Localization effects on transport properties in chains of oscillators

Cédric Bernardin
(University of Côte d'Azur)

ICTS INTERNATIONAL CENTRE for THEORETICAL SCIENCES
TATA INSTITUTE OF FUNDAMENTAL RESEARCH
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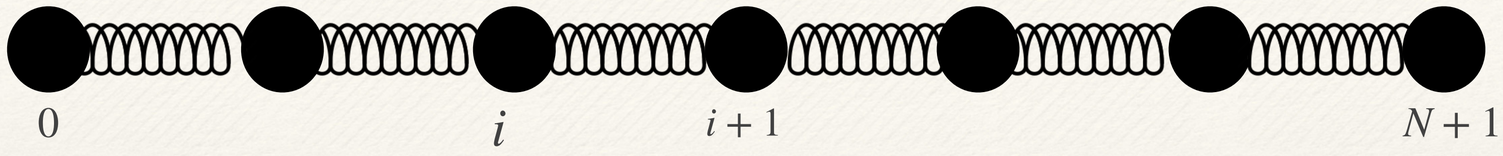
Part I: chains of haemonic oscillators with random masses

Part II: chains of harmonic oscillators with random charges in presence of a magnetic field

Chains of oscillators with random masses

(joint with F. Huveneers and S. Olla)

Harmonic chain of N oscillators



m_i : mass of particle i

$p_i = m_i v_i$: momentum of particle i

q_i : position of particle i

$$r_i = q_{i+1} - q_i$$

Newton's equations in the bulk of the system

$$\dot{r}_i = \frac{p_{i+1}}{m_{i+1}} - \frac{p_i}{m_i}, \qquad \dot{p}_i = r_i - r_{i-1},$$

Physical boundary conditions:

Fixed bc: $q_0 = 0, \quad q_{N+1} = 0$

Free bc: $q_0 = q_1, \quad q_N = q_{N+1}$

Periodic bc:

3 physical conserved quantities (in the bulk):

$$\begin{cases} \text{energy:} & \sum_i e_i, \quad e_i = \frac{p_i^2}{2m_i} + \frac{r_i^2}{2} \\ \text{momentum:} & \sum_i p_i \\ \text{elongation/stretch:} & \sum_i r_i \end{cases}$$

but many other ones (integrable dynamics) : energy of each normal mode ψ^k

$$\frac{d}{dt}\left(\langle p, \psi^k \rangle^2 + \frac{\langle r, \nabla \psi^k \rangle^2}{\omega_k^2} \right) = 0 \qquad M^{-1}(-\Delta)\psi^k = \omega_k^2 \psi^k, \qquad \langle \psi^j, M\psi^k \rangle = \delta(j-k)$$

($M = \mathrm{Diag}(\mathrm{m}_1, \ldots, \mathrm{m}_\mathrm{N})$, ω_k dispertion relation)

Standard Gibbs Ensembles (SGE)

$$\rho^{\mathrm{G}}(r,p) = \frac{1}{Z_{\mathrm{G}}} \exp\left\{ -\frac{\beta}{2} \sum_{i=1}^{N} m_x \left(\frac{p_i}{m_i} - \frac{\mathsf{p}}{\overline{m}} \right)^2 - \frac{\beta}{2} \sum_{i=1}^{N-1} (r_i - \mathsf{r})^2 \right\}$$

Generalized Gibbs Ensembles (GGE)

$$\rho^{\mathrm{GGE}}(r,p) = \frac{1}{Z_{GGE}} \exp\left\{ -\sum_{n=1}^{N} \lambda_n \, Q_n^{(N)}(r,p) \right\}$$

conserved quantities (sum of local observables)

Hydrodynamic limit in hyperbolic time scale for the ordered chain ($m_x = m$ constant)

Start initially the system in a local SGE (associated to macroscopic profiles $\beta, \mathsf{r}, \mathsf{p}$):

$$\rho^{\mathrm{G}}_{\mathrm{loc}}(r,p) = \frac{1}{Z_{\mathrm{loc}}} \exp\Big\{ -\frac{1}{2}\sum_{i=1}^{N} \beta(i/N) m \Big(\frac{p_i}{m} - \frac{\mathsf{p}(i/N)}{m}\Big)^2 - \frac{1}{2}\sum_{i=1}^{N-1} \beta(i/N)(r_i - \mathsf{r}(i/N))^2 \Big\}$$

