

Integrability breaking in extended Hamiltonian systems

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CEREMADE
UMR CNRS 7534

Seminar Dynamical systems and PDEs, april 2021

Plan

- I - Diffusive transport
- II - Slowing down transport: Frequency mismatch
- III - Rigorous results
- IV - Puzzles at $T = 0$
- V - Many-body localization
- VI - Technical: Green-Kubo formula, role of the noise

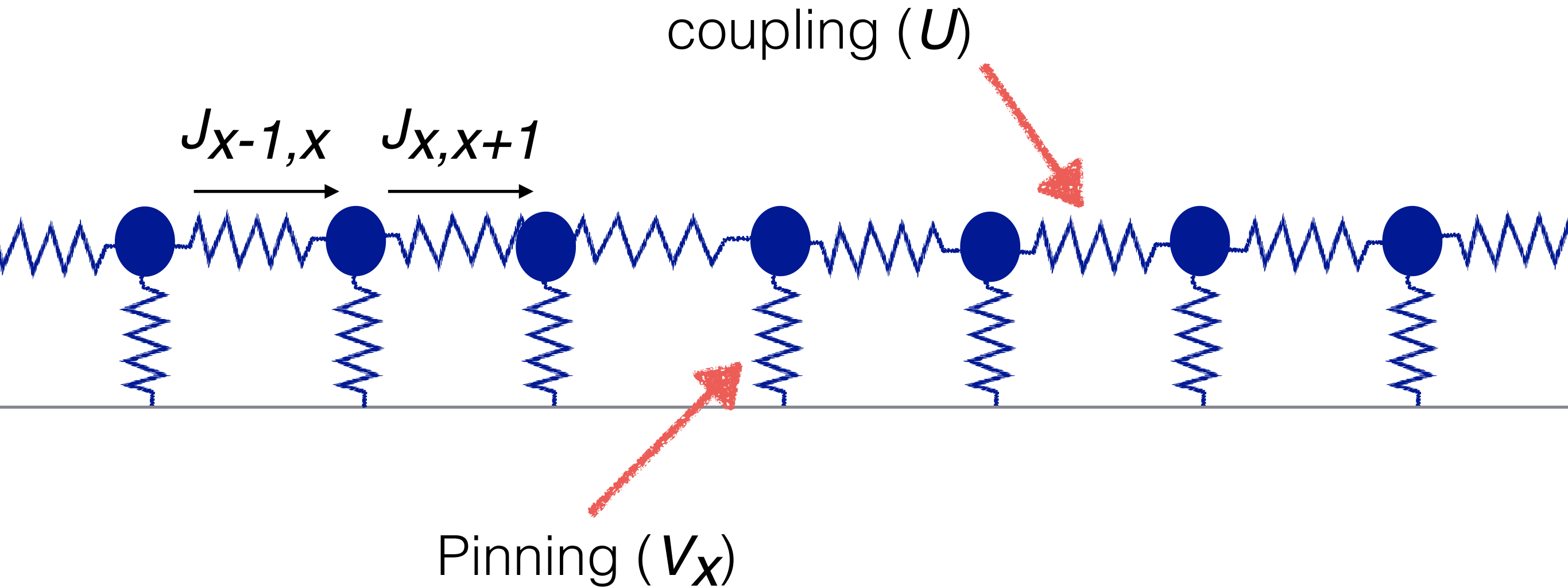
Main collaborator



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I - Transport

Chain of oscillators



$$H(p, q) = \sum_{x=1}^L \frac{p_x^2}{2m} + V_x(q_x) + \sum_{x=1}^{L-1} U(q_x - q_{x+1})$$

