can be taken as uniformly randomly distributed. Because the magnetic fields are functions of the positions, this means that the fields themselves are random, with a distribution that is easily derived from the position dependence of the fields. All in all, what we have is that the velocity vector turns at each kick by a random amount, the probability distribution of which is known. Let us consider the change in energy for the

couple $(i, i+1)$ before $(e_i = \frac{1}{2}v_i^2)$ and after $(e_i' = \frac{1}{2}v_i'^2)$ a kick:

$$
\begin{aligned}
e_i' &= c^2(B_i)\, e_i + s^2(B_i)\, e_{i+1} + 2\, s(B_i)\, c(B_i)\, \sqrt{e_i e_{i+1}} \\
e_{i+1}' &= s^2(B_i)\, e_i + c^2(B_i)\, e_{i+1} - 2\, s(B_i)\, c(B_i)\, \sqrt{e_i e_{i+1}}
\end{aligned}
\tag{22}
$$

where, of course, $e_i' + e_{i+1}' = e_i + e_{i+1}$. Suppose now that x_i, x_{i+1} are well approximated by independent uniform random process on the interval $[0, 2\pi]$. Then the magnetic field (10) will be a random variable and, with this particular choice for G, its probability distribution in the interval $[-2K\pi, 2K\pi]$ will be

$$
p(B) = \begin{cases}
\dfrac{1}{2K\pi}\left(1 + \dfrac{1}{2K\pi}x\right) & x \in [-2K\pi, 0] \\[2mm]
\dfrac{1}{2K\pi}\left(1 - \dfrac{1}{2K\pi}x\right) & x \in [0, 2K\pi].
\end{cases}
\tag{23}
$$

The mean energy of a couple of particles will be redistributed according to the rule

$$
\begin{aligned}
\langle e_i' \rangle &= x_K \langle e_i \rangle + (1 - x_K) \langle e_{i+1} \rangle \\
\langle e_{i+1}' \rangle &= (1 - x_K) \langle e_i \rangle + x_K \langle e_{i+1} \rangle
\end{aligned}
\tag{24}
$$

since

$$
\begin{aligned}
\langle c^2(B_i) \rangle &= \int_{-2K\pi}^{2K\pi} \cos^2(B)p(B)\,\mathrm{d}B = \frac{1}{2}\left(1 + \left(\frac{\sin(2K\pi)}{2K\pi}\right)^2\right) = x_K \\
\langle s^2(B_i) \rangle &= \frac{1}{2}\left(1 - \left(\frac{\sin(2K\pi)}{2K\pi}\right)^2\right) = 1 - x_K \\
\langle s(B_i)c(B_i) \rangle &= 0.
\end{aligned}
\tag{25}
$$

Here expectation values are taken over an ensemble of systems having the same velocities but random positions. If we choose K to be an integer or a half-integer, the dynamical rule (24) becomes (*only as far as the means are concerned*) that of the stochastic model introduced by Kipnis, Marchioro and Presutti [28]–[30], where the total energy of a particle pair is equally redistributed between the two ($x = 1/2$).

Let us give here a short computation of the heat conductivity in the case $K = 1$. The idea is to use first self-averaging with respect to the noise and then stationarity. The local 'temperature' is defined as twice the kinetic energy $T_i(t) = \langle v_i^2(t) \rangle$. Using (15), (16) and imposing stationarity $T_i(t) = T_i(t+1) = T_i$ one obtains the following recursion relation:

$$
\begin{aligned}
T_1 &= T_L \\
-T_{i-2} + 2T_i - T_{i+2} &= 0 & i &= 2, 4, 6, \ldots, N-2 \\
T_{i+1} &= T_i & i &= 0, 2, 4, 6, \ldots, N \\
T_N &= T_R.
\end{aligned}
\tag{26}
$$