If the dynamics was ergodic when fixing the values of the three physical conserved quantities, we would expect that **propagation of local SGE holds at time** tN , i.e. the state $\langle \cdot \rangle_{tN}$ of the system at this time should be `close' to a new local SGE with macroscopic profiles $\beta_t = 1/\mathbf{T}_t$, $\mathbf{p}_t$, $\mathbf{r}_t$ such that

$$\mathbf{e}_t(y) = \mathbf{T}_t(y) + \frac{\mathbf{p}_t^2(y)}{2m} + \frac{\mathbf{r}_t^2(y)}{2}$$

and $\mathbf{r}$, $\mathbf{p}$, $\mathbf{e}$ solutions of the Euler equations:

$$\begin{cases} \partial_t \mathbf{r}_t(y) = \dfrac{1}{m}\partial_y \mathbf{p}_t(y), \qquad \mathbf{r}_t(0) = \mathbf{r}_t(1) = 0, \\ \partial_t \mathbf{p}_t(y) = \partial_y \mathbf{r}_t(y), \\ \partial_t \mathbf{e}_t(y) = \dfrac{1}{m}\partial_y(\mathbf{r}_t(y)\mathbf{p}_t(y)) \,. \end{cases}$$

$$\partial_t \mathbf{T}_t(y) = 0$$

This propagation of local equilibrium is usually false but weaker forms may hold, e.g. if the initial temperature profile is constant in space (and then in time).

Doyon-Spohn's generalized hydrodynamics theory for integrable systems shows that generalized Euler equations are still valid by assuming propagation of local GGE instead of propagation of local SGE.

Hydrodynamic limit in hyperbolic time scale for the disordered chain (m_x i.i.d. random variables)

$$\overline{m} = \langle m_i \rangle$$

Theorem: [B. Huveneers, Olla CMP'20]

Start the sytem with a local SGE

$$\rho^{\mathrm{G}}_{\mathrm{loc}}(r,p) = \frac{1}{Z_{\mathrm{loc}}} \exp\Big\{ -\frac{1}{2}\sum_{i=1}^{N} \beta(i/N) m_i \Big(\frac{p_x}{m_i} - \frac{\mathsf{p}(i/N)}{\overline{m}}\Big)^2 - \frac{1}{2}\sum_{i=1}^{N-1} \beta(i/N)(r_i - \mathsf{r}(i/N))^2 \Big\}$$

Then for any test function $f : [0,1] \to \mathbb{R}$ we have almost surely with respect to the masses realization that

$$\lim_{N\to\infty} \frac{1}{N}\sum_i f(i/N)\langle r_i\rangle_{tN} = \int_0^1 f(y)\ \mathbf{r}_t(y)\ dy$$

$$\lim_{N\to\infty} \frac{1}{N}\sum_i f(i/N)\langle p_i\rangle_{tN} = \int_0^1 f(y)\ \mathbf{p}_t(y)\ dy$$

$$\lim_{N\to\infty} \frac{1}{N}\sum_i f(i/N)\langle e_i\rangle_{tN} = \int_0^1 f(y)\ \mathbf{e}_t(y)\ dy$$

with

$$\begin{cases} \partial_t \mathbf{r}_t(y) = \dfrac{1}{\overline{m}}\partial_y \mathbf{p}_t(y), \qquad \mathbf{r}_t(0) = \mathbf{r}_t(1) = 0, \\ \partial_t \mathbf{p}_t(y) = \partial_y \mathbf{r}_t(y), \\ \partial_t \mathbf{e}_t(y) = \dfrac{1}{\overline{m}}\partial_y(\mathbf{r}_t(y)\mathbf{p}_t(y)) \,. \end{cases}$$

The previous result **which does not hold for the ordered harmonic chain** is a consequence of **localization effects** induced by the presence of random masses

Anderson localization implies localization of the eigenmodes ψ^k but the localization length ζ_k diverges when one approaches the ground state

$$\zeta_k \sim \omega_k^2 \sim \left(\frac{k}{N}\right)^2$$

For $k \gg \sqrt{N}$ normal modes are localized and do not transport energy.
For $k \ll \sqrt{N}$ normal modes are delocalized and in fact are close to the normal modes of the ordered chain.

A local SGE gives weight only to modes with small wave number.

Hence everything happens like if the disordered harmonic chain was an ordered harmonic chain without normal modes with large wave number.

Performing computations with this assumption gives the Euler equations.

