Thermal conductivity of classical disordered lattices in the weak coupling regime

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supported by ERC MALADY

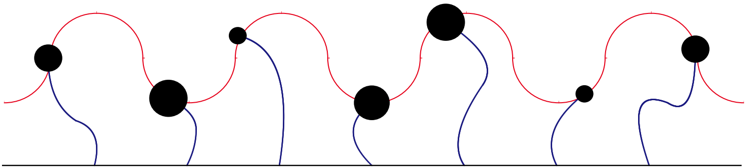
ICMP, Aalborg 2012

Issue

General goal: Thermal transport in solids from molecular dynamics

More precisely: Integrable dynamics $\sim$ anomalous transport (often).
Generic anharmonic interactions and-or disorder ?

Typical model of solids: a classical chain of oscillators



$$H(q,p) = \sum_x H_x(q,p) = \sum_x \left\{ \frac{p_x^2}{2} + U_x(q_x) + V(q_{x+1} - q_x) \right\}$$

Conductivity

Conservation of energy:

$$dH_x/dt = J_{x-1,x} - J_{x,x+1}$$

Let

$$N = \text{Volume} = \text{Number of atoms}$$
$$\langle \cdot \rangle_T = \text{Gibbs measure at temperature } T$$

Green-Kubo conductivity:

$$\kappa(T) = \lim_{t\to\infty} \lim_{N\to\infty} \frac{1}{T^2} \left\langle \left(\frac{1}{\sqrt{t}} \int_0^t \frac{1}{\sqrt{N}} \sum_x J_{x,x+1}(s)\, ds \right)^2 \right\rangle_T$$

Very difficult to analyze due to long time correlations

In the hydrodynamic regime, we expect

$$\partial_t T = \partial_x \big(\kappa(T) \partial_x T \big)$$

Perturbative regime

- Example 1: (Lefevere-Schenkel, Aoki-Lukkarinen-Spohn)

$$H(q,p) \;=\; \sum_x \{p_x^2 + q_x^2 + \epsilon\, q_x^4 + (q_{x+1} - q_x)^2\}$$

  Ballistic motion of energy gets destroyed by anharmonic potentials.

- Example 2: (Liverani-Olla, Dolgopyat-Liverani) Roughly speaking:

$$H(q,p) \;=\; \sum_x \{p_x^2 + U(q_x) + \epsilon\, V(q_{x+1} - q_x)\} \quad \text{with} \quad U \;\text{“chaotic”}$$

  The system is close to a stochastic system for energy alone.

- We expect

$$\kappa(T \sim 1, \epsilon) \;\sim\; \begin{cases} 1/\epsilon^2 & \text{in Example 1} \\ \epsilon^2 & \text{in Example 2} \end{cases} \qquad \text{as} \quad \epsilon \to 0$$

What about disordered chains ?

Example: Pinned 1-dimensional disordered harmonic chain:

$$H(q,p) \;=\; \frac{1}{2}\sum_x \{p_x^2 + \omega_x^2\, q_x^2 + (q_{x+1} - q_x)^2\}$$

with

$$0 \;<\; c_- \;\leq\; \omega_x^2 \;\leq\; c_+ \;<\; +\infty \qquad \text{i.i.d. random variables.}$$

Harmonic interactions:

- Linear equations of motions,
- Strictly equivalent to Anderson model for a single electron,
- All eigenmodes are localized,
- $\kappa(T) = 0$ for all $T > 0$ (only local oscillations).

Harmonic interactions are not expected to be very generic however...

Adding anharmonic potentials (I)

- Dhar and Lebowitz '08: Numerics for a 1-d chain analogous to

$$H(q,p) \;=\; \sum_x \{p_x^2 + \omega_x^2\, q_x^2 + (q_{x+1} - q_x)^2 + \epsilon\, q_x^4\} \quad \text{with} \quad \omega_x^2 \;\text{ i.i.d.}$$

Localization - Delocalization transition expected at $\epsilon = 0$:

$$\kappa(T \sim 1, \epsilon) \;>\; 0 \quad \text{for} \quad \epsilon > 0.$$

- Oganesyan, Pal, Huse '09: Numerics for a 1-d classical spin chain

$$H(\mathbf{S}) \;=\; \sum_x \left\{\boldsymbol{\omega}_x \cdot \mathbf{S}_x + \epsilon\, \mathbf{S}_x \cdot \mathbf{S}_{x+1}\right\} \quad \text{with} \quad \boldsymbol{\omega}_x \;\text{ i.i.d.}$$

Findings by Dhar and Lebowitz are confirmed. Moreover

$$0 \;<\; \kappa(T \sim 1, \epsilon) \;\to\; 0 \quad \text{very fast} \quad \text{as} \;\; \epsilon \to 0.$$

Adding anharmonic potentials (II)

- Basko '11: Theoretical analysis of a Dhar-Lebowitz like chain. Arnold diffusion invoked to explain positive conductivity. Roughly speaking, the message is

$$\kappa(\epsilon) \;\sim\; \mathrm{e}^{-\log^2(1/\epsilon)} \quad \text{for} \;\; \epsilon \;>\; 0.$$

- Flach, and many others: Numerics for Dhar-Lebowitz like chains
  - at positive temperature
  - for an initially localized wave packet ("zero temperature")

  predict

$$\kappa(T, \epsilon \sim 1) \;\sim\; T^{\alpha} \quad \text{as} \;\; T \to 0 \qquad \text{for some} \;\; \alpha > 0.$$

  Possibly conflicting with aforementioned results.