$$(p, q) \in \mathbb{R}^{2L}$$

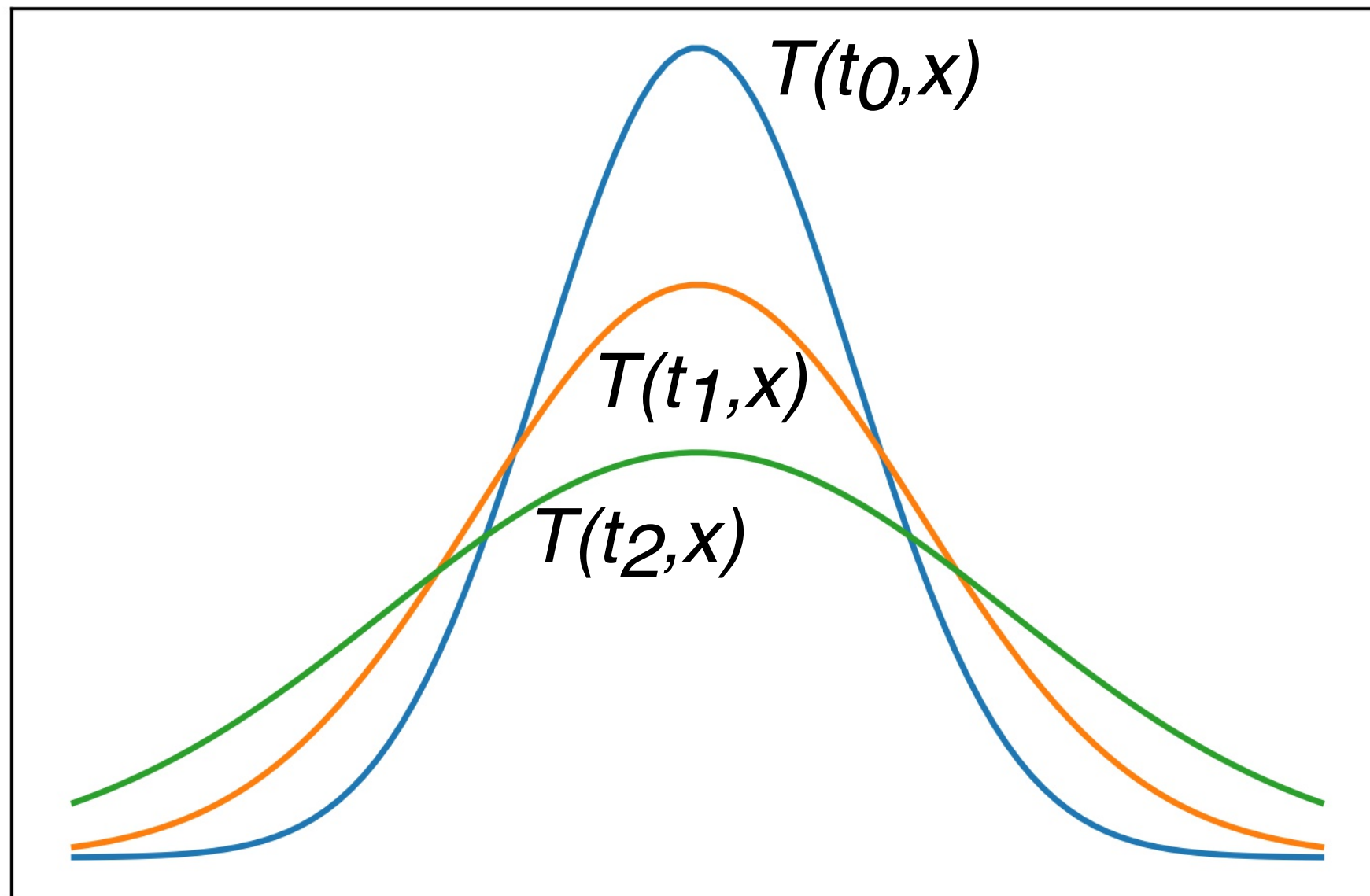
Conservation of energy

$$H(p, q) = \sum_{x=1}^L H_x(p, q)$$

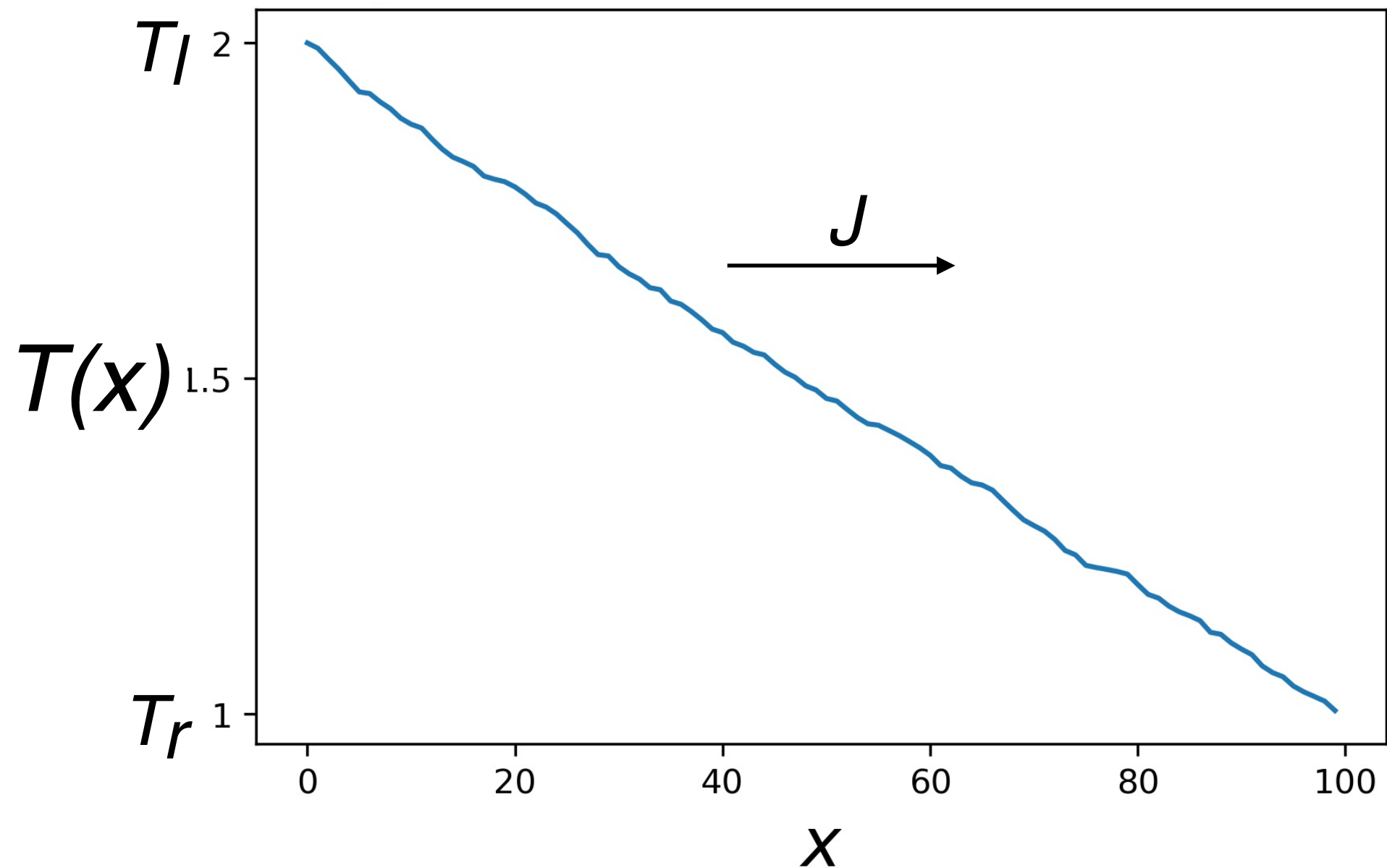
$$\frac{dH_x}{dt} = j_{x-1,x} - j_{x,x+1}$$

$$j_{x,x+1} = \frac{p_x}{m} U'(q_x - q_{x+1})$$

1) Time evolution of an energy profile



2) Steady state profile



$$J = \langle \dot{j}_{x,x+1}(t) \rangle_{NESS} \quad \forall t, x$$

Scaling of J with L ?