Conclusion and comments:

- Euler equations can be obtained rigorously [Olla-Varadhan-Yau'93] for an ordered harmonic chain by restoring artificially ergodicity (add an energy-monentum conservative stochastic noise). The mechanism to derive Euler equations is the same (the noise destroys the high modes of the harmonic chain).

- Hydrodynamic limits gives the typical evolution of the empirical conserved quantities. What is the form of the fluctuations?

- In the case of ordered harmonic chain + energy-momentum conservative noise: superdiffusion of energy driven by a fractional Laplacian of order $3/4$ [Jara-Komorowski-Olla'15, B.-Jara-Gonçalves'16].

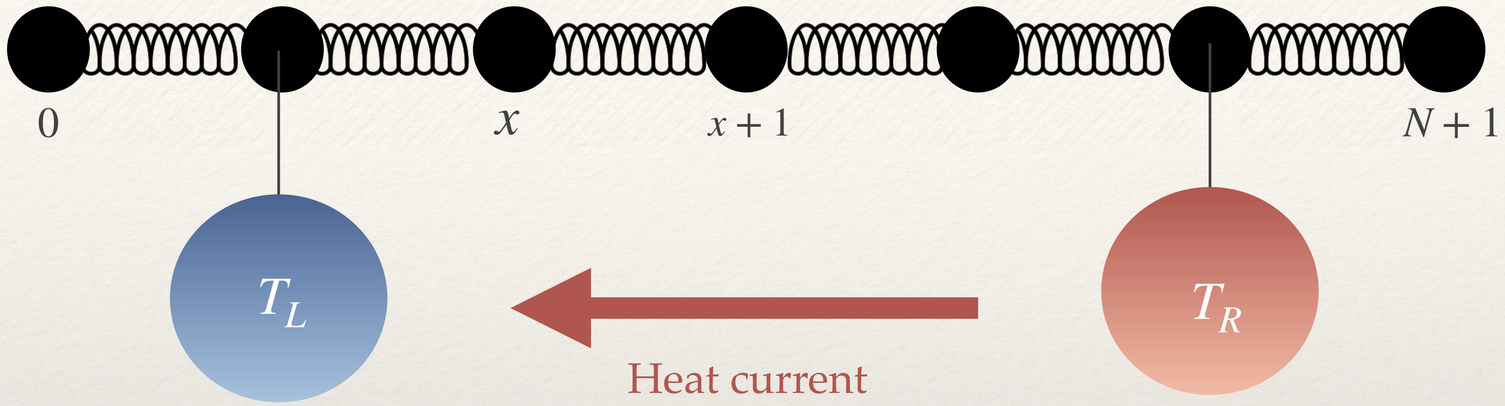
- Not clear the same occurs for the disordered harmonic chain (without noise).

- See also Arxiv preprint by Amirali Hannani for a similar result for a quantum disordered harmonic chain.

Chains of oscillators with random charges in presence of a magnetic field

(joint with J. Bhat, G. Cane and A. Dhar)

A different setting to study transport of energy is to consider the chain in contact at the extremities with thermal Langevin baths at different temperatures at the boundaries

