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Conductivity and Fourier's law for a system of harmonic oscillators perturbed by a noise conserving energy and momentum.

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We consider a system of harmonic oscillators perturbed by a stochastic dynamics conserving momentum and energy. We compute the effective thermal conductivity via Green-Kubo formula. In the limit as the size N of the system goes to infinity, conductivity remains finite if a pinning (on site potential) is present or in dimension $d \ge 3$. In the unpinned case conductivity diverges like Nin dimension 1 and like $\ln N$ in dimension 2. Then we consider the open system in contact with 2 heat bath at different temperature in the stationary state. We prove that the conductivity of the open system coincides with the Green-Kubo formula, and a corresponding Fourier's law in the cases of finite conductivity. Mathematical complete proofs of these results are in reference [1].

PACS numbers: 44.10+i,05.60-k,63.10.+a Keywords: Thermal conductivity, Fourier's law, non-equilibrium systems, Green-Kubo formula, anomalous heat transport

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

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

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 heat baths at temperature T_{ℓ} and T_r respectively, the steady state current should be proportional to $(T_{\ell} - T_r)/N$.

The derivation of the macroscopic Fourier's law for thermal conduction from a microscopic deterministic Hamiltonian dynamics is one of the main problems in non-equilibrium statistical mechanics (cf. [2] and [3] for recent reviews on the subject). Even the existence of the transport coefficients (conductivity), defined by the Green-Kubo formula, cannot be proven, because of the (poorly understood) slow decay of the space-time correlations in deterministic systems. Furthermore in Hamiltonian mechanical system is not proven that the conductivity κ appearing in the Fourier's law is connected to the Green-Kubo definition through the space time integral of equilibrium correlation of the energy current [2].

In some low dimensional systems $(d \leq 2)$ anomalous thermal conductivity is observed numerically [4] and experimentally in nanotubes technology. The anomalous conductivity in low dimension has attracted a lot of attention in the literature, and it has been suggested that conservation of momentum is an important ingredient [5].

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 energy current J is independent of the length N of the system

(i.e. Fourier law is not satisfied) [6].

In non-linear cases, as in Fermi-Pasta-Ulam systems without pinning (on-site) potential, numerical evidence shows a conductivity diverging like N^{α} , with $\alpha < 1$ in one dimension, and like log N in dimension 2 (cf. [3] and references in there). Finite conductivity is observed numerically in all pinned cases, as long as some nonlinearity is present in the interaction.

We study here a system of harmonic (linear) coupled oscillators where the hamiltonian dynamics is perturbed by a random exchange of momentum between nearest neighbors atoms. Each atom can be pinned or not by an harmonic on site potential. The random exchange of momentum conserves the total momentum and the total energy. In dimension 1 we consider a random exchange of momentum between nearest and second nearest neighbors atoms that has the same conservation laws. Because of the conservation laws, this noise introduces a certain non-linearity in the model. In some sense this stochastic perturbation of the dynamics simulates (qualitatively) the long time (chaotic) effect of the deterministic nonlinear model.

We compute explicitly and rigorously 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 $N \to \infty$ in $d \ge 3$ 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. 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. We prove then, in the finite conductivity cases, Fourier law for the open system in contact with thermal reservoirs at different temperatures are specified on the prove then in the finite conductivity cases.

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Other explicitely solvable models have been proposed before as perturbation of the harmonic chain (in [7] and [8] only the number of particles is conserved, in [11] only energy and number of particles). In all these cases conductivity is finite.

First we consider the dynamics of the closed system of length N with periodic boundary conditions. The Hamiltonian of the harmonic system is given by

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

The atoms are here labeled by $\mathbf{x} \in \Pi_N^d$, the d-dimensional discrete thorus of lenght N. We denote with ∇ and Δ respectively the discrete gradient and the discrete Laplacian on Π_N^d . The position $\mathbf{q}_{\mathbf{x}}$ should be interpreted here as the displacement of the atom \mathbf{x} from an equilibrium position (that can be \mathbf{x} itself). The parameter $\alpha > 0$ is the strength of the interparticle springs, and $\nu \geq 0$ is the strength of the pinning (on-site potential).