A simple model (I)

Weakly coupled integrable dynamics:

$$H(q,p) \;=\; \sum_x \left\{ p_x^2 + \omega_x^2\, q_x^2 + \epsilon\, q_x^4 + \epsilon\, (q_{x+1} - q_x)^2 \right\}$$

Theorem 1: For almost all realization of the disorder, for $T \sim 1$,

$$\lim_{t\to\infty} \lim_{\epsilon\to 0} \lim_{N\to\infty} \epsilon^{-n} \left\langle \left(\frac{1}{\sqrt{\epsilon^{-m} t}} \int_0^{\epsilon^{-m} t} \frac{1}{\sqrt{N}} \sum_x J_{x,x+1}(s)\, \mathrm{d}s \right)^2 \right\rangle_T \;=\; 0$$

for all $n \geq 1$ and all large enough $m \geq n$.

Remark 1: The result extends to higher dimensions.

Remark 2: Interesting for $n \geq 1$ large and $m >> n$ very large. We conjecture

$$\kappa(T \sim 1, \epsilon) = \mathcal{O}(\epsilon^n) \qquad \text{for all } \; n \geq 1.$$

A simple model (II)

Theorem 2: Dynamics generated by

$$L = A + \epsilon^n S, \qquad n \geq 1,$$

with

$$\begin{aligned} A &= \text{Hamiltonian generator}, \\ Su &= \sum_x \{u(\dots, -p_x, \dots) - u(\dots, p_x, \dots)\}. \end{aligned}$$

Then, for almost all realizations of the disorder, and for all $n \geq 1$,

$$\kappa(T \sim 1, \epsilon) = \mathcal{O}(\epsilon^n) \qquad \text{as} \quad \epsilon \to 0.$$

Remark 1: The noise S crudely models chaotic effects due to nonlinearities.

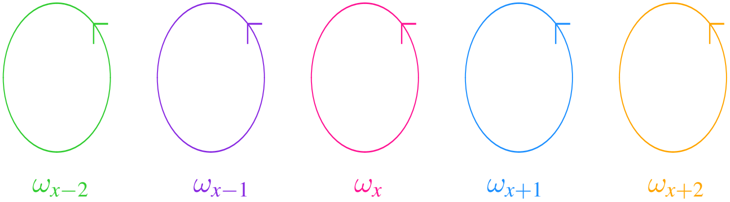
Remark 2: Striking contrast with the chain

disordered harmonic + noise $\epsilon\, S$

where $\kappa(T, \epsilon) \sim \epsilon$ (joint work with Cédric Bernardin).

Why is it so ?

Basic phenomenon: uncoupled atoms oscillates at different frequencies



Since $\langle J_{x,x+1} \rangle = 0$ for all microcanonical surfaces of the uncoupled dynamics,

$$\int_0^t J_{x,x+1}(s)\,\mathrm{d}s \;\leq\; C \quad \text{as} \quad t \to \infty$$

typically, and for the uncoupled evolution.

Symmetry! Generator exchanges p-symmetric and p-antisymmetric functions.

Allows us to iterate this observation at higher perturbative orders.

A bit more formally...

- Let
$$L \ = \ \text{generator of the dynamics.}$$
Perturbative analysis for typical currents:
$$\begin{aligned} J_{x,x+1} &= \ -L\, u_{x,x+1} \ + \ \epsilon^{n+1}\, G_{x,x+1} \\ &= \ \text{Oscillation} \ + \ \epsilon^{n+1}\, \text{New current.} \end{aligned}$$

- Some currents are atypical:

Resonances occur if $|\omega_x - \omega_{x+1}|$ is too small.

Conservation of energy implies for example
$$\begin{aligned} J_{x,x+1} \ &= \ L\, H_x \ + \ J_{x-1,x} \\ \text{Resonant} \ &= \ \text{Oscillation} \ + \ \text{Non resonant.} \end{aligned}$$

Related models

- Oganesyan-Pal-Huse spin chain
  The result holds with some hypotheses on the random magnetic field.

- Dhar-Lebowitz chain
  Exponential localization of eigenmodes: the substitution

$$\epsilon\,(q_x - q_{x+1})^2 \;\longrightarrow\; 1\,(q_x - q_{x+1})^2$$

is not harmful (not rigorous!)

Remark: Exact scaling

$$\kappa(T,\epsilon) \;=\; \kappa(r\,T,\epsilon/r) \quad \text{for all} \quad r > 0.$$

We also conjecture

$$\kappa(T,\epsilon\sim 1) \;=\; \mathcal{O}(T^n) \quad \text{as} \quad T\to 0 \qquad \text{for all} \quad n\geq 1.$$

Decay as $t^{-1/(2+n)}$ of some solutions of $\partial_x T = \partial_x(T^n\partial_x T)$,
phenomenological equation for spreading of initially localized packets.

A quartic chain ?

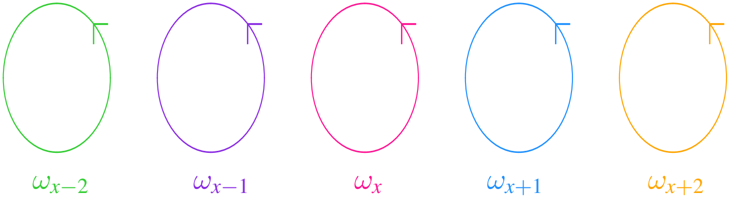
Hamiltonian

$$H(q,p) = \sum_x H_x = \sum_x \{p_x^2 + q_x^4 + \epsilon\,(q_{x+1} - q_x)^2\}$$

For the uncoupled dynamics ($\epsilon = 0$):

- Gibbs measure is product: H_x selected at random.
- Each atom oscillates at a frequency $\omega_x \sim H_x^{1/4}$.

We recover the picture



Full picture less clear: resonances may now travel along the chain...
(ongoing work with Wojciech De Roeck)