This can be easily checked starting from a configuration $(T_L, T_2, T_2, T_4, T_4, \ldots, T_{N-2}, T_{N-2}, T_R)$, making it evolve through the two kicks, and demanding that the same configuration is recovered. From the solution of the system (26), a linear temperature profile is obtained (apart from the fact that the sites are in pairs):

$$
T_i = T_L + \frac{(T_R - T_L)}{N}i.
\tag{27}
$$
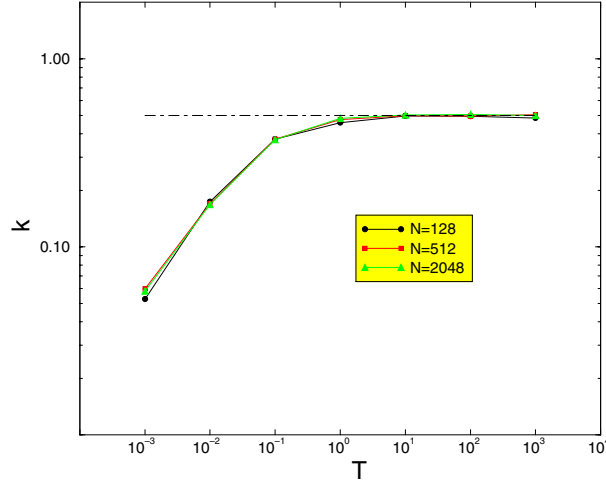
Figure 3. Thermal conductivity k versus the temperature (note the log–log scale). The dashed line corresponds to the value $k = 1/2$. Results are plotted for three different N values (see legend). Here only a single trajectory has been used in the application of the Green–Kubo formula. However the good overlap between the three curves indicates reliability of the computation.

It is easy to write a time-dependent version of (26), and check that the convergence to this profile is rapid, independently of the length of the chain, as it is essentially a diffusion equation.

Between t and $t + 1/2$ we consider the local flux of the odd sites, while between $t + 1/2$ and $t + 1$ we consider the local flux on the even sites. Self-averaging plus stationarity gives

$$
\begin{aligned}
j_0 &= \tfrac{1}{2}(T_L + T_1) - T_L \\
j_i &= \tfrac{1}{2}(T_i + T_{i+1}) - T_i \qquad i = 1, 2, \dots, N - 1 \\
j_N &= \tfrac{1}{2}(T_R + T_N) - T_N.
\end{aligned}
\tag{28}
$$

The solution is an average site-independent local flux

$$
j_i = \frac{1}{2}\frac{T_R - T_L}{N}
\tag{29}
$$

and a spatial average flux

$$
J = \frac{1}{N}\sum_{i=0}^{N} j_i = \frac{1}{2}\frac{T_R - T_L}{N}.
\tag{30}
$$

Putting together (27) and (30) we verify the Fourier law $J = k\nabla T$ with a heat conductivity $k = 1/2$.

In figure 3 we report the result of microcanonical simulations at different temperatures. One can see that for temperatures $T \geq 10$ the heat conductivity is basically constant and its numerical value coincides with the value we have just calculated in the high temperature regime.

4.4. Momentum-conserving model

We now run the arguments for a momentum-conserving model. Consider a coupling between three sites which is given by a magnetic field in the direction $(1, 1, 1)$. The analogue of (11) for this case is

$$R_i(t) = \frac{1}{3} \begin{pmatrix} 1 + 2\,c(B_i) & 1 - c(B_i) + \sqrt{3}\,s(B_i) & 1 - c(B_i) - \sqrt{3}\,s(B_i) \\ 1 - c(B_i) - \sqrt{3}\,s(B_i) & 1 + 2\,c(B_i) & 1 - c(B_i) + \sqrt{3}\,s(B_i) \\ 1 - c(B_i) + \sqrt{3}\,s(B_i) & 1 - c(B_i) - \sqrt{3}\,s(B_i) & 1 + 2\,c(B_i) \end{pmatrix} \quad (31)$$

where now

$$\begin{aligned} c(B_i) &= \cos(\sqrt{3}B_i(t)) \\ s(B_i) &= \sin(\sqrt{3}B_i(t)). \end{aligned} \quad (32)$$

