Momentum Conserving Model with Anomalous Thermal Conductivity in Low Dimensional Systems

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Anomalous large thermal conductivity has been observed numerically and experimentally in one- and two-dimensional systems. There is an open debate about the role of conservation of momentum. We introduce a model whose thermal conductivity diverges in dimensions 1 and 2 if momentum is conserved, while it remains finite in dimension $d \geq 3$. We consider a system of harmonic oscillators perturbed by a nonlinear stochastic dynamics conserving momentum and energy. We compute explicitly the time correlation function of the energy current $C_J(t)$, and we find that it behaves, for large time, like $t^{-d/2}$ in the unpinned cases, and like $t^{-d/2-1}$ when an on-site harmonic potential is present. This result clarifies the role of conservation of momentum in the anomalous thermal conductivity in low dimensions.

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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. 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. [1,2] 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 dimension 1, and like $\log N$ in dimension 2 (cf. [2], and references therein). If some nonlinearity is present in the interaction, finite conductivity is observed numerically in all pinned cases, and it is expected in all three-dimensional cases [1,2], as long as some nonlinearity is present in the interaction. Consequently it has been suggested that conservation of momentum is an important ingredient for the anomalous conductivity in low dimension [3].

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. Nonlinearity 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 [4]. In fact, in the harmonic crystal the normal modes of the vibrations (phonons) do not interact and follow ballistic motion. A finite asymptotic conductivity instead should result eventually by the diffusive behavior of phonons due to phonon-phonon interaction caused by anharmonicity.

Since conductivity in nonlinear 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 nonlinear model.

We study in this Letter a stochastic model where conductivity can be explicitly computed, and diverges in dimension 1 and 2 when momentum is conserved, while it remains finite in dimension 3. So this is the only explicitly solvable model that has a behavior qualitatively consistent with numerical simulations.

We consider a system of harmonic (linear) coupled oscillators where the Hamiltonian dynamics are perturbed by a random exchange of momentum between nearest neighbor atoms. The random exchange of momentum conserves total momentum and 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 nonlinearity in the model.

We compute explicitly the time correlation function at equilibrium of the energy currents $C_J(t)$ [cf. Eq. (12)], and we find that, as $t \sim +\infty$, $C_J(t) \sim t^{-d/2}$ if the system is unpinned, while $C_J(t) \sim t^{-d/2-1}$ if an on-site potential is present. Conductivity, defined by the Green-Kubo formula, is then finite only in dimension $d \geq 3$ or for the pinned system. This indicates a divergence of the conductivity of the finite system κ_N as $N^{1/2}$ in the unpinned one-dimensional case, and as $\log N$ in the unpinned two-dimensional case.

Other explicitly solvable models have been proposed before as perturbation of the harmonic chain (in [5,6] only the number of particles is conserved, and in [7] only energy and the number of particles are conserved). In all these models, 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 stochastic dynamics where the probability density distribution on the phase space at time t, denoted by $P(t, \mathbf{q}, \mathbf{p})$, evolves following the Fokker-Planck equation (cf. [8]):

$$\frac{\partial P}{\partial t} = (-A + \gamma S)P = L^* P.$$

Here $L = A + \gamma S$ is the generator of the process, L^* is the adjoint operator, and A is the usual Hamiltonian vector field

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

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

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

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

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

where $\mathbf{e}_1, \ldots, \mathbf{e}_d$ is the canonical basis of $\mathbb{Z}^d$. Observe that this noise conserves the total momentum $\sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}}$ and energy $\mathcal{H}_N$; i.e.,

$$S\sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} = 0, \qquad S\mathcal{H}_N = 0.$$

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.