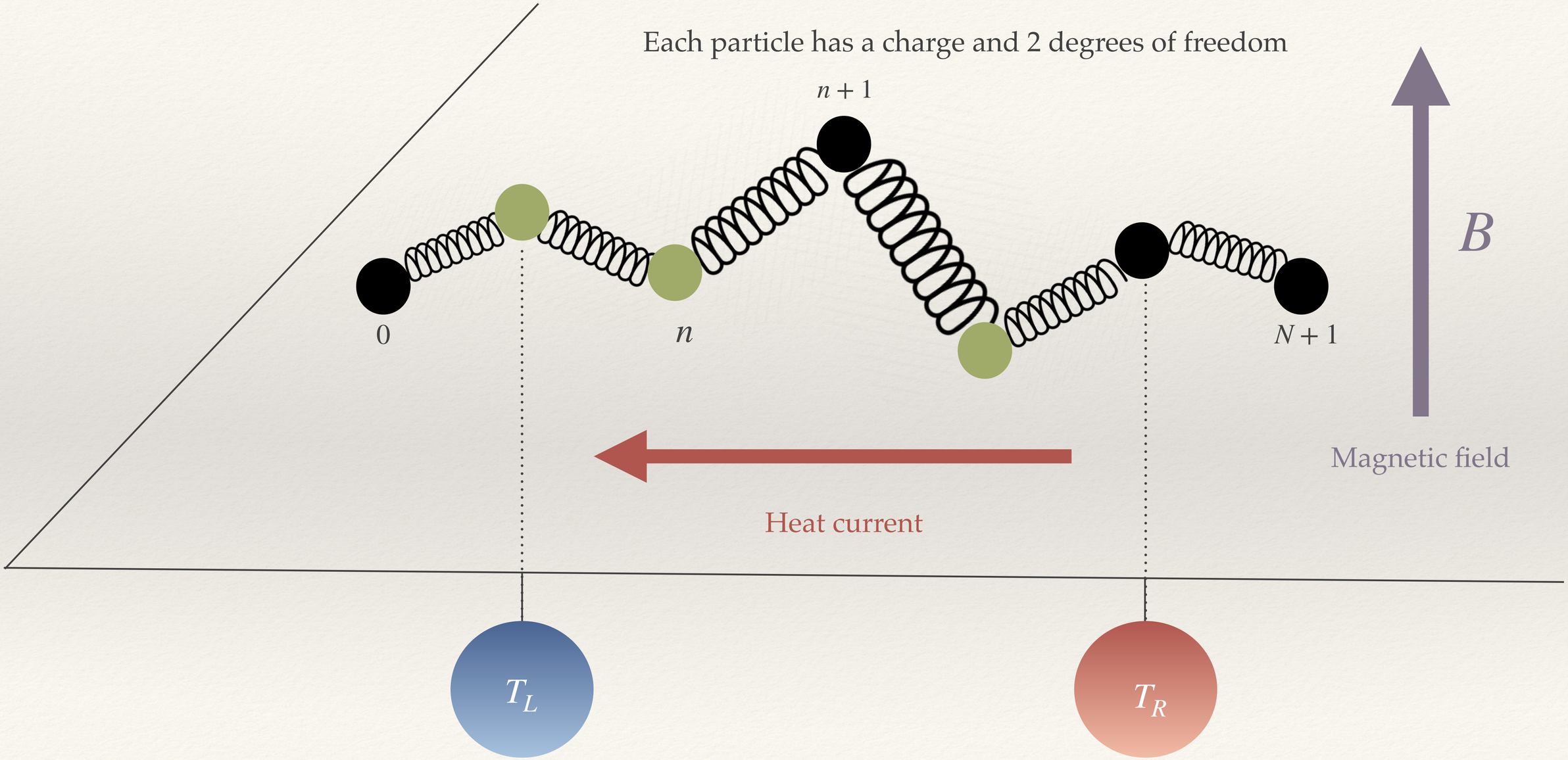


Question: what is the scaling of the heat current J_N in the NESS as $N \to \infty$ ($J_N \sim N^{-1}$ corresponds to Fourier's law)?

- Ordered chain: transport is ballistic, i.e. $J_N \sim 1$ [Rieder, Lieb, Lebowitz'67]
- Disordered chain: transport is affected by Anderson localization effects

$$J_N \sim 1/N^{1/2} \text{ for free b.c. and } J_N \sim 1/N^{3/2} \text{ for fixed b.c.}$$

Huge Litterature: [Ajanki, Casher, Chaudury, Dhar, Greer, Ishii, John, Huveneers, Kundu, Lee, Lebowitz, Lepri, Livi, O'Connor, Politi , Matsuda, Rubin, Roy, Saito …]


Each particle has a charge and 2 degrees of freedom
$n+1$
0
n
$N+1$
B
Magnetic field
Heat current
T_L
T_R

Equations of motion:

$$\begin{cases} \ddot{x}_n = (x_{n+1} + x_{n-1} - c_n x_n) + B_n \dot{y}_n + \eta_L^x(t)\delta_{n,1} + \eta_R^x(t)\delta_{n,N} - (\gamma\delta_{n,1} + \gamma\delta_{n,N})\dot{x}_n \ , \\ \ddot{y}_n = (y_{n+1} + y_{n-1} - c_n y_n) - B_n \dot{x}_n + \eta_L^y(t)\delta_{n,1} + \eta_R^y(t)\delta_{n,N} - (\gamma\delta_{n,1} + \gamma\delta_{n,N})\dot{y}_n \ . \end{cases}$$

B_n i.i.d. random variables
(random charge times B)

$$\begin{cases} c_n = 2 \quad \text{for fixed b.c.} \\ c_n = 2 - \delta_{n,1} - \delta_{n,N} \quad \text{for free b.c.} \end{cases}$$

$$\langle \eta_{L/R}(t)\eta_{L/R}(t')\rangle \ = \ \sqrt{2\gamma T_{L/R}}\ \delta(t-t')$$