How to model the baths?

Most popular: Langevin thermostats

$$\dot{\mathbf{p}}_1 = -\frac{\partial H}{\partial \mathbf{q}_1} - \gamma \mathbf{p}_1 + \sqrt{2\gamma m T_\ell} \xi_\ell$$

$$\dot{\mathbf{p}}_L = -\frac{\partial H}{\partial \mathbf{q}_L} - \gamma \mathbf{p}_L + \sqrt{2\gamma m T_r} \xi_r$$

Common expectations:

1) There exists a unique NESS

2) Local equilibrium sets in:

Fix a site x . Given a local observable O_x , as $L \rightarrow \infty$

$$\langle O_x \rangle_{\text{NESS}} \rightarrow \langle O_x \rangle_{T(x/L)}$$

for some appropriate temperature T

Common expectations:

3) Fourier's law: As $L \rightarrow \infty$

$$\mathbf{J} = -\kappa(\mathbf{T}(\mathbf{x}/L)) \frac{1}{L} \nabla \mathbf{T}(\mathbf{x}/L) + o(1/L)$$



Thermal conductivity



Normal scaling of the current

What do we know about κ ?

1) From thermodynamics: $\kappa(T) > 0$

Entropy increases: current flows from hot to cold

Cf. J-P Eckmann, C-A Pillet and L Rey-Bellet, JSP 1998

2) It is expressed by the Green-Kubo formula:

$$\kappa(T) = \frac{1}{T^2} \lim_{t \rightarrow \infty} \lim_{L \rightarrow \infty} \left\langle \left(\frac{1}{\sqrt{t}} \int_0^t \frac{1}{\sqrt{L}} \sum_{x=1}^{L-1} j_{x,x+1}(s) ds \right)^2 \right\rangle_T$$

Reminder: Gibbs state

$$\langle f \rangle_T = \frac{1}{Z(T)} \int_{\mathbb{R}^{2L}} f(p, q) e^{-H(p, q)/T}$$

$$Z(T) \quad s.t. \quad \langle 1 \rangle_T = 1 \quad (\textit{probability measure})$$

II - Frequency mismatch

2 harmonic oscillators

$$H = \frac{p_1^2}{2m} + \frac{\omega_1^2 q_1^2}{2} + g \frac{(q_1 - q_2)^2}{2} + \frac{p_2^2}{2m} + \frac{\omega_2^2 q_2^2}{2}$$

There are two eigenmodes = eigenvectors of

$$\begin{pmatrix} \omega_1 & g \\ g & \omega_2 \end{pmatrix}$$

The eigenvectors are localized if $|g| \ll |\omega_1 - \omega_2|$

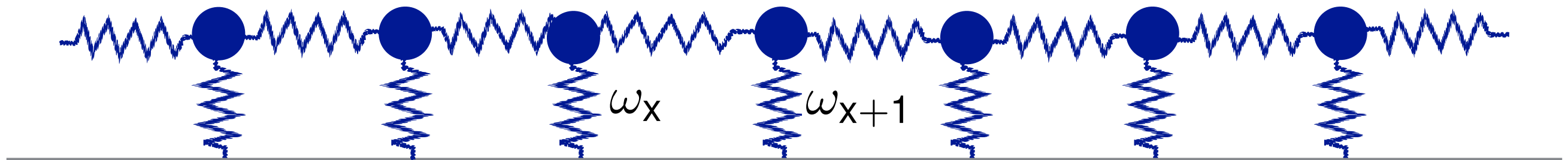
$$v_1 \sim (1, 0) \quad v_2 \sim (0, 1)$$