These dynamics can also be written in terms of the solutions of the stochastic differential equations:

$$d\mathbf{p}_{\mathbf{x}} = -(\nu I - \Delta)\mathbf{q}_{\mathbf{x}}dt + 2\gamma\Delta\mathbf{p}_{\mathbf{x}}dt + \sqrt{\gamma}d\mathbf{n}_{\mathbf{x}}(t), \quad (1)$$

where of course $\dot{\mathbf{q}}_{\mathbf{x}} = \mathbf{p}_{\mathbf{x}}$ and $\mathbf{n}_{\mathbf{x}}(t)$ are defined by the Ito stochastic integrals

$$\mathbf{n}_{\mathbf{x}}(t) = \frac{1}{2\sqrt{d-1}}\sum_{\|\mathbf{y}-\mathbf{x}\|=1}\sum_{i,j}^d \int_0^t (X_{\mathbf{x},\mathbf{y}}^{i,j}\mathbf{p}_{\mathbf{x}})(s)dw_{\mathbf{x},\mathbf{y}}^{i,j}(s).$$

Here $w_{\mathbf{x},\mathbf{y}}^{i,j}(t) = w_{\mathbf{y},\mathbf{x}}^{i,j}(t)$ are independent standard Wiener processes. In $d = 1$ the expression is similar with the term $2\gamma\Delta\mathbf{p}_{\mathbf{x}}$ replaced by $(\gamma/6)\Delta(4p_x + p_{x+1} + p_{x-1})$.

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

$$J_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t) = \int_0^t j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(s)ds + M_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t). \quad (2)$$

In the above, $M_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t)$ is the Ito stochastic integral defined by

$$M_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t) = \sqrt{\frac{\gamma}{d-1}}\sum_{i,j}^d \int_0^t (X_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^{i,j}e_{\mathbf{x}})(s)dw_{\mathbf{x},\mathbf{y}}^{i,j}(s).$$

The instantaneous energy currents $j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}$ satisfy the equation

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

and can be written as

$$j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} = j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^a + \gamma j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^s. \quad (3)$$

The first term in (3) is the Hamiltonian contribution to the energy current

$$j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^a = -\frac{\alpha}{2}(\mathbf{q}_{\mathbf{x}+\mathbf{e}_k} - \mathbf{q}_{\mathbf{x}}) \cdot (\mathbf{p}_{\mathbf{x}+\mathbf{e}_k} + \mathbf{p}_{\mathbf{x}}), \quad (4)$$

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

$$\gamma j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^s = -\gamma\nabla_{\mathbf{e}_k}\mathbf{p}_{\mathbf{x}}^2 \quad (5)$$

and in $d = 1$ is

$$\gamma j^s_{x,x+1} = -\gamma \nabla \varphi(p_{x-1}, p_x, p_{x+1}),$$
$$\varphi(p_{x-1}, p_x, p_{x+1}) = \tfrac{1}{6}[p^2_{x+1} + 4p^2_x + p^2_{x-1} + p_{x+1}p_{x-1} - 2p_{x+1}p_x - 2p_x p_{x-1}].$$

Consider the dynamics of the closed system on $\mathbb{T}^d_N$ in microcanonical equilibrium. The microcanonical distribution is usually defined as the uniform measure on the energy surface $\mathcal{H} = N^d e$, for a given $e > 0$. Our dynamics conserve also $(\sum \mathbf{p_x})^2 + \nu(\sum \mathbf{q_x})^2$. Notice that the dynamics is invariant under the change of coordinates $\mathbf{p}'_\mathbf{x} = \mathbf{p_x} - \sum_\mathbf{y} \mathbf{p_y}$ and $\mathbf{q}'_\mathbf{x} = \mathbf{q_x} - \sum_\mathbf{y} \mathbf{q_y}$. Consequently, without any loss of generality, we can fix $\sum \mathbf{p_x} = 0$ and $\sum \mathbf{q_x} = 0$ in the microcanonical measure.

