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A momentum conserving model with anomalous thermal conductivity in low dimension

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Anomalous large thermal conductivity has been observed numerically and experimentally in one and two dimensional systems. All explicitly solvable microscopic models proposed until now did not explain this phenomenon and there is an open debate about the role of conservation of momentum. We introduce a model whose thermal conductivity diverges in dimension 1 and 2, while it remains finite in dimension 3. We compute the finite-size thermal conductivity of a system of harmonic oscillators perturbed by a non-linear stochastic dynamics conserving momentum and energy. In the limit as the size N of the system goes to infinity, conductivity diverges like N in dimension 1 and like $\ln N$ in dimension 2. Conductivity remains finite if $d \geq 3$ or if a pinning (on site potential) is present. This result clarifies the role of conservation of momentum in the anomalous thermal conductivity.

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When a small gradient of temperature ∇T is applied to a material, we expect that, in the steady state, the heat current satisfies Fourier's law

$$\langle J \rangle = -\kappa \nabla T$$

where κ is the conductivity of the material. So if the system has length N and the left and right ends are in contact with thermostats at temperature T_ℓ and T_r respectively, the current, in the steady state, should be proportional to $(T_\ell - T_r)/N$.

There has been interest in the question of validity of Fourier's law for low dimensional systems ($d \leq 2$), where standard arguments based on linear response break down (cf. [1] and [2] for a review on the subject). Anomalous large conductivity is observed experimentally in carbon nanotubes and numerically in Fermi-Pasta-Ulam (FPU) systems without pinning (on-site potential), where numerical evidence shows a conductivity diverging like N^α , with $\alpha < 1$ in one dimension, and like $\log N$ in dimension 2 (cf. [2] and references of [2]). Finite conductivity is observed numerically in all pinned cases, and it is expected in all 3 dimensional cases, as long as some non-linearity is present in the interaction [1, 2]. Consequently it has been suggested that conservation of momentum is an important ingredient for the anomalous conductivity in low dimension [4].

In insulating crystals heat is transported by lattice vibrations, and since the pioneering work of Debye, systems of coupled anharmonic oscillators have been used as microscopic models for heat conduction. Non-linearity is extremely important, in fact in the linear case the average energy current $\langle J \rangle$ is independent of the length N of the system, i.e. the conductivity κ_N diverges like N [5].

Since conductivity in non-linear systems is difficult to compute or estimate analytically, it is natural to model the nonlinearities by stochastic perturbations of the linear dynamics. In some sense these stochastic perturbations simulate (qualitatively) the long time (chaotic) effect of the deterministic non-linear model.

We study in this letter a stochastic model that conserves energy and momentum, where conductivity can be explicitly computed, and diverges in dimension 1 and 2, while it remains finite in dimension 3. All the explicitly solvable models previously proposed in the literature have finite conductivity in all dimension (see discussion at the end of this letter).

We consider a system of harmonic (linear) coupled oscillators where the Hamiltonian dynamics are perturbed by a random exchange of momentum between nearest neighbors atoms. The random exchange of momentum conserves the total momentum and the total energy. We construct this noise with a diffusion on the surface of constant kinetic energy and momentum. Because of the conservation laws, this noise introduces a certain non-linearity in the model.

We compute explicitly the conductivity κ_N of the finite closed system of linear size N , by using Green-Kubo formula for the dynamics in the microcanonical ensemble. We find that it has a finite explicit limit as $N \rightarrow \infty$ in $d \geq 3$ or in the pinned cases, while it diverges like N in the unpinned 1-dimensional case, and like $\log N$ in the unpinned 2-dimensional case.

Most of the numerical simulations on FPU models concern open systems with boundaries in contact with thermal reservoirs. In low dimension, since conductivity diverges, the connection with the Green-Kubo formula for the finite system is not always clear in the deterministic

cases. So for our model we compute also the thermal conductivity of the open system in contact with thermal reservoirs at different temperatures and we show that it coincides with the Green-Kubo definition.

Other explicitly solvable models have been proposed before as perturbation of the harmonic chain (in [6] and [7] only the number of particles is conserved, in [11] only energy and the number of particles). In all these cases conductivity is always finite.

