Heat conduction in disordered harmonic lattices with energy conserving noise

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Outline

- Introduction: Heat conduction in $1D$ systems.
    - Disordered harmonic chains
    - Ordered anharmonic chains
    - Disordered anharmonic chains: effect of interactions on localization.
- Stochastic models of heat conduction.
- Analytically tractable model to study effects of interactions on localization .
    - Exact results.
    - Numerical results.
- Discussion.

Fourier's Law

For small $\Delta T = T_L - T_R$ and system size L :

$$\text{Fourier's law implies :} \quad J \sim \kappa \frac{\Delta T}{L}$$

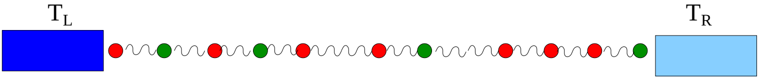
The thermal conductivity κ is expected to be an intrinsic material property.

- Fourier's law is not generally valid in low-dimensional systems . κ depends on system size L.
- Necessary and sufficient conditions for validity of Fourier's law ?
  Role of anharmonicity, disorder and dimensionality.

Bonetto, Lebowitz, Rey-Bellet, Math. Phys. (2000) .

Lepri, Livi, Politi, Phys. Rep. (2003) .
Dhar , Adv. Phys. (2008) .

Disordered Harmonic systems: Results in $1D$



Exact expression for nonequilibrium heat current ["Landauer-like" formula for phonons.]
In classical case:

$$J = \frac{k_B \Delta T}{2\pi} \int_0^\infty d\omega \, T(\omega) \,,$$

where $T(\omega)$ is the phonon transmission function.

[Casher and Lebowitz (1971), Rubin and Greer (1971), Dhar and Roy (2006)].

Anderson localization implies: $T(\omega) \sim e^{-L/\ell(\omega)}$ with $\ell(\omega) \sim 1/\omega^2$ for $\omega \to 0$.

Disordered Harmonic systems: $1D$

Hence frequencies $\omega \lesssim L^{-1/2}$ "do not see" the randomness and can carry current. These are the ballistic modes.

Hence $\quad J \sim \int_0^{L^{-1/2}} T(\omega) d\omega.$

Form of $T(\omega)$ (at small ω) depends on boundary conditions.

Fixed BC: $\quad T(\omega) \sim \omega^2 \quad J \sim 1/L^{3/2}$
Free BC: $\quad T(\omega) \sim \omega^0 \quad J \sim 1/L^{1/2}$

If all sites are pinned then low frequency modes are cut off. Hence we get:

$$Pinned\ case: \qquad J \sim e^{-L/\ell}.$$

Matsuda, Ishii, Rubin/Greer, Casher/Lebowitz, Dhar.
Exact results: Verheggen (1979), Ajanki / Huveneers (2010).

One dimensional disordered harmonic chain

- Almost all normal modes of the chain are localized and their amplitude at the boundaries is exponentially small (in L) leading to transmission decaying exponentially.
- Low frequency modes are extended and transmit energy.
- No Fourier's law: Strong boundary condition dependence.
- Heat insulator in pinned case.

One-dimensional systems with nonintegrable interactions

Momentum conserving system: FPU - model

$$H = \sum_{\ell=1}^{N} \frac{p_\ell^2}{2m} + \sum_{\ell=1}^{N+1} \left[k_2 \frac{(q_\ell - q_{\ell-1})^2}{2} + k_3 \frac{(q_\ell - q_{\ell-1})^3}{3} + \lambda \frac{(q_\ell - q_{\ell-1})^4}{4} \right] .$$

Momentum non-conserving system: ϕ^4 - model

$$H = \sum_{\ell=1}^{N} \left[\frac{p_\ell^2}{2m} + k_o \frac{q_\ell^2}{2} \right] + \sum_{\ell=1,N+1} k_2 \frac{(q_\ell - q_{\ell-1})^2}{2} + \sum_{\ell=1}^{N} \lambda \frac{q_\ell^4}{4} .$$

Simulations:

- Momentum conserving: $\kappa \sim L^{1/3}$ ($L^{2/5}$, $L^{1/2}$?) .
- Momentum nonconserving (pinned case): $\kappa \sim L^0$

Systems with non-integrable Hamiltonian dynamics

Theory

- Momentum conserving:

  MC (Lepri, Livi, Politi, Delfini) $\kappa \sim L^{1/3}, \; L^{1/2}$ (odd, even)

  RG (Narayan, Ramaswamy) $\kappa \sim L^{1/3}$ (universal)

  Kinetic theory (Pereverzev, Lukkarinen, Spohn) $\kappa \sim L^{2/5}$. (even)

- Momentum nonconserving (pinned case): $\kappa \sim L^0$.