QUESTION: Asymptotics of the average heat current J_N in the NESS for $N \gg 1$

Non Equilibrium Green Function ([Casher-Lebowitz.'71, Dhar et al. '01-'20]) approach gives us an explicit expression of J_N

Same NEGF structure found for electron transport in superconducting wires [Bhat-Dhar'20-21]

$$\mathcal{T}_N(\omega) = \frac{2\gamma^2}{\pi}\,\omega^2 \left[\frac{1}{|F_N^+(\omega)|^2} + \frac{1}{|F_N^-(\omega)|^2}\right]$$

$$\boxed{J_N = 2(T_L - T_R)\int_0^\infty d\omega\, \mathcal{T}_N(\omega)}$$

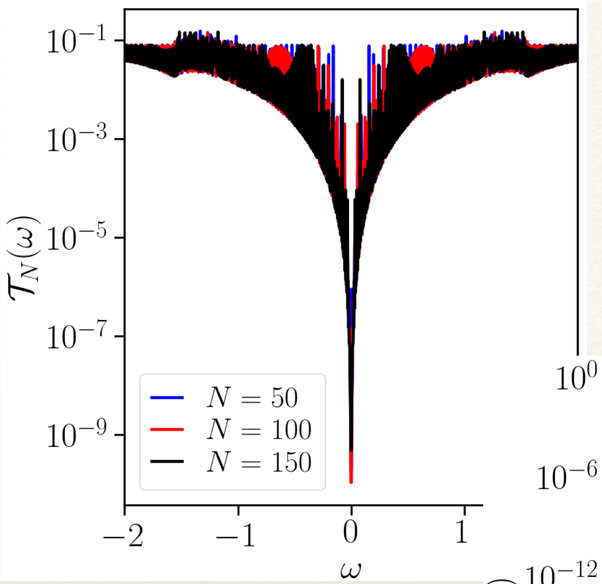
$$F_N^\pm := F_N^\pm(\omega) = f_N^\pm + i\gamma\omega(g_N^\pm + f_{N-1}^\pm) - \gamma^2\omega^2 g_{N-1}^\pm$$

$$f_{n+1}^\pm = (c_{n+1} - \omega^2 \pm \omega B_{n+1})f_n^\pm - f_{n-1}^\pm, \quad f_0^\pm = 1, \quad f_1^\pm = c_1 - \omega^2 \pm \omega B_1\ ,$$
$$g_{n+1}^\pm = (c_{n+1} - \omega^2 \pm \omega B_{n+1})g_n^\pm - g_{n-1}^\pm, \quad g_0^\pm = 0, \quad g_1^\pm = 1\ .$$

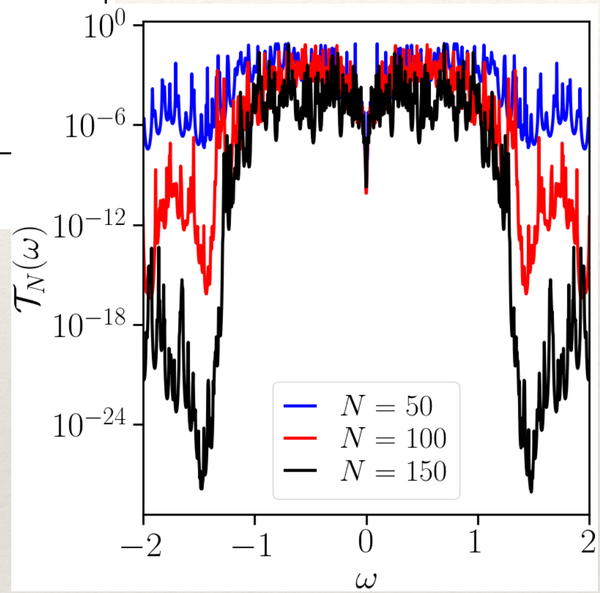
- <u>$B_n = B$ constant:</u> $J_N \sim 1$, i.e. ballistic transport (exact computation of the transmission coefficient $\mathcal{T}_N$)
- <u>$Var(B_n) > 0$ then Anderson localization effects:</u>

$$U_{n+1} = \begin{pmatrix} 2 - \omega^2 - \omega B_{n+1} & -1 \\ 1 & 0 \end{pmatrix} U_n, \quad \text{where} \quad U_n := \begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix}$$