In order to compute the conductivity by the Green-Kubo formula, we consider the dynamics of the closed system of length N with periodic boundary conditions. The Hamiltonian is given by

$$\mathcal{H}_N = \frac{1}{2} \sum_{\mathbf{x}} [\mathbf{p}_{\mathbf{x}}^2 + \mathbf{q}_{\mathbf{x}} \cdot (\nu I - \alpha \Delta) \mathbf{q}_{\mathbf{x}}].$$

The atoms are labeled by $\mathbf{x} \in \mathbb{T}_N^d$, the d -dimensional discrete torus of length N . We denote with ∇ and Δ respectively the discrete gradient and the discrete Laplacian on \mathbb{T}_N^d . $\{\mathbf{q}_{\mathbf{x}}\}$ are the displacements of the atoms from their equilibrium positions. The parameter $\alpha > 0$ is the strength of the interparticles springs, and $\nu \geq 0$ is the strength of the pinning (on-site potential).

We consider the stochastic dynamics corresponding to the Fokker-Planck equation

$$\frac{\partial P}{\partial t} = (A + \gamma S)P = LP.$$

where A is the usual Hamiltonian vector field

$$A = \sum_{\mathbf{x}} \{\mathbf{p}_{\mathbf{x}} \cdot \partial_{\mathbf{q}_{\mathbf{x}}} + [(\alpha \Delta - \nu I) \mathbf{q}_{\mathbf{x}}] \cdot \partial_{\mathbf{p}_{\mathbf{x}}}\}$$

while S is the generator of the stochastic perturbation and $\gamma > 0$ is a positive parameter that regulates its strength. The operator S acts only on the momentums $\{\mathbf{p}_{\mathbf{x}}\}$ and generates a diffusion on the surface of constant kinetic energy and constant momentum. This is defined as follows. For every nearest neighbor atoms \mathbf{x} and \mathbf{z} , consider the $d-1$ dimensional surface of constant kinetic energy and momentum

$$\mathbb{S}_{e,\mathbf{p}} = \{(\mathbf{p}_{\mathbf{x}}, \mathbf{p}_{\mathbf{z}}) \in \mathbb{R}^{2d} : \mathbf{p}_{\mathbf{x}}^2 + \mathbf{p}_{\mathbf{z}}^2 = e ; \mathbf{p}_{\mathbf{x}} + \mathbf{p}_{\mathbf{z}} = \mathbf{p}\}.$$

The following vector fields are tangent to $\mathbb{S}_{e,\mathbf{p}}$

$$X_{\mathbf{x},\mathbf{z}}^{i,j} = (p_{\mathbf{z}}^j - p_{\mathbf{x}}^j)(\partial_{p_{\mathbf{z}}^i} - \partial_{p_{\mathbf{x}}^i}) - (p_{\mathbf{z}}^i - p_{\mathbf{x}}^i)(\partial_{p_{\mathbf{z}}^j} - \partial_{p_{\mathbf{x}}^j}).$$

so $\sum_{i,j=1}^d (X_{\mathbf{x},\mathbf{z}}^{i,j})^2$ generates a diffusion on $\mathbb{S}_{e,\mathbf{p}}$. In $d \geq 2$ we define

$$S = \frac{1}{2(d-1)} \sum_{\mathbf{x}} \sum_{i,j,k} \left(X_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^{i,j} \right)^2$$

where $\mathbf{e}_1, \dots, \mathbf{e}_d$ is canonical basis of \mathbb{Z}^d . Observe that total momentum $\sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}}$ and energy \mathcal{H}_N are thus conserved by these dynamics, i.e.

$$L \sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} = 0, \quad L \mathcal{H}_N = 0$$

In dimension 1, in order to conserve total momentum and total kinetic energy, we have to consider a random exchange of momentum between three consecutive atoms, and we define $S = \frac{1}{6} \sum_{x \in \mathbb{T}_N^1} (Y_x)^2$ where

$$Y_x = (p_x - p_{x+1}) \partial_{p_{x-1}} + (p_{x+1} - p_{x-1}) \partial_{p_x} + (p_{x-1} - p_x) \partial_{p_{x+1}}$$

which is vector field tangent to the surface of constant energy and momentum of the three particles involved.