We consider the dynamics generated by the operator

$$L = A + \gamma S \tag{2}$$

where A is the usual Hamiltonian vector field

$$A = \sum_{\mathbf{x}} \left\{ \mathbf{p}_{\mathbf{x}} \cdot \partial_{\mathbf{q}_{\mathbf{x}}} + \left[(\alpha \Delta - \nu I) \mathbf{q}_{\mathbf{x}} \right] \cdot \partial_{\mathbf{p}_{\mathbf{x}}} \right\}$$
$$= \sum_{\mathbf{x}} \sum_{j=1}^{d} \left\{ p_{\mathbf{x}}^{j} \partial_{q_{\mathbf{x}}^{j}} + (\alpha \Delta - \nu I) q_{\mathbf{x}}^{j} \partial_{p_{\mathbf{x}}^{j}} \right\}$$
(3)

while S is the generator of the stochastic perturbation and $\gamma > 0$ is a positive parameter that regulates its strength. In $d \ge 2$ we choose as generator of the noise

$$S = \frac{1}{2(d-1)} \sum_{\mathbf{x}} \sum_{i,j,k} \left(X_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^{i,j} \right)^2 \tag{4}$$

where $\mathbf{e}_1, \ldots, \mathbf{e}_d$ is canonical basis of \mathbb{R}^d , and

$$X_{\mathbf{x},\mathbf{z}}^{i,j} = (p_{\mathbf{z}}^j - p_{\mathbf{x}}^j)(\partial_{p_{\mathbf{z}}^i} - \partial_{p_{\mathbf{x}}^i}) - (p_{\mathbf{z}}^i - p_{\mathbf{x}}^i)(\partial_{p_{\mathbf{z}}^j} - \partial_{p_{\mathbf{x}}^j}).$$
(5)

In dimension 1, in order to conserve the total momentum, we have to consider a random exchange between nearest and second nearest neighbors, and we define $S = \frac{1}{6} \sum_{x \in \mathbb{T}_N^1} (Y_x)^2$ where

$$Y_x = (p_x - p_{x+1})\partial_{p_{x-1}} + (p_{x+1} - p_{x-1})\partial_{p_x} + (p_{x-1} - p_x)\partial_{p_{x+1}}.$$
(6)

Observe that total momentum $\sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}}$ and energy \mathcal{H}_N are conserved by these dynamics. Defining the energy of the atom \mathbf{x} as

$$e_{\mathbf{x}} = \frac{1}{2} \|\mathbf{p}_{\mathbf{x}}\|^2 + \frac{\alpha}{4} \sum_{\mathbf{y}: \|\mathbf{y} - \mathbf{x}\| = 1} \|\mathbf{q}_{\mathbf{y}} - \mathbf{q}_{\mathbf{x}}\|^2 + \frac{\nu}{2} \|\mathbf{q}_{\mathbf{x}}\|^2 \quad (7)$$

the energy conservation law can be read locally as

$$Le_{\mathbf{x}} = \sum_{k} \left(j_{\mathbf{x}-\mathbf{e}_{k},\mathbf{x}} - j_{\mathbf{x},\mathbf{x}+\mathbf{e}_{k}} \right)$$

where $j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}$ is the instantaneous energy current between \mathbf{x} and $\mathbf{x} + \mathbf{e}_k$, that can be written as

$$j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k} = j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^a + \gamma j_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}^s \quad . \tag{8}$$

The first term in (8) is the hamiltonian contribution to the energy current

$$j^{a}_{\mathbf{x},\mathbf{x}+\mathbf{e}_{k}} = -\frac{\alpha}{2}(\mathbf{q}_{\mathbf{x}+\mathbf{e}_{k}} - \mathbf{q}_{\mathbf{x}}) \cdot (\mathbf{p}_{\mathbf{x}+\mathbf{e}_{k}} + \mathbf{p}_{\mathbf{x}}) \qquad (9)$$

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

$$\gamma j_{\mathbf{x},\mathbf{x}+\mathbf{e}_{k}}^{s} = -\gamma \nabla_{\mathbf{e}_{k}} \|\mathbf{p}_{\mathbf{x}}\|^{2}$$
(10)

and in d = 1

$$\gamma j_{x,x+1}^{s} = -\gamma \nabla \varphi(p_{x-1}, p_x, p_{x+1})$$
$$\varphi(p_{x-1}, p_x, p_{x+1}) = \frac{1}{6} [p_{x+1}^2 + 4p_x^2 + p_{x-1}^2 + p_{x+1}p_{x-1} - 2p_{x+1}p_x - 2p_x p_{x-1}]$$
(11)

The total energy current between $\mathbf{x}, \mathbf{x} + \mathbf{e}_k$ up to time t is then given by

$$J_{\mathbf{x},\mathbf{x}+\mathbf{e}_{k}}(t) = \int_{0}^{t} j_{\mathbf{x},\mathbf{x}+\mathbf{e}_{k}}(s) \, ds + M_{\mathbf{x},\mathbf{x}+\mathbf{e}_{k}}(t) \qquad (12)$$

where $M_{\mathbf{x},\mathbf{x}+\mathbf{e}_k}(t)$ is a martingale, i.e. a term that, for every initial condition, has null average with respect to the noise of the dynamics.