- Long wavelength modes lead to slow decay of current-current correlations and hence to anomalous transport.

- Value of current depends on BCs, but exponents do not.

Effect of interaction on localization (Numerical results)

(A) Disordered FPU model (Dhar and Saito)

$$H = \sum_{\ell=1,N} \frac{p_\ell^2}{2m_\ell} + \sum_{\ell=1,N+1} k\frac{(q_\ell - q_{\ell-1})^2}{2} + \lambda\,\frac{(q_\ell - q_{\ell-1})^4}{4}\ .$$

(B) Disordered ϕ^4 model (Dhar and Lebowitz)

$$H = \sum_{\ell=1,N} [\frac{p_\ell^2}{2m_\ell} + k_o\frac{q_\ell^2}{2}] + \sum_{\ell=1,N+1} k\frac{(q_\ell - q_{\ell-1})^2}{2} + \sum_{\ell=1,N} \lambda\,\frac{q_\ell^4}{4}\ .$$

$\{m_\ell\} = [m - \Delta, m + \Delta]$.

Disorder $\rightarrow \Delta$ Anharmonicity $\rightarrow \lambda$.

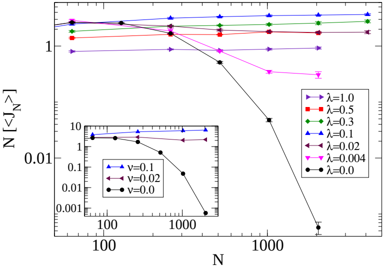
Simulations:

Case (A) $\lambda = 0 : \kappa \sim L^{1/2}\ ,\ L^{-1/2}$ $\lambda > 0\ :\ \kappa \sim L^{1/3}\ .$

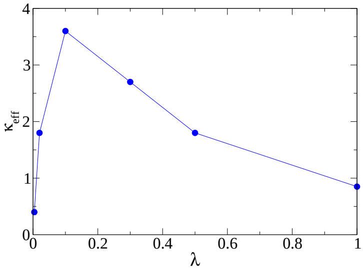
Case (B) $\lambda = 0 : \kappa \sim e^{-cL}\ ,$ $\lambda > 0\ :\ \kappa \sim L^{0}\ .$

Numerical results: Pinned case

Dhar/Lebowitz (2008)



Dramatic transition: $e^{-cN/\ell} \longrightarrow \frac{1}{N}$
for small amount of interaction.



$$\kappa \sim (\lambda T)^a$$

$a = 1/2$ [$a = 4$ – Flach *etal* (2011)]

Effect of interactions on localization

- Many-body localization — In the $\lambda - \Delta$ plane, is there a conductor-insulator transition ?
- Transport mechanism: Destruction of localization ?, Hopping of energy between localized states ?
- Small λ behaviour of $\kappa(\lambda)$.

Look at analytically tractable models to address these questions.

Stochastic models of heat conduction

MOTIVATION

- Analytically tractable.
- Physical relevance: one hopes that they effectively mimic anharmonicity and environmental degrees of freedom.

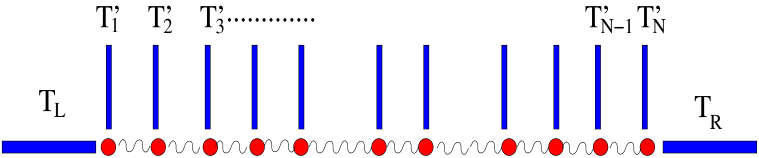
Purely Stochastic dynamics (Local energy conservation)

- Kipnis-Marchioro-Presutti model for heat conduction in harmonic oscillator chain .
- Creutz model for heat conduction in Ising model .