Defining the energy of the atom \mathbf{x} as

$$e_{\mathbf{x}} = \frac{1}{2} \mathbf{p}_{\mathbf{x}}^2 + \frac{\alpha}{4} \sum_{\mathbf{y}:|\mathbf{y}-\mathbf{x}|=1} (\mathbf{q}_{\mathbf{y}} - \mathbf{q}_{\mathbf{x}})^2 + \frac{\nu}{2} \mathbf{q}_{\mathbf{x}}^2,$$

the energy conservation law can be read locally as

$$e_{\mathbf{x}}(t) - e_{\mathbf{x}}(0) = \sum_{k=1}^d (J_{\mathbf{x}-\mathbf{e}_k,\mathbf{x}}(t) - J_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t))$$

where $J_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t)$ is the total energy current between \mathbf{x} and $\mathbf{x} + \mathbf{e}_k$ up to time t . This can be written as

$$J_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t) = \int_0^t j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(s) ds + M_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t). \quad (1)$$

In the above $M_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t)$ is a martingale, i.e. a term that, for every initial condition, has zero average with respect to the noise of the dynamics, while the instantaneous energy currents $j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}$ satisfy the equation

$$L e_{\mathbf{x}} = \sum_{k=1}^d (j_{\mathbf{x}-\mathbf{e}_k,\mathbf{x}} - j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k})$$

and can be written as

$$j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} = j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^a + \gamma j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^s. \quad (2)$$

The first term in (2) is the Hamiltonian contribution to the energy current

$$j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^a = -\frac{\alpha}{2} (\mathbf{q}_{\mathbf{x}+\mathbf{e}_k} - \mathbf{q}_{\mathbf{x}}) \cdot (\mathbf{p}_{\mathbf{x}+\mathbf{e}_k} + \mathbf{p}_{\mathbf{x}}) \quad (3)$$

while the noise contribution in $d \geq 2$ is

$$\gamma j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^s = -\gamma \nabla_{\mathbf{e}_k} \mathbf{p}_{\mathbf{x}}^2 \quad (4)$$

and in $d = 1$ is

$$\gamma j_{x,x+1}^s = -\gamma \nabla \varphi(p_{x-1}, p_x, p_{x+1})$$

$$\varphi(p_{x-1}, p_x, p_{x+1}) =$$

$$\frac{1}{6} [p_{x+1}^2 + 4p_x^2 + p_{x-1}^2 + p_{x+1}p_{x-1} - 2p_{x+1}p_x - 2p_xp_{x-1}]$$

We define conductivity using the microcanonical version of the Green-Kubo formula. Consider the closed system on \mathbb{T}_N^d in the microcanonical measure. This is

defined as the uniform measure on the energy surface defined by $\mathcal{H} = N^d e$, for a given $e > 0$. If $nu > 0$, for any given e , this is the unique stationary measure. In the unpinned case $\nu = 0$, since also total momentum is conserved, we also fix this to be zero: $\sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} = 0$. The conductivity of the finite system in the direction \mathbf{e}_1 is defined as

$$\kappa_N^{1,1} = \lim_{t \rightarrow \infty} \frac{1}{2e^2 t} \frac{1}{N^d} \sum_{\mathbf{x}} \mathbb{E} (J_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}(t) J_{0, \mathbf{e}_1}(t))$$

where \mathbb{E} is the expectation starting with the microcanonical distribution. Using the explicit expression of the total current (1), because of the periodic boundary conditions all gradient terms disappear, and the martingale term gives a term equal to γd . The contribution of $j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}^a$ is

$$\begin{aligned} & \frac{1}{e^2 N^d} \sum_{\mathbf{x}} \int_0^\infty \mathbb{E} (j_{0, \mathbf{e}_1}^a(0) j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}^a(t)) dt \\ &= -\frac{1}{e^2 N^d} \left\langle j_{0, \mathbf{e}_1}^a(0) L^{-1} \left(\sum_{\mathbf{x}} j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}^a \right) \right\rangle_N \end{aligned} \quad (5)$$

where $\langle \cdot \rangle_N$ denotes the microcanonical expectation. We can compute explicitly

$$L^{-1} \left(\sum_{\mathbf{x}} j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}^a \right) = \frac{\alpha}{\gamma} \sum_{\mathbf{x}, \mathbf{y}} g(\mathbf{x} - \mathbf{y}) \mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}$$

where $g(\mathbf{z})$ is the solution of the equation

$$4\Delta g(\mathbf{z}) = (\delta(\mathbf{z} - \mathbf{e}_1) - \delta(\mathbf{z} + \mathbf{e}_1))$$

for $d \geq 2$, or

$$\frac{1}{3}\Delta [4g(z) + g(z+1) + g(z-1)] = (\delta(z-1) - \delta(z+1))$$

for $d = 1$. Substituting in (5), and using equivalence of ensembles estimates (cf [8] for the details) we have

$$\kappa_N^{1,1} = \gamma d + \frac{\alpha^2}{2\gamma} \sum_{\mathbf{z}} g(\mathbf{z}) \langle (\mathbf{q}_{\mathbf{z} + \mathbf{e}_1} - \mathbf{q}_{\mathbf{z} - \mathbf{e}_1}) \cdot \mathbf{q}_0 \rangle_N + o_N(1) \quad (6)$$