We define conductivity first using the microcanonical version of the Green-Kubo formula. Consider the closed system on Π_N^d in the microcanonical measure with fixed energy $\mathcal{H} = N^d T$. In the unpinned case $\nu = 0$, we also fix the momentum $\sum_{\mathbf{x}} \mathbf{p}_{\mathbf{x}} = 0$. The conductivity in the direction \mathbf{e}_1 is defined as

$$\kappa_{1,1} = \lim_{N \to \infty} \lim_{t \to \infty} \frac{1}{2T^2 t} \frac{1}{N^d} \sum_{\mathbf{x}} \mathbb{E} \left(J_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}(t) J_{0,\mathbf{e}_1}(t) \right)$$
(13)

where \mathbb{E} is the expectation of the system starting with the microcanonical distribution. Using the explicit expression of the total current (12), all gradient terms disappear, the martingale term gives $d\gamma$, while the contribution of $j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}$ is

$$\lim_{N \to \infty} \frac{1}{T^2} \frac{1}{N^d} \sum_{\mathbf{x}} \int_0^\infty \mathbb{E} \left(j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1}^a(t) j_{0, \mathbf{e}_1}^a(0) \right) dt.$$
(14)

We look now for solution u of the equation

$$\sum_{\mathbf{x}} j^a_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1} = L_N u \tag{15}$$

and we have

$$\sum_{\mathbf{x}} \int_{0}^{\infty} \mathbb{E} \left(j_{\mathbf{x},\mathbf{x}+\mathbf{e}_{1}}^{a}(t) j_{0,\mathbf{e}_{1}}^{a}(0) \right) dt = -\sum_{\mathbf{x}} \left\langle u j_{\mathbf{x},\mathbf{x}+\mathbf{e}_{1}}^{a} \right\rangle_{N}$$
(16)

where $\langle \cdot \rangle_N$ denotes the microcanonical expectation. Equation (15) has an explicit solution given by

$$u = \frac{\alpha}{\gamma} \sum_{\mathbf{x}, \mathbf{y}} g(\mathbf{x} - \mathbf{y}) \mathbf{p}_{\mathbf{x}} \cdot \mathbf{q}_{\mathbf{y}}$$
(17)

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

$$4\Delta g(\mathbf{z}) = (\delta(\mathbf{z} - \mathbf{e}_1) - \delta(\mathbf{z} + \mathbf{e}_1))$$
(18)

for $d \geq 2$, or

$$\frac{1}{3}\Delta \left[4g(z) + g(z+1) + g(z-1)\right] = \left(\delta(z-1) - \delta(z+1)\right)$$
(19)

for d = 1. Substituting in (16), and using equivalence of ensembles estimates (see [1] for the rigorous mathematical details) we have

$$-\sum_{\mathbf{x}} \left\langle u j_{\mathbf{x},\mathbf{x}+\mathbf{e}_{1}}^{a} \right\rangle_{N}$$

$$= \frac{\alpha^{2} T N^{d}}{2\gamma} \sum_{\mathbf{z}} g(\mathbf{z}) \left\langle (\mathbf{q}_{\mathbf{z}+\mathbf{e}_{1}} - \mathbf{q}_{\mathbf{z}-\mathbf{e}_{1}}) \cdot \mathbf{q}_{0} \right\rangle_{gc,T} + o(N^{d})$$
(20)

where $\langle \cdot \rangle_{gc,T}$ is the expectation with respect to the infinite volume grand-canonical measure at temperature T and average momentum 0, i.e. the centered gaussian measure with covariance operator $T(\nu I - \alpha \Delta)^{-1}$. The function g is intended here as the solution of (18) or (19) on \mathbb{Z}^d . In dimension 1 and 2, if $\nu = 0$, the grand-canonical measure is intended for the differences $\{\mathbf{q}_{\mathbf{x}+\mathbf{e}_j} - \mathbf{q}_{\mathbf{x}}, \mathbf{x} \in \mathbb{Z}^d, j = 1, \dots d\}.$

A simple Fourier analysis shows that, if $\nu = 0$ (i.e. the unpinned case), (20) diverge like N^2 in dimension 1 and like $N^2 \log N$ in dimension 2. In all other cases we have the following expression for the conductivity

$$\kappa_{1,1} = \gamma d + \frac{\alpha^2 d}{2\gamma} \sum_{\mathbf{z}} \left(g(\mathbf{z} - \mathbf{e}_1) - g(\mathbf{z} + \mathbf{e}_1) \right) \Gamma(0, \mathbf{z})$$
(21)

where Γ is the kernel of the operator $(\nu I - \alpha \Delta)^{-1}$ on \mathbb{Z}^d . Observe that this expression diverges for $\gamma \to 0$, as expected since deterministic harmonic oscillators have infinite conductivity [6].