Hamiltonian + Stochastic dynamics

- Self-Consistent Reservoirs (Momentum Non-conserving)
  (Bolsterli, Rich, Visscher)
- Local momentum exchange dynamics (Both momentum conserving and non-conserving)
  (Basile, Bernardin, Olla)
  (Delfini, Lepri, Livi, Politi, Mejia-Monasterio)
  (Bernardin)

Self-consistent reservoirs



$$
\begin{aligned}
m_1 \ddot{q}_1 &= -\Phi_{1m} q_m \;+\; [\,-\gamma \dot{q}_1 + (2\gamma T_L)^{1/2} \eta_1(t)\,] \;+\; [\,-\gamma_1' \dot{q}_1 + (2\gamma_1' T_1')^{1/2} \zeta_1(t)\,] \\
m_\ell \ddot{q}_\ell &= -\Phi_{\ell,m} q_m \;+\; [\,-\gamma_\ell' \dot{q}_\ell + (2\gamma_\ell' T_\ell')^{1/2} \zeta_\ell(t)\,] \quad \ell = 2, \ldots, N-1\,, \\
m_N \dot{q}_N &= -\Phi_{Nm} q_m \;+\; [\,-\gamma \dot{q}_N + (2\gamma T_R)^{1/2} \eta_N(t)\,] \;+\; [\,-\gamma_N' \dot{q}_N + (2\gamma_N' T_N')^{1/2} \zeta_N(t)\,]\,.
\end{aligned}
$$

Self-consistency condition: Zero net current into side reservoirs.

$$\langle\, p_\ell^2 / m_\ell \,\rangle = T_\ell'\,, \qquad \ell = 1, 2, \ldots, N.$$

Self-consistent reservoirs

- Model introduced by Bolsterli, Rich, Visscher (1970):
  "Simulation of nonharmonic interactions in a crystal by self-consistent reservoirs"
- Ordered harmonic chain: solved exactly by Bonetto, Lebowitz and Lukkarinen (2004).
  Fourier's law satisfied and κ is finite.
- Disordered harmonic chain: numerically studied by Rich and Visscher.
  - Finite conductivity, independent of boundary conditions.
  - CONJECTURE: In the limit of vanishing coupling to side reservoirs,
    the conductivity $\kappa \longrightarrow$ a finite value.

    NOTE: In absence of side-reservoirs:

    $$\kappa \longrightarrow \infty \quad \text{free} \quad \text{BCs.}$$

    $$\kappa \longrightarrow 0 \quad \text{fixed} \quad \text{BCs.}$$
- Momentum non-conserving. Energy conserved, on average.

Stochastic models with local momentum/energy conservation

Momentum and energy conserving models

- Basile,Bernardin,Olla: 3-particle collisions

$$p_{\ell-1} + p_\ell + p_{\ell+1} = \text{constant}$$
$$p_{\ell-1}^2 + p_\ell^2 + p_{\ell+1}^2 = \text{constant.}$$

- Delfini, Lepri, Livi, Politi, Mejia-Monasterio: 2 particle collisions

$$p_\ell \leftrightarrow p_{\ell+1} \ .$$

- Ordered harmonic chain: $\kappa \sim L^{1/2}$.
  [numerical and analytical results]

Energy conserving (Momentum non-conserving)

- Bernardin: 2-particle collisions

$$p_\ell^2 + p_{\ell+1}^2 = \text{constant.}$$

- Present study: Momentum flip model

$$p_\ell \leftrightarrow -p_\ell \ .$$

- Ordered and disordered harmonic chain: $\kappa \sim L^0$.
  [numerical and analytical results]

Definition of model studied by us

$$
\begin{aligned}
H &= \sum_{\ell=1,N} \left[\frac{p_\ell^2}{2m_\ell} + k_o \frac{q_\ell^2}{2} \right] + \sum_{\ell=2,N} k \frac{(q_\ell - q_{\ell-1})^2}{2} + k' \left[\frac{q_1^2}{2} + \frac{q_N^2}{2} \right] \\
&= \frac{1}{2} \left[p\hat{M}^{-1}p + q\hat{\Phi}q \right] ,
\end{aligned}
$$

$k_o = 0$: Unpinned case Free BC ($k' = 0$), Fixed BC ($k' > 0$)

$k_o > 0$: Pinned case .