A simple Fourier analysis shows that, if $\nu = 0$ (i.e. the unpinned case), (6) diverge like N in dimension 1 and like $\log N$ in dimension 2. In all other cases $\kappa_N^{1,1}$ converge to a finite limit $\kappa^{1,1}$ given by

$$\kappa^{1,1} = \gamma d + \frac{\alpha^2 d}{2\gamma} \sum_{\mathbf{z}} (g(\mathbf{z} - \mathbf{e}_1) - g(\mathbf{z} + \mathbf{e}_1)) \Gamma(0, \mathbf{z})$$

where Γ is the kernel of the operator $(\nu I - \alpha \Delta)^{-1}$ on \mathbb{Z}^d . Observe that this expression diverges for $\gamma \rightarrow 0$, as expected since deterministic harmonic oscillators have infinite conductivity [5].

We consider now the open case where the finite system is in contact with 2 heat baths at different temperatures T_ℓ and T_r . We model these external thermal baths with Ornstein-Uhlenbeck processes at given temperatures. Let $\Xi_N = \{1, \dots, N\} \times \mathbb{T}_N^{d-1}$. Hence Ξ_N is a box of $(\mathbb{Z}^d)^N$ of length N with periodic boundary conditions in any direction different from the first direction. Atoms are now labeled by $\mathbf{x} \in \Xi_N$ and the dynamics is generated by the operator

$$L = A + \gamma S + B_\ell + B_r$$

where A and S are defined as before (with the laplacian Δ taken with Neumann boundary conditions), while B_ℓ and B_r are the contributions of the heat baths defined by

$$\begin{aligned} B_\ell &= \frac{1}{2} \sum_{\mathbf{x} \in \Xi_N} \delta_1(x_1) (T_\ell \partial_{\mathbf{p}_{\mathbf{x}}}^2 - \mathbf{p}_{\mathbf{x}} \cdot \partial_{\mathbf{p}_{\mathbf{x}}}) \\ B_r &= \frac{1}{2} \sum_{\mathbf{x} \in \Xi_N} \delta_N(x_1) \sum_{j=1}^d \left(T_r \partial_{p_{\mathbf{x}}^j}^2 - p_{\mathbf{x}}^j \partial_{p_{\mathbf{x}}^j} \right). \end{aligned}$$

If $T_\ell = T_r = T$ the centered gaussian product measure of variance T is the unique stationary state. When $T_\ell \neq T_r$, this system has still a unique stationary measure, but it cannot be computed explicitly but one can show that is not gaussian [8]. Let us denote the expectation with respect to this stationary measure with $\langle \cdot \rangle_{ss, N}$. The conductivity of this finite system can be defined as

$$\kappa_N^{ss} = \frac{N \langle j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1} \rangle_{ss, N}}{T_\ell - T_r}.$$

We prove that

$$\kappa_N^{ss} \underset{N \rightarrow \infty}{\sim} \kappa_N^{1,1}.$$

This is a consequence of a decomposition of the energy current in a space derivative plus a time derivative. In order to keep notations simple, let us consider the case $d = 1$. Define the functions

$$h_x = \frac{\alpha}{\gamma} \sum_z g(z) p_{x+z} q_x$$

and

$$\begin{aligned} \phi_x &= \frac{\alpha}{2\gamma} \sum_{z \geq 1} g(z) \left[\sum_{y \geq 1}^z \psi_{x+y}^z + \alpha(q_{x-z-1} q_x - q_{x-z} q_{x-1}) \right] \\ &\quad + \frac{\alpha}{2} (p_{x-1} + p_x) q_x + \gamma \varphi(p_{x-1}, p_x, p_{x+1}) \end{aligned}$$

where

$$\psi_x^z = p_{x-z} p_y + q_{x-z} (\alpha \Delta - \nu I) q_x.$$

Then by explicit calculation one can write

$$j_{x, x+1} = -\nabla \phi_x + L h_x \quad . \quad (7)$$

It follows that $\langle j_{x,x+1} \rangle_{ss,N} = -\nabla \langle \phi_x \rangle_{ss,N}$. By stationarity, this expected current is constant in x , so

$$N \langle j_{x,x+1} \rangle_{ss,N} = \sum_x \langle j_{x,x+1} \rangle_{ss,N} \\ = \langle \phi_1 \rangle_{ss,N} - \langle \phi_N \rangle_{ss,N} .$$