Lyapunov exponent: $$\lambda(\omega) = \lim_{n\to\infty} \frac{1}{2n}\left\langle \log \|U_n(\omega)\| \right\rangle = \lim_{n\to\infty} \frac{1}{n}\left\langle \log |u_n(\omega)| \right\rangle > 0$$



constant magnetic field



random magnetic field

$$\langle J_N \rangle \approx 2(T_L - T_R)\int_0^{\omega_{max}^N} d\omega \lim_{N\to\infty} \langle \mathcal{T}_N(\omega) \rangle = 2(T_L - T_R)\int_0^{\omega_{max}^N} d\omega \mathcal{T}_\infty(\omega)$$

cutoff of frequencies in terms of the Lyapunov exponent

$$1/\lambda(\omega_{max}^N) = N$$

Transmission coefficient of the ordered chain with constant magnetic field equal to $\langle B \rangle$ and Frre/fixed b.c.

Numerical study of the transmission coefficient $\mathcal{T}_N(\omega)$

$\lambda(\omega) \sim$? for $\omega \to 0$

Study of the Lyapunov exponent for $\omega \to 0$

$$\lambda(\omega) = \lim_{n\to\infty} \frac{1}{n} \left\langle \log|u_n(\omega)| \right\rangle$$

where $\quad u_{n+1} + u_{n-1} - 2u_n = -\omega\langle B\rangle u_n - \omega(B_{n+1} - \langle B\rangle)u_n + \mathcal{O}(\omega^2)$

In the continuous limit we get $\quad \ddot{u}_t = -\omega\langle B\rangle u_t - \omega\sigma\xi_t u_t, \quad \sigma^2 = \mathrm{Var}(B_n), \quad \xi_t$ standard white noise

$$\lambda_*(\omega) = \lim_{t\to\infty} \frac{1}{t} \left\langle \log|u_t| \right\rangle$$

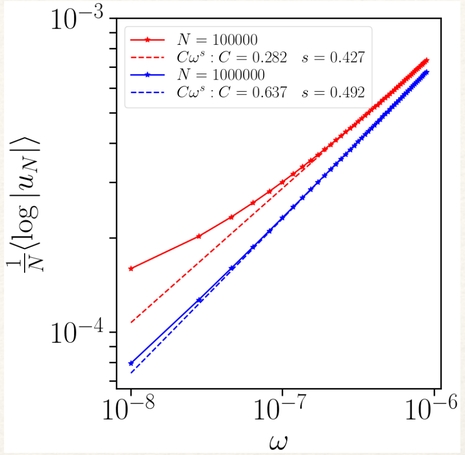
[Wihstutz, Pardoux '81-88]

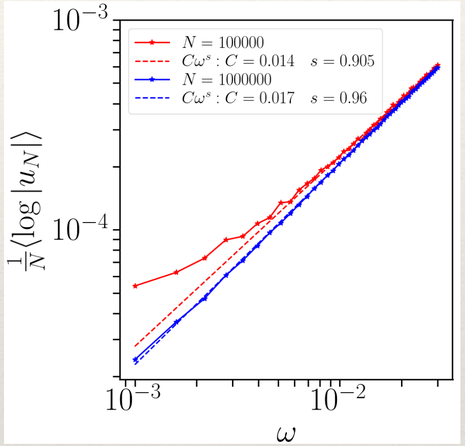
$\langle B\rangle = 0, \quad \lambda_*(\omega) \sim \omega^{2/3}$

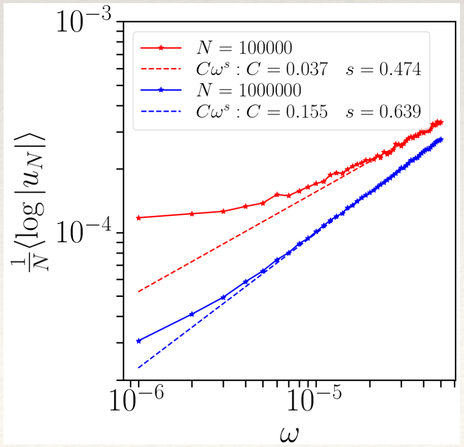
$\langle B\rangle > 0, \quad \lambda_*(\omega) \sim \omega$