The system's time evolution has:

1. A deterministic part described by the Hamiltonian above.
2. A momentum flipping noise at all sites: transition $p_\ell \to -p_\ell$ occurs with a rate λ.
3. Particles at the boundaries $\ell = 1$ and $\ell = N$ which are attached to Langevin heat baths at temperatures T_L and T_R respectively.

Thermal conductivity

- Non-equilibrium definition:

$$\kappa = \lim_{L\to\infty} \frac{\langle J\rangle\, L}{\Delta T}$$

$$J \;=\; \text{Current density}\ .$$

- From Green-Kubo formulation:

$$\kappa_{GK} = \lim_{z\to 0} \lim_{L\to\infty} \frac{1}{LT^2} \int_0^\infty dt\; e^{-zt}\, \langle \mathcal{J}(0)\mathcal{J}(t)\rangle\ .$$

$$\mathcal{J} \;= \text{Total current}\ .$$

Master equation for time evolution

Let $x = (q_1, q_2, ..., q_N, p_1, p_2, ..., p_N) = (x_1, x_2, ...x_{2N})$

$P(x,t)$: phase-space probabilty distribution .

Master equation:

$$\frac{\partial P(x)}{\partial t} = \sum_{\ell,m} \hat{a}_{\ell,m} x_m \frac{\partial P}{\partial x_\ell} + \sum_{\ell,m} \frac{\hat{d}_{\ell,m}}{2} \frac{\partial^2 P}{\partial x_\ell \partial x_m} + \lambda \sum_{\ell} [\, P(..., -p_\ell, ...) - P(..., p_\ell, ...)\,] \,,$$

$$\text{where} \quad \hat{a} = \begin{pmatrix} 0 & -\hat{M}^{-1} \\ \hat{\Phi} & \hat{M}^{-1}\hat{\Gamma}^{-1} \end{pmatrix} \qquad \hat{d} = \begin{pmatrix} 0 & 0 \\ 0 & 2\hat{T}\hat{\Gamma} \end{pmatrix} .$$

$$\hat{T}_{\ell,\ell} = T_L \delta_{\ell,1} + T_R \delta_{\ell,N}$$

$$\hat{\Gamma}_{\ell,\ell} = \gamma(\delta_{\ell,1} + \delta_{l,N})$$

Equations for pair-correlations

Define pair-correlation matrix:

$$\hat{c} = \begin{pmatrix} \hat{u} & \hat{z} \\ \hat{z}^T & \hat{v} \end{pmatrix} , \quad \text{where } \hat{u}_{\ell,m} = \langle q_\ell q_m \rangle \, , \hat{v}_{\ell,m} = \langle p_\ell p_m \rangle \, , \hat{z}_{\ell,m} = \langle q_\ell p_m \rangle \, .$$

Closed equation of motion for $\hat{c}$:

$$\frac{d\hat{c}}{dt} = -\hat{a}\hat{c} - \hat{c}\hat{a}^T + \hat{d} + \left(\frac{d\hat{c}}{dt}\right)_{col} .$$

Term from flip dynamics is given by:

$$\left(\frac{d\hat{c}}{dt}\right)_{col} = -2\lambda \begin{pmatrix} 0 & \hat{z} \\ \hat{z}^T & 2(\hat{v} - \hat{v}_D) \end{pmatrix} , \quad \text{where } [\hat{v}_D]_{\ell,\ell} = \hat{v}_{\ell,\ell} = \langle \, p_\ell^2 \, \rangle \, .$$

In steady state $d\hat{c}/dt = 0$ gives:

$$\hat{a}\hat{c} + \hat{c}\hat{a}^T - \left(\frac{d\hat{c}}{dt}\right)_{col} = \hat{d}$$

With $\gamma'_\ell = 2 \, \lambda \, m_\ell$ and $\langle \, p_\ell^2 / m_\ell \, \rangle = T'_\ell$, the above equations are identical to the correlation equations for model with self-consistent reservoirs.

Pair-correlations in NESS

- Steady state current given by $J = k \langle x_\ell \; v_{\ell+1} \rangle$. Exact solution available for ordered case – BLL (2004).
- Closed equations for correlation in all orders. However NON-GAUSSIAN unlike self-consistent reservoir model .
- $N^2 + N(N+1)$ linear equations for same number of unknown variables . Accurate numerical solution possible for disordered case and both steady state current and temperature profiles can be obtained.