By the thermalization due to the heat baths, one can show that $\langle \phi_1 \rangle_{ss,N} \sim T \ell \kappa_N^{1,1}$ and $\langle \phi_N \rangle_{ss,N} \sim T_r \kappa_N^{1,1}$. This argument can be made rigorous by a proper localization of the functions h and ϕ and an entropy production argument [8]. A decomposition similar to (7) is valid also in $d \geq 2$. One can use directly (7) in the Green-Kubo formula (), obtaining the same result as above, by noticing that in the periodic case $\sum_x \nabla \phi_x = 0$ and that $\sum_x h_x = L^{-1} (\sum_{\mathbf{x}} j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^a)$.

Discussion. The exact results presented in this letter concerning the stochastic model we introduced, suggest some indications about the role of conservation of momentum and of confinement (pinning) in the heat conduction for the nonlinear deterministic Hamiltonian case. In fact the behavior of the conductivity that we proved in our stochastic model is (qualitatively) the same as the one indicated by numerical simulation for the deterministic non-linear FPU models, at least if $d \geq 2$ or for pinned models. In the one dimensional unpinned case we have a divergence like N . In non-linear FPU type of interaction, a behavior like N^α , with $0 < \alpha < 1$ is numerically observed. Numerical simulation cannot be conclusive about the value of α and there is an intense debate in the literature on this value (cf. [2]). As suggested recently by R. Livi [9], probably there is not a universal behavior of the conductivity in 1-dimensional systems (unlike the logarithmic behavior of the 2-dimensional systems) and the value of α may depend on the specific non linearity of the interaction.

In our calculation two factors determine the anomalous conductivity in low dimension: the conservation of momentum **and** the unboundness of the fluctuations of the positions $\{\mathbf{q}_{\mathbf{x}}\}$ in the equilibrium states. This would explain why the 1-dimensional coupled-rotors model, that conserves momentum, has finite conductivity [10]. Observe that in [11] we consider the unpinned 1-dimensional harmonic chain with noise that conserves only energy, and we prove that conductivity is finite in any dimension. These two examples suggest that both factors are necessary for the anomalous conductivity also for deterministic Hamiltonian non-linear systems.

About Fourier's law in non-equilibrium stationary state driven at the boundary by two thermal reservoirs, we have seen how this can be proven by a decomposition formula like (7), that in fact connects the conductivity of the open system to the Green-Kubo formula. Anomalous conductivity in low dimension is due to strong non-locality of the involved functions h and ϕ . Models for

which the current can be written as $\nabla \phi$ with a local ϕ are called *gradient models* in the mathematical literature of hydrodynamic limits. The Kipnis-Marchioro-Presutti model [13] is of this type, so is the Giardinà-Kurchan model in the high temperature approximation [12]. All gradient models have finite conductivity, if the equilibrium average of the function ϕ is finite. Hamiltonian deterministic models are always non-gradient. Our situation is non-gradient since the energy current has a gradient component $\gamma j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^s$ that comes from the contribution of the noise to the transport, and a non-gradient term $j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}^a$ that comes from the Hamiltonian mechanism, and whose slow decay of space-time correlations is responsible for the eventual anomalous conductivity in low dimensions.

One can consider a system of coupled anharmonic oscillators perturbed by the same noise considered in this article. We expect, qualitatively, a similar behavior of the conductivity, probably diverging like N^α in dimension 1 with $\alpha < 1$, and some logarithmic divergence in dimension 2. To prove this behavior, and prove Fourier's law in $d \geq 3$, is still a mathematically challenging problem, even though easier than the original non-linear deterministic case. The difficulty will be in proving the decomposition formula for the current (7). This decomposition will be valid only in some approximate sense. In general we expect conductivity depending on the temperature T .

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