A simple choice for $B_i = G(x_i, x_{i+1}, x_{i+2})$ is

$$G(x_i, x_{i+1}, x_{i+2}) = K[(x_i + x_{i+1} + x_{i+2}) - 3\pi]. \quad (33)$$

Clearly, the velocity in the $(1, 1, 1)$ direction (the sum of the three velocities) is not affected. If we now alternate kicks which couple sites $(1, 2, 3), (4, 5, 6), (7, 8, 9), \ldots$ with kicks which couple sites $(2, 3, 4), (5, 6, 7), (8, 9, 10), \ldots$, we obtain a map that at each kick conserves the total sum of the velocities (and, of course, the energy).

We can repeat the argument in the previous section to obtain the high energy limit. We set the multiplicative constant K to $1/\sqrt{3}$, for simplicity. If we consider that at each step the positions x_i, x_{i+1}, x_{i+2} are uniform and independently random with the choice (33), we have that

$$\langle c(B_i) \rangle = \langle s(B_i) \rangle = \langle c(B_i)s(B_i) \rangle = 0 \quad (34)$$

$$\langle c^2(B_i) \rangle = \langle s^2(B_i) \rangle = \tfrac{1}{2} \quad (35)$$

and we see that the average energies evolve during a kick as

$$\begin{pmatrix} \langle e_i' \rangle \\ \langle e_{i+1}' \rangle \\ \langle e_{i+2}' \rangle \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \langle e_i \rangle \\ \langle e_{i+1} \rangle \\ \langle e_{i+2} \rangle \end{pmatrix}. \quad (36)$$

Again we can easily find an equation for the T_i, and check that the profile is linear, with the only difference that now the sites come in triplets:
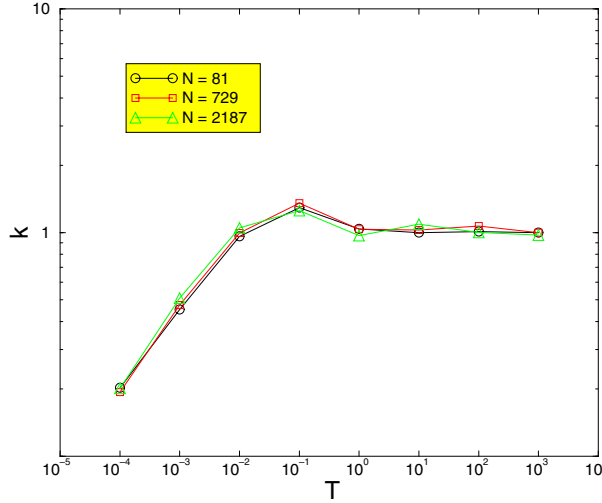
$$(T_L, T_L, T_3, T_3, T_3, T_6, T_6, T_6, \ldots, T_{N-3}, T_{N-3}, T_{N-3}, T_R) \quad (37)$$

and the temperatures satisfy

$$-T_{i-3} + 2T_i - T_{i+3} = 0 \qquad i = 3, 6, 9, \ldots, N - 3. \quad (38)$$

From this we easily obtain a value for the thermal conductivity $k = 1$.

The numerical simulations do agree with this value in the high temperature regime and give a finite heat conductivity at each temperature; see figure 4.

Figure 4. As figure 3 but for the momentum-conserving case. The analytical high temperature value is $k = 1$.

5. A stochastic minimal model

As was done in the previous section for the discrete time model we study here a high temperature limit which becomes a continuous time model, by replacing the magnetic fields with suitable random processes.