Green-Kubo conductivity

No Langevin baths for end-particles, periodic BCs. Master equation is:

$$
\begin{aligned}
\frac{\partial P(x)}{\partial t} &= LP(x) \, , \\
\text{where } L &= A + \lambda S \, , \\
AP(x) &= \sum_{\ell=1}^{N} \left[-\frac{p_\ell}{m_\ell} \frac{\partial P(x)}{\partial q_\ell} + \sum_{m=1}^{N} \Phi_{\ell,m} q_m \frac{\partial P(x)}{\partial p_\ell} \right] \qquad \textit{Hamiltonian part} \, , \\
SP(x) &= \sum_{\ell} [\, P(\ldots, -p_\ell, \ldots) - P(\ldots, p_\ell, \ldots) \,] \qquad \textit{Stochastic part} .
\end{aligned}
$$

The Green-Kubo thermal conductivity κ_{GK} is:

$$
\begin{aligned}
\kappa_{GK} &= \lim_{z \to 0} \lim_{N \to \infty} \frac{1}{NT^2} \int_0^\infty dt \; e^{-zt} \, \langle \mathcal{J}(0) \mathcal{J}(t) \rangle \\
&= \lim_{z \to 0} \lim_{N \to \infty} \frac{1}{NT^2} \, \langle \, \mathcal{J} \, (z - L)^{-1} \, \mathcal{J} \, \rangle \, .
\end{aligned}
$$

Green-Kubo conductivity

The total current which is carried entirely by the Hamiltonian part can be written in the following form:

$$\mathcal{J} = \frac{k}{2} \sum_{\ell=1}^{N} \frac{p_\ell}{m_\ell} (q_{\ell+1} - q_{\ell-1})$$

With this and the forms of A and S it follows:

$$\begin{aligned} A\mathcal{J}P_{eq} &= \sum_{\ell,j} \frac{\Phi_{\ell,j} q_j}{m_\ell} (q_{\ell+1} - q_{\ell-1}) P_{eq} \\ \text{and} \quad S\mathcal{J}P_{eq} &= -2\mathcal{J}P_{eq} \; . \end{aligned}$$

Ordered case: $A\mathcal{J}P_{eq} = 0$.

Green-Kubo conductivity

Ordered case (exact expression for κ).

$$\kappa_{GK} \quad = \quad \lim_{z\to 0}\lim_{N\to\infty}\frac{1}{T^2N}\int dx\;\mathcal{J}\;\frac{1}{z+2\lambda}\;\mathcal{J}\;P_{eq} = \lim_{N\to\infty}\frac{\langle \mathcal{J}^2\rangle}{2\lambda T^2 N}\;.$$

$$\kappa_{GK} = \frac{kD}{8\lambda m}\;, \qquad \text{where} \quad D = \frac{4k}{2k+k_o+[(k_o)(4k+k_o)]^{1/2}}\;.$$

Same as result for κ for self-consistent reservoirs.– BLL (2004)

Disordered case (lower and upper bounds):

$$\frac{kD}{8\lambda[m](1+k\frac{[1/m]-1/[m]}{4\lambda^2 D})} \;\leq\; [\kappa_{GK}] \;\leq\; \frac{kD}{8\lambda}\left[\frac{1}{m}\right]$$

– Bernardin (2008)

Numerical results

Motivations:

- Bounds show that κ_{GK} finite for any finite lambda. For $\lambda \to 0$ — $\kappa_{LB} \sim \lambda$, $\kappa_{UB} \sim 1/\lambda$.
  Not clear what happens at $\lambda \to 0$.
- Comparing κ (from NESS) with κ_{GK}.

- Apply temperature difference ΔT and compute J for different system sizes. Use two methods:

  —- From numerical solution of steady state equations for pair-correlations .

  —- Direct non-equilibrium simulations .

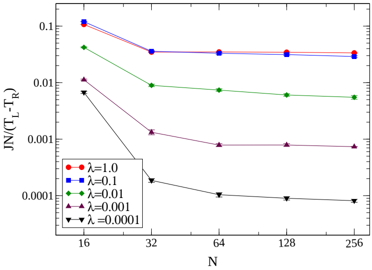
- Plot $\kappa_N = JN/\Delta T$ and check if this saturates for large N . Hence obtain κ.