Let us define $\mathfrak{I}_{\mathbf{e}_1} = \sum_\mathbf{x} j_{\mathbf{x},\mathbf{x}+\mathbf{e}_1} = \sum_\mathbf{x} j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}$. We are interested in computing the correlation function:

$$C_{1,1}(t) = \lim_{N\to\infty} \frac{1}{N^d} \mathbb{E}(\mathfrak{I}_{\mathbf{e}_1}(t)\mathfrak{I}_{\mathbf{e}_1}(0)), \tag{6}$$

where $\mathbb{E}$ is the expectation starting with the microcanonical distribution defined above. By explicit calculation we can solve the equation

$$(\lambda - L)^{-1}\mathfrak{I}_{\mathbf{e}_1} = -\frac{\alpha}{\gamma}\sum_{\mathbf{x},\mathbf{y}} g_{\lambda,N}(\mathbf{x} - \mathbf{y})\mathbf{p_x} \cdot \mathbf{q_y}, \tag{7}$$

where $g_{\lambda,N}(\mathbf{x})$ is the solution of the equation

$$\frac{2\lambda}{\gamma} g_{\lambda,N}(\mathbf{x}) - 4\Delta g_{\lambda,N}(\mathbf{x}) = [\delta(\mathbf{x} + \mathbf{e}_1) - \delta(\mathbf{x} - \mathbf{e}_1)] \tag{8}$$

on $\mathbb{T}^N_d$ for $d \geq 2$, while in one dimension it solves

$$\frac{2\lambda}{\gamma} g_{\lambda,N}(x) - \frac{1}{3}\Delta[4g_{\lambda,N}(x) + g_{\lambda,N}(x+1) + g_{\lambda,N}(x-1)] = [\delta(x+1) - \delta(x-1)]. \tag{9}$$

Consequently, for $\lambda > 0$, we can write the Laplace transform of $C_{1,1}(t)$ as

$$\int_0^\infty e^{-\lambda t} C_{1,1}(t)dt = \lim_{N\to\infty} \langle j^a_{0,\mathbf{e}_1}(\lambda - L)^{-1}\mathfrak{I}_{\mathbf{e}_1}\rangle_N, \tag{10}$$

where $\langle \cdots \rangle_N$ denotes the expectation with respect to the microcanonical measure.

By substituting (7) in (10) and using equivalence of ensembles estimates (see [8] for details), we have

$$\int_0^\infty e^{-\lambda t} C_{1,1}(t)dt = \frac{\alpha^2 e^2}{2d\gamma}\sum_\mathbf{z} g_\lambda(\mathbf{z})[\Gamma(0, \mathbf{z} + \mathbf{e}_1) - \Gamma(0, \mathbf{z} - \mathbf{e}_1)], \tag{11}$$

where Γ is the kernel of the operator $(\nu I - \alpha\Delta)^{-1}$ on $\mathbb{Z}^d$, while g_λ is the solution of Eq. (8) in $\mathbb{Z}^d$ or Eq. (9) in $\mathbb{Z}$. We compute explicitly (11) and invert the Laplace transform obtaining

$$C_{1,1}(t) = \frac{e^2}{4\pi^2 d}\int_{[0,1]^d} (\partial_{k^1}\omega(\mathbf{k}))^2 e^{-t\gamma\psi(\mathbf{k})} d\mathbf{k}, \tag{12}$$

where $\omega(\mathbf{k}) = [\nu + 4\alpha\sum_{j=1}^d \sin^2(\pi k^j)]^{1/2}$ is the dispersion relation of the system, and

$$\psi(\mathbf{k}) = \begin{cases} 8\sum_{j=1}^d \sin^2(\pi k^j) & \text{if } d \geq 2, \\ 4/3\sin^2(\pi k)[1 + 2\cos^2(\pi k)] & \text{if } d = 1. \end{cases} \tag{13}$$

Since around $\mathbf{k} = 0$ we have $\psi(\mathbf{k}) \sim \mathbf{k}^2$ and $(\partial_{k^1}\omega(\mathbf{k}))^2 \sim (\alpha k^1)^2(\nu + \alpha^2\mathbf{k}^2)^{-1}$, we have the following asymptotic behavior:

$$C_{1,1}(t) \sim_{t\to\infty} \begin{cases} t^{-d/2} & \text{if } \nu = 0, \\ t^{-d/2-1} & \text{if } \nu > 0. \end{cases} \tag{14}$$

By the Green-Kubo formula [9], the conductivity in the direction $\mathbf{e}_1$ is given by

$$\kappa^{1,1} = \lim_{t\to\infty} \frac{1}{2e^2 t} \lim_{N\to\infty} \sum_\mathbf{x} \mathbb{E}(J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t) J_{0,\mathbf{e}_1}(t)). \tag{15}$$