5.1. The Fokker–Planck equation

In the limit in which the field is very weak, and the velocities (and hence the energy) are very large, we get a velocity field that is randomly exchanging momentum, but in small amounts each step. The deterministic equations of motion (3) can then be replaced by a system of Langevin equations with multiplicative noise

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = \sum_{j=1}^{N} B_{ij} v_j \tag{39}$$

with the B_{ij} of the nearest-neighbour form (6):

$$B_{ij} = B_i(t)(\delta_{i,j+1} - \delta_{i+1,j}) \tag{40}$$

and B_i white, Gaussian random variables with[4]

$$\langle B_j(t) \rangle = 0 \qquad \langle B_j(t) B_k(t') \rangle = 2\, \delta_{jk}\, \delta(t - t'). \tag{41}$$

Standard techniques [38] yield the following Fokker–Planck equation for the evolution of the velocity probability distribution:

$$\frac{\partial P}{\partial t} = -\sum_{i=1}^{N} L_{i,i+1}^2 P \tag{42}$$

---

[4] This being a multiplicative process, the convention (Ito, Stratonovitch, ...) should be specified. In fact, the precise definition will be implicit in the Fokker–Planck equation (42), (43).

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where the operators $L_{i,i+1}$ are 'angular momentum' operators corresponding to the Laplacian on the sphere:

$$L_{i,i+1} = v_i \frac{\partial}{\partial v_{i+1}} - v_{i+1} \frac{\partial}{\partial v_i}. \tag{43}$$

If we add to the bulk system the interaction with two heat baths connected to the first and last particles (respectively at temperatures T_L and T_R) and represented as Ornstein–Uhlenbeck processes, we arrive at

$$\frac{\partial P}{\partial t} = \sum_{i=1}^{N} L_{i,i+1}^2 P + \partial_1(v_1 P) + T_L \partial_1^2 P + \partial_N(v_N P) + T_R \partial_N^2 P. \tag{44}$$

This diffusion process has also been considered by Olla [39], in combination with a deterministic harmonic part.

One can also easily write a momentum-conserving variant. Indeed, considering the low field version of the conserving map, we get

$$\frac{\partial P}{\partial t} = - \sum_{i=1}^{N} \{L_{i,i+1} + L_{i+1,i+2} + L_{i+2,i}\}^2 P \tag{45}$$

where in a closed chain the indices are understood modulo N.

5.2. Expectation values

We would like to compute the energy and flux expectation values and also energy correlations. One may derive an equation of motion for these quantities directly from the Fokker–Planck equation. Multiplying for instance (44) by v_i^2 and integrating the resulting equations, i.e.

$$\frac{\partial}{\partial t} \int v_i^2 P(v) \, \mathrm{d}^N v = \int v_i^2 \left(\sum_{i=1}^{N} L_{i,i+1}^2 P(v) \right) \mathrm{d}^N v$$

$$+ \int v_i^2 \left(\partial_1(v_1 P(v)) + T_L \partial_1^2 P(v) \right) \mathrm{d}^N v$$

$$+ \int v_i^2 \left(\partial_N(v_N P(v)) + T_R \partial_N^2 P(v) \right) \mathrm{d}^N v, \tag{46}$$

by using repeatedly integration by parts (with $v_i \partial_i = \partial_i v_i - 1$), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle v_1^2 \rangle = -4\langle v_1^2 \rangle + 2\langle v_2^2 \rangle + 2T_L$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle v_i^2 \rangle = 2\langle v_{i-1}^2 \rangle - 4\langle v_i^2 \rangle + 2\langle v_{i+1}^2 \rangle \qquad \text{for } i = 2, \ldots, N-1 \tag{47}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle v_N^2 \rangle = -4\langle v_N^2 \rangle + 2\langle v_{N-1}^2 \rangle + 2T_R.$$

