Microscopic Hamiltonian dynamics perturbed by a conservative noise

Cédric Bernardin (with G. Basile and S. Olla)

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Introduction

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• Fourier's law : Consider a macroscopic system in contact with two heat baths with different temperatures $T_{\ell} \neq T_r$. When the system reaches its steady state $\langle \cdot \rangle_{ss}$, one expects Fourier's law holds:

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- J(q) is the energy current; T(q) the local temperature; κ(T) the conductivity.
- If system has (microscopic) size N, finite conductivity means $< J >_{ss} \sim N^{-1}$.

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$$\mathcal{H} = \sum_{x \in \Lambda} \left\{ rac{p_x^2}{2m_x} + rac{W(q_x)}{2} + \sum_{y \sim x} rac{V(q_x - q_y)}{4}
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- Non linearity is extremely important to have normal heat conduction.
- But it is not sufficient : It has been observed experimentally and numerically for nonlinear chains that if d ≤ 2 and momentum is conserved (⇔ W = 0, unpinned) then conductivity is still infinite (finite otherwise).

Motivations/Goal

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- If Fourier's law does not hold, κ_N ~ N^δ, universality of the diverging order δ of the conductivity?
- Numerical simulations are not conclusive ($\delta \in [0.25; 0.47]$ for the same models) and subject of intense debate.

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Noise 1 = only energy conservative Noise 2 = energy and momentum conservative

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Construction of the noise

Example : Noise 1, energy conserving, $m_x = 1$, d=1

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• Noise 2, $d \ge 1$... are of the same type. $(\square) (\square)$

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Evaluation of the conductivity

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with M martingale (mean 0 w.r.t. any initial condition)

$$j_{x,x+e_k} = -\frac{1}{2} (\nabla V) (q_{x+e_k} - q_x) \cdot (p_{x+e_k} + p_x) - \gamma \nabla_{e_k} p_x^2$$

$$[\kappa_{GK}]_{1,1}(T) = \lim_{t \to \infty} \lim_{N \to \infty} \frac{1}{2T^2} \mathbb{E}_{eq.} \left(\left[\frac{1}{\sqrt{tN^d}} \sum_{x \in \mathbb{T}_N^d} J_{x,x+e_1}(t) \right]^2 \right)$$

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Theorem (B., Olla, JSP'05)

- κ_{GK} is finite (pinned or unpinned) in any dimension.
- Fourier's law holds and linear response theory is correct: System of length N in contact with two Langevin baths at temperature T_ℓ and T_r in its steady state

$$\lim_{N \to \infty} N < j_{x,x+1} >_{ss} = \kappa_{GK} (T_r - T_\ell)$$

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Theorem (B., '08)

Harmonic system with random masses and energy conservative noise 1. The conductivity defined by Green-Kubo formula is strictly positive and bounded above:

$$0 < c_{-} \leq \kappa_{KG} \leq C_{+} < +\infty$$

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Noise 2: energy/momentum conserving

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Theorem (Basile, B., Olla, PRL'06)

$$C_{1,1}(t) = \lim_{N \to \infty} \left\langle \left(\sum_{x} j_{x,x+e_1}(t) \right), j_{0,e_1}(0) \right\rangle_{eq}$$
$$C_{1,1}(t) = \frac{T^2}{4\pi^2 d} \int_{[0,1]^d} (\partial_{k^1} \omega(k))^2 e^{-t\gamma \psi(k)} dk$$

where ω is the dispertion relation of the harmonic chain

$$\omega(k) = (\nu + 4\alpha \sum_{j=1}^{d} \sin^2(\pi k^j))^{1/2}, \quad \psi(k) \sim k^2$$

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Corollary

•
$$C_{1,1}(t) \sim t^{-d/2}$$
 in the unpinned case ($\nu = 0$)
• $C_{1,1}(t) \sim t^{-d/2-1}$ in the pinned case ($\nu > 0$)

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Corollary

If the system is unpinned ($\nu = 0$) then "truncated" Green-Kubo formula for κ_N gives:

$$\begin{cases} \kappa_N \sim N^{1/2} \text{ if } d = 1\\ \kappa_N \sim \log N \text{ if } d = 2 \end{cases}$$

In all other cases κ_N is bounded in N and converges to κ_{GK} .

Results : Anharmonic case, Canonical version of GK

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Theorem (Basile, B., Olla'08)

• For $d \ge 3$, if W > 0 is "general" or if W = 0 and $0 < c_{-} \le V$ " $\le C_{+} < +\infty$ then

$$\kappa_N \leq C.$$

• For d = 2, if W = 0 and $0 < c_{-} \le V'' \le C_{+} < \infty$

 $\kappa_N \leq C(\log N)^2.$

• For d = 1, if W = 0 and $0 < c_{-} \le V'' \le C_{+} < \infty$, then

$$\kappa_N \leq C\sqrt{N}.$$

 In any dimension, if V are quadratic and W > 0 is "general" then κ_N ≤ C.

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Thermal conductivity increases with strength of the noise !!!

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Thermal conductivity increases with strength of the noise !!!

Theoretical arguments are controversial. For FPU (β):
Anharmonic case : Numerical simulations, (EPJ'08) , Basile, Delfini, Lepri, Livi, Olla, Politi

• Simulations (d = 1) for unpinned systems with energy/momentum conservative noise 2. The strength of the noise is regulate by γ . Then $\kappa_N \sim N^{\delta}$.

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- Function h_λ is local in the energy conservative case and non-local in the energy/momentum case. For d ≥ 3 or ν > 0, the decay of h_λ is sufficient to assure a finite conductivity.

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$$\delta T = T_r - T_\ell$$
 is small

$$f_{ss} = \mathbf{1} + \delta T h_0 + o((\delta T)^2)$$

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$$(N^{-1} - \gamma S)^{-1} \left(\sum_{x} j_{x,x+e_1} \right) = \sum_{j=1}^{d} \sum_{x,y} G_N(x-y) \rho_x^j V'(q_{y+e_1}^j - q_y^j)$$

where $G_N(z)$ is the solution of the resolvent equation

$$N^{-1}G_N(z) - 2\gamma(\Delta G_N)(z) = -\frac{1}{2}[\delta_0(z) + \delta_{e_1}(z)]$$