By explicit calculation one can show (see [8] for details)

$$\kappa^{1,1} = \frac{\gamma}{d} + \frac{1}{2e^2}\int_0^\infty C_{1,1}(t)dt = \frac{\gamma}{d} + \frac{1}{8\pi^2 d\gamma}\int_{[0,1]^d} \frac{(\partial_{k^1}\omega(\mathbf{k}))^2}{\psi(\mathbf{k})} d\mathbf{k}. \tag{16}$$

By (14), if $d \geq 3$ or if $\nu > 0$, the integral on the right-hand side of (16) is finite.

If $\nu = 0$ and $d \leq 2$, by (14) the time integral in (16) diverges and conductivity is infinite. Following Ref. [2] (p. 46), one can estimate the dependence of the conductivity of the finite open system of length N with thermic baths at the boundary imposing a temperature gradient, by restricting the time integral in (16) to times smaller than the "transit time" N/v_s, where v_s is the sound velocity of the lattice defined as $v_s = \lim_{\mathbf{k}\to 0}\partial_{k^1}\omega(\mathbf{k}) = 1$. This gives a finite size conductivity κ_N diverging like $N^{1/2}$ in dimension 1, and like $\log N$ in dimension 2.

Discussion.—The exact results presented in this Letter concerning the stochastic model we introduced give some indications about the role of conservation of momentum and of confinement (pinning) in heat conduction for the nonlinear deterministic Hamiltonian case. In fact, the decay of the energy current correlations and consequently the behavior of the conductivity that we proved in our stochastic model are (qualitatively) the same as those indicated by numerical simulation for the deterministic nonlinear FPU

models. Furthermore, a recent paper [10] on the one-dimensional unpinned purely quartic FPU model suggests the same decay of the time correlations of energy current as in our stochastic model.

In the one-dimensional case we can give the following euristic explanation of the effect of the noise in these harmonic systems. In deterministic harmonic systems the energy of each mode is conserved, in both pinned or unpinned chain; so if modes are created by initial or boundary conditions, they cannot interact and they move ballistically. This causes ballistic transport and diverging conductivity, in both cases (cf. [4,11]). The effect of the energy-momentum conservative noise we have introduced is to scatter modes randomly with rate proportional to k^2, for small wave number k. The *velocity* of the k mode is given by the gradient of the dispersion function $\nabla\omega(k)$. In the unpinned chain, $\nabla\omega(k) \sim 1$ for small k, so small wave number modes have little probability to be scattered, and their movement results in a ballistic contribution to energy transport, while modes with large k scatter fast and consequently they diffuse. Properly averaging over all modes, one obtains a current proportional to $N^{-1/2}$, i.e., a conductivity diverging like $N^{1/2}$. In the pinned chain, small wave number modes move very slowly [$\nabla\omega(k) \sim k$], so there is a high probability they will be scattered and then diffuse while they cross the system. Consequently, in this case, conductivity is finite.

In [7] we considered the unpinned one-dimensional harmonic chain with noise that conserves only energy, and proved that conductivity is finite in any dimension. In this last case, all modes are scattered with a constant rate (independent of k).

In the nonlinear FPU type of interaction, a behavior $\kappa_N \sim N^\alpha$, with $0 < \alpha < 1$, is observed numerically. But numerical simulations are not conclusive about the value of α and there is an intense debate in the literature on this value (cf. [2]). As suggested recently by Livi [12], in one-dimensional systems the value of α may depend on the specific nonlinearity of the interaction (unlike the logarithmic behavior of the two-dimensional systems). The nonlinearity creates some scattering of the long-wave modes, which results in a breaking of the ballistic transport and in a superdiffusive behavior of these modes. An extreme case is given by the one-dimensional coupled-rotors model, which is an example of a nonlinear chain that conserves momentum and has finite conductivity [13]. In this example, rotobreathers (isolated rotors with high kinetic energy that turn very fast) scatter waves that try to pass through them (cf. [14]).

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