- Study two different cases

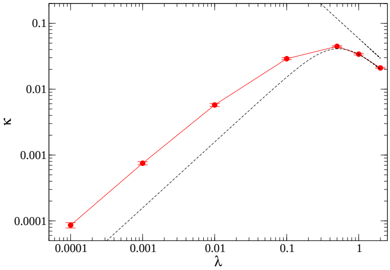
  (i) Unpinned system with fixed and free BCs .

  (ii) Pinned system .

Numerical results: Pinned case



$JN/\Delta T$ - versus - system size
for different values of λ



Conductivity-versus-λ
κ follows the lower bound κ_{GK}.
$\kappa \sim 1/\lambda$ at large λ .
$\kappa \sim \lambda$ at small λ .

Pinned case: discusion

Heuristic argument for small λ behaviour .

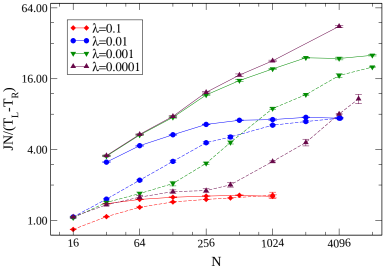
- For $\lambda = 0$, all phonon modes are localized within length-scales $\ell_L \sim \frac{k}{k_o} \left(\frac{m}{\Delta}\right)^2$.
- For small λ, mean free path of phonons $\ell \sim 1/\lambda$.

  Since $\ell >> \ell_L$, localized states are not destroyed completely.
- There is diffusion of energy between the localized states with a diffusion constant $\sim \ell_L^2 \lambda$. Hence:

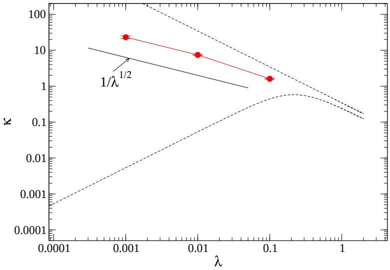
$$\kappa \sim \frac{k^2 m^4}{k_o^2 \Delta^4} \lambda \, .$$

This is consistent with numerical data .

Numerical results: Unpinned case



$J\,N/\Delta T$ - versus - system size for different values of λ for free and fixed BCs.



κ - versus - λ
$\kappa \sim 1/\lambda^{1/2}$ at small λ .
$\kappa \sim 1/\lambda$ at large λ .

Unpinned case: discussion

- κ is independent of BCs for all $\lambda > 0$. Diffusive heat transport.
- Need large *N* to reach the correct asymptotic diffusive limit.
  Effective mean free path $\ell \sim 1/\lambda$.
  To see diffusion of the low frequency ballistic modes, one needs $N \gtrsim \ell$ or $N \gtrsim 1/\lambda$.

Heuristic argument for small λ behaviour:

- In absence of noise, localization length $\ell_L \sim 1/\omega^2$.
- Hence all modes with $\ell_L < \ell$ or $\omega > \lambda^{1/2}$ stay localized.
- The low frequency modes $0 < \omega < \lambda^{1/2}$ become diffusive with mean free paths $\sim 1/\lambda$ thus resulting in a conductivity:

$$\kappa \sim \lambda^{1/2} \times \frac{1}{\lambda} \sim \frac{1}{\lambda^{1/2}} .$$

Thus $\kappa \to \infty$ as $\lambda \to 0$ unlike conjecture of Rich/Visscher.

Summary and open questions

Refn: Dhar, Venkateshan, Lebowitz, PRE **83**, 021108 (2011)

- Analytically tractable model to study effect of interactions in disordered harmonic systems .
- Mapping to model of self-consistent reservoirs and exact bounds for GK conductivity .
- For pinned case exact proof of insulator - conductor transition for arbitrarily small value of λ. Different from many-body localization in quantum systems .
- For $\lambda \to 0$, $\kappa \sim \lambda$ (pinned case), $\kappa \sim 1/\lambda^{1/2}$ (unpinned case) . Rigorous proof ?
- NESS: Deviation from Gaussian measure. Does this vanish in the thermodynamic limit ?

Other Questions:

- Heat conduction in disordered harmonic crystals in higher dimensions: effect of noisy dynamics.
- Equivalent quantum dynamics.
- Heat conduction in disordered harmonic chains with momentum-conserving noisy dynamics.