In the stationary state $(\mathrm{d}/\mathrm{d}t)\langle v_i^2 \rangle = 0$, so the temperature profile is obtained as the solution of a linear system of equations. The solution is

$$T_i = T_L + \frac{(T_R - T_L)}{N+1} \, i. \tag{48}$$

In the stationary state there is a net heat current J flowing through the lattice. This can be calculated by directly measuring the energy exchange with the two baths. The energy flux from the left reservoir to the first particle is

$$\langle J_1 \rangle = \langle v_1^2 \rangle - T_L \tag{49}$$

while the energy flux from the last particle to the right reservoir is

$$\langle J_N \rangle = \langle v_N^2 \rangle - T_R. \tag{50}$$

In both cases, by using (48) we obtain

$$\langle J_1 \rangle = \langle J_N \rangle = J = \frac{(T_R - T_L)}{N+1}. \tag{51}$$

Putting together (48) and (51) we find that the Fourier law holds for the stochastic model with a heat conductivity $k = 1$.

5.3. The stationary measure

We show here that the stationary measure in the presence of heat flow cannot be of either Gaussian or product form. First of all, the evolution operator is invariant with respect to change in sign of any single velocity, and hence $P(v_1 \ldots v_N) = P(T_1, \ldots, T_N)$, i.e. the velocities only appear as even powers.
Proposing a Gaussian measure of the form

$$P(v_1 \ldots v_N) \sim \exp\left(-\tfrac{1}{2} \sum_{ij} A_{ij} v_i v_j\right) \tag{52}$$

and substituting into (44), we get

$$\left[\sum_{ij} A_{ij} v_i v_j\right]^2 = \left[\sum_{ij} A_{ij}^2 v_i v_j\right]\left(\sum v_i^2\right) \qquad \forall v \in \mathbb{R}^N. \tag{53}$$

Going to the diagonal basis $A = A_i \delta_{ij}$, this equation implies $(A_i - A_l)^2 = 0$, i.e., A is proportional to the identity. This is impossible if there is heat flow.
Let us see that a product measure

$$P(v_1 \ldots v_N) = \prod_{i=1}^{N} p_i(v_i) \tag{54}$$

is in general not possible if there is heat flow. In the stationary state we have

$$\frac{L_{\mathrm{FP}} P}{P} = \sum_{i=1}^{N} \frac{L_{i,i+1}^2 p_i(v_i) p_{i+1}(v_{i+1})}{p_i(v_i) p_{i+1}(v_{i+1})} = 0. \tag{55}$$

Because of their different arguments, each term must vanish separately; thus,

$$(L_{i-1,i}^2 + L_{i,i+1}^2) p_{i-1}(v_{i-1}) p_i(v_i) p_{i+1}(v_{i+1}) = 0. \tag{56}$$

This is an equation of the form $(L_x^2 + L_y^2)\psi = 0$ (with L_x, L_y the $SU(2)$ operators), which can only be satisfied by the quantum numbers $(l, m) = (00)$, the spherically symmetric

function. In our case this means that

$$p_1(x)p_2(y)p_3(z) = g(x^2 + y^2 + z^2) \tag{57}$$

which is a product only if we have an isotropic Gaussian, again impossible in the presence of heat flow.

The equations of motion for n-point correlation functions of these models are linear and form a closed set. This is a strong suggestion that the models may be integrable, but we shall not pursue this line here.

6. Conclusions

We have studied a family of models of heat transport whose high energy limit is analytically solvable. The intermediate energies are easy to simulate; the approach to the asymptotic value can be easily tested. The momentum-conserving version of the model has finite conductivity, providing further confirmation of the fact that in itself momentum conservation does not imply anomalous conductivity.

It would be nice in the future to investigate, in the simple framework of 'magnetic kicks' that we have introduced, a system which also has a potential energy. For example one could start from a system of coupled linear oscillators, establishing a connection with the work of Olla [39].

Another interesting problem is solving the Fokker–Planck equation to find the stationary distribution of our system. This could shed some light also on the stochastic model introduced by Presutti *et al* [29]. There again the stationary measure is a product measure only locally (i.e. in the approximation to first order in L^{-1}).

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