One can also start with the grand-canonical version of the Green-Kubo formula obtaining the same expression.

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 $\Xi_N = \{1, \ldots, N\} \times \prod_N^{d-1}$. 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

$$L = A + \gamma S + B_{\ell} + B_r \tag{22}$$

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 contribution of the heat bath defined by

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

When $T_{\ell} \neq T_r$, this system has a unique stationary measure [1]. 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

$$\kappa_{ss}(N, T_r, T_\ell) = \frac{N \left\langle j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1} \right\rangle_{ss, N}}{T_\ell - T_r}$$

Open question for the non-linear deterministic case is if $\lim_{L\to\infty} \lim_{T_\ell\to T_r=T} \kappa_{ss}(N, T_r, T_\ell)$ exists and, in this case, if this limit is equal to $\kappa_{1,1}$. We prove that this is the case in our model:

- in the unpinned cases $\kappa_{ss}(N) \sim N$ in dimension 1 and $\kappa_{ss}(N) \sim \ln N$ in dimension 2,
- in all cases where conductivity is finite

$$\lim_{N \to \infty} N \left\langle j_{\mathbf{x}, \mathbf{x} + \mathbf{e}_1} \right\rangle_{ss, N} = \kappa_{1, 1} (T_\ell - T_r)$$
(23)

(i.e. the Fourier's law).

The connection between Green-Kubo formula and the heat transport coefficient appearing in the Fourier law in the open system subject to a gradient of temperature 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 with with $\nu > 0$. The following argument does extend in all other case as long $d \geq 3$ or $\nu > 0$. Define the functions

$$h = \frac{\alpha}{\gamma} \sum_{z} g(z) \ p_z q_0 \tag{24}$$

and

$$\phi = \frac{\alpha}{2\gamma} \sum_{z \ge 1} g(z) \left[\sum_{y \ge 1}^{z} \tau_{y} \psi_{z} + \alpha (q_{-z-1}q_{0} - q_{-z}q_{-1}) \right] \\ + \frac{\alpha}{2} (p_{-1} + p_{0})q_{0} + \gamma \varphi (p_{-1}, p_{0}, p_{1})$$
(25)

where $\{\tau_y\}$ is the shift operator on the configuration space, and

$$\psi_z = p_{-z}p_0 + q_{-z}(\alpha\Delta - \nu I)q_0.$$

Then by explicit calculation one can write

$$j_{x,x+1} = -\nabla \tau_x \phi + L \tau_x h \quad . \tag{26}$$

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

$$N < j_{x,x+1} >_{ss,N} = \sum_{x} < j_{x,x+1} >_{ss,N}$$
$$= < \tau_1 \phi >_{ss,N} - < \tau_N \phi >_{ss,N}$$

By the thermalization due to the heat baths, one can prove local equilibrium around the boundaries, and prove that

This argument can be made rigorous by a proper localization of the functions h and ϕ and an entropy production argument [1]. A decomposition similar to (26) is valid also in $d \ge 2$. One can use directly (26) in the Green-Kubo formula (13), obtaining the same result as above, by noticing that in the periodic case $\sum_x \nabla \tau_x \phi = 0$ and that $\sum_x \tau_x h = u$ as defined by (17).

Discussion. The exact and mathematically rigorous results presented in this letter concerning the stochastic model we considered, suggest some indications about the role of conservation of momentum and of confinement (pinning) in the heat conduction for the nonlinear and 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. [3]). As suggested recently by R. Livi [9], probably there is not an 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 in 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 $\{\mathbf{q_x}\}$ in the equilibrium states. This would explain why the 1-dimensional coupled-rotors model has finite conductivity, still conserving momentum [10]. Observe that in [11] we consider the unpinned 1-dimensional case with only energy conserved (with noise that dissipates momentum), and we prove that conductivity is finite. These two examples suggest that both factors are necessary for the anomalous conductivity also for deterministic Hamiltonian non-linear systems.

About the Fourier's law in the 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 (26). 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 model are always nongradient. Our situation is non-gradient since the energy current has a non-gradient term $j^a_{\mathbf{x},\mathbf{x}+\mathbf{e}_1}$ that comes from the hamiltonian mechanism.

One can consider a system of coupled anharmonic oscillators perturbed by the same noise considered in this article. Establishing Fourier law 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, that will be valid only in some approximate sense. In general we expect that the conductivity will depend on the temperature T.

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