$\langle B\rangle < 0, \quad \lambda_*(\omega) \sim \omega^{1/2}$

$$\boxed{\lambda(\omega) \approx \lambda_*(\omega)}$$

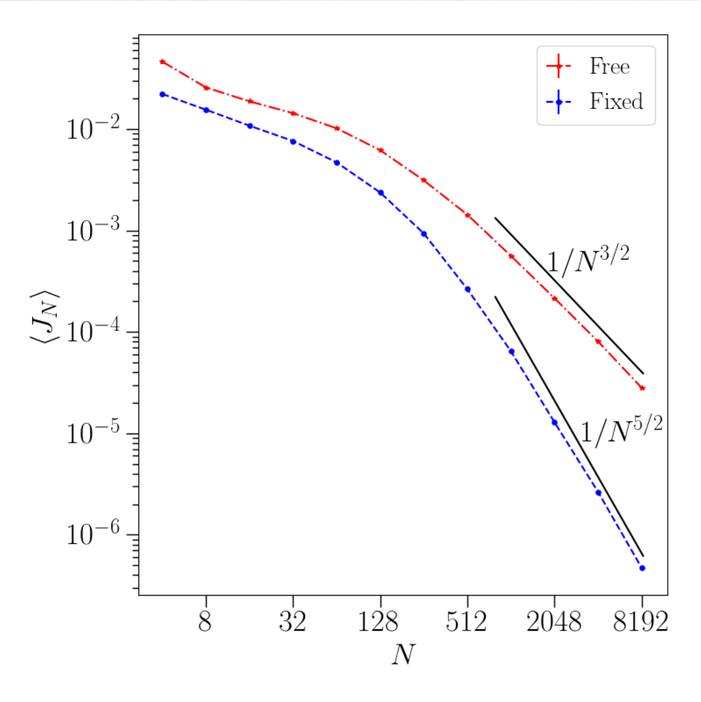


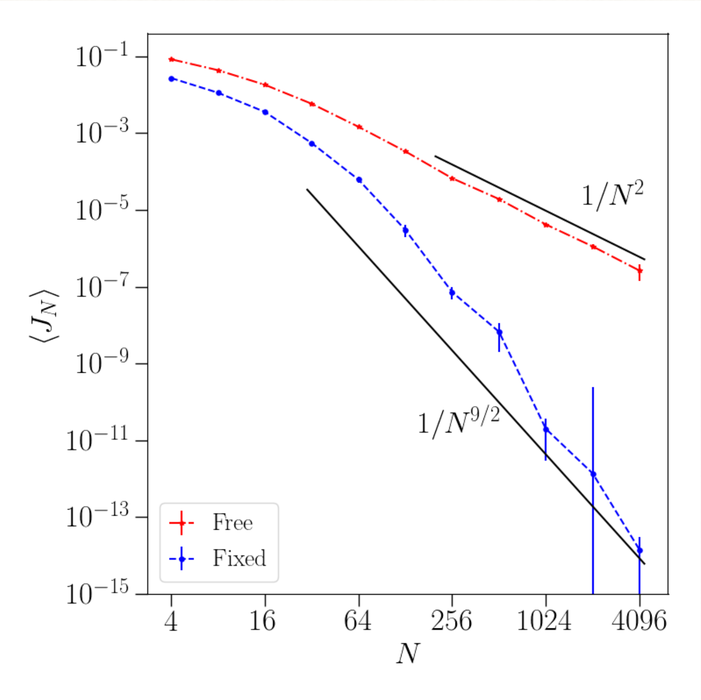




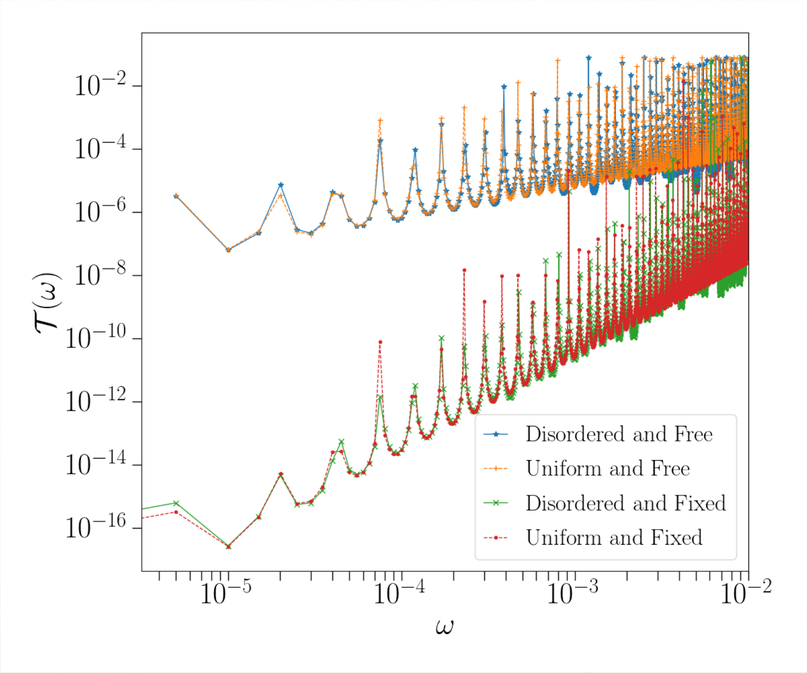
Prediction for $\langle J_N \rangle$

Boundary Conditions	Average magnetic field	$\mathcal{T}_\infty(\omega)$	$\lambda(\omega)$	Power law for the current $\langle J_N \rangle$
Fixed	$\langle B \rangle \neq 0$	$\sim \omega^{3/2}$	$\sim \omega$	$\sim 1/N^{5/2}$
Fixed	$\langle B \rangle = 0$	$\sim \omega^{2}$	$\sim \omega^{2/3}$	$\sim 1/N^{9/2}$
Free	$\langle B \rangle \neq 0$	$\sim \omega^{1/2}$	$\sim \omega$	$\sim 1/N^{3/2}$
Free	$\langle B \rangle = 0$	$\sim \omega^{0}$	$\sim \omega^{2/3}$	$\sim 1/N^{3/2}$

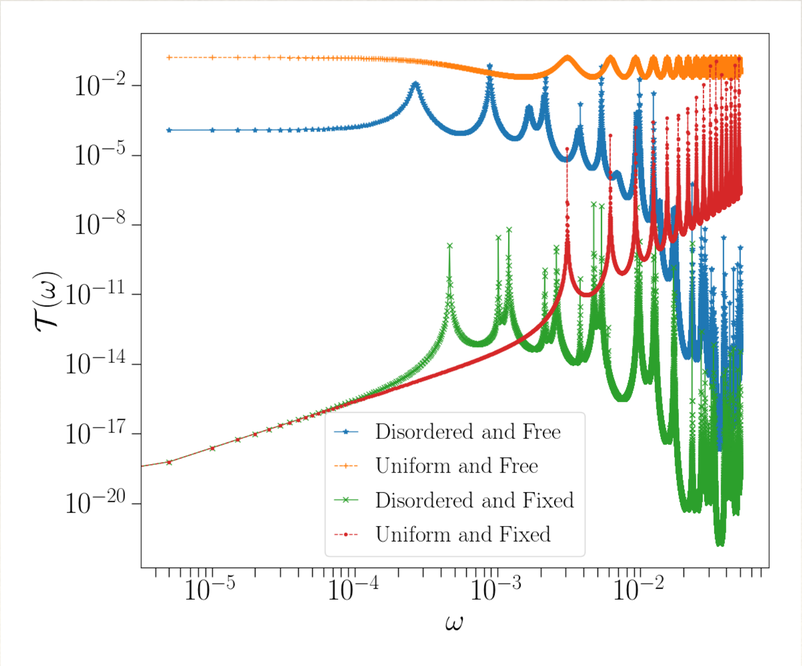




$\langle B \rangle \neq 0$



$\langle B \rangle = 0$



Conclusion and comments:

- Transport properties for a chain of harmonic oscillators in the presence of a random magnetic field are different from a harmonic chain with random masses. We obtained theoretically the behavior of the Lyapunov exponents in the three regimes with a good agreement with numerics. However, if $\langle B \rangle = 0$, it seems false to approximate the average of the transmission coefficient by the one of the chain with 0 magnetic field.

- The model with constant magnetic field and some energy-momentum conserving noise has been investigated in [Saito, Sasada, Suda'18]. There superdiffusion of energy driven by a fractional Laplacian of exponent $5/6$ appears. [Cane'21] investigated intermediate regimes when $B = B(N)$ is small exhibiting new fractional Laplacian exponents.

- Can we establish rigorously predictions done here (and predict correctly the size of the current for $\langle B \rangle = 0$?

- Can we establish hydrodynamic limits in hyperbolic time scale for a harmonic chain in the presence of a random magnetic field like in the case of random masses by taking advantage of the localization effects?

- Can we precise the form of the fluctuations for a harmonic chain in the presence of a random magnetic field?