Anderson Localization

Disordered harmonic chain : $(\mathbf{p}, \mathbf{q}) \in \mathbb{R}^{2L}$

$$H(\mathbf{p}, \mathbf{q}) = \frac{1}{2} \sum_{1 \leq x \leq L} p_x^2 + \omega_x^2 q_x^2 + g(q_x - q_{x+1})^2$$

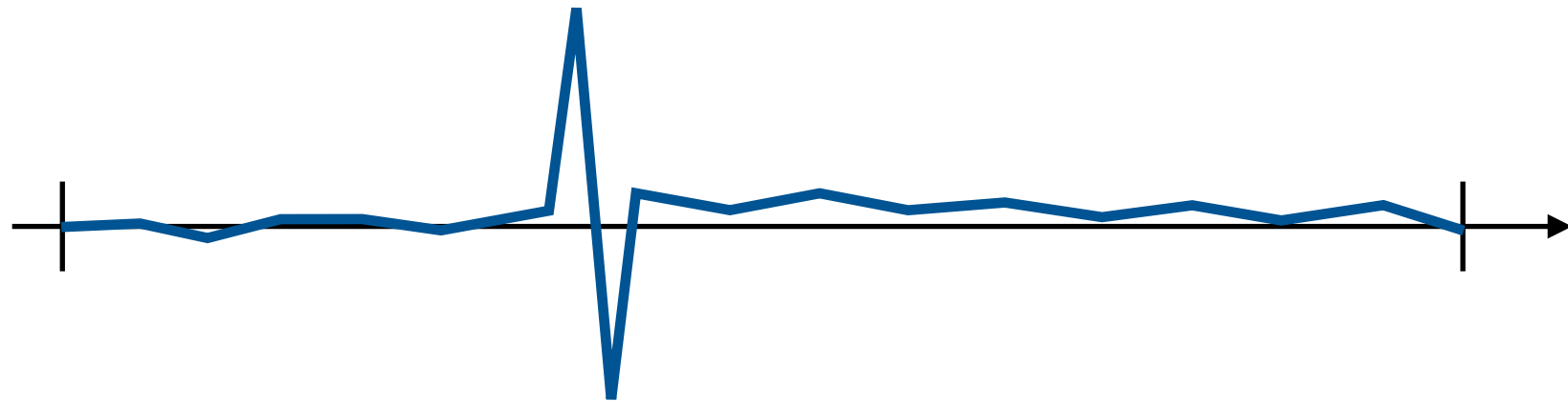
$$0 < \omega_- < \omega_x < \omega_+ \quad \text{iid}$$



Newton : $\ddot{\mathbf{q}} = (g\Delta - V)\mathbf{q}, \quad V_{x,y} = \delta(x - y)\omega_x^2$

Localized eigenmodes

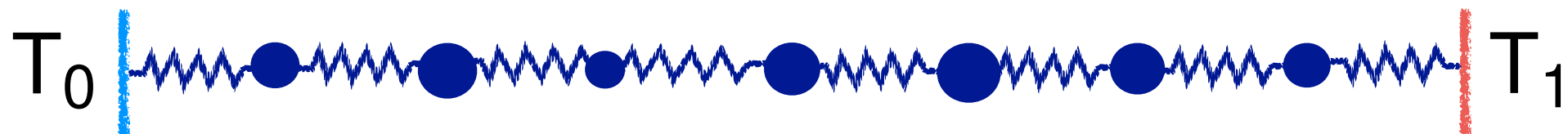
Eigenmodes of $g\Delta - V$



$d = 1$: localized for all values of g

$d > 2$: localized if $|g| \ll \Delta\omega$

With heat baths:



Very bad coupling, thus: $J \sim e^{-L/\xi}, \quad \xi > 0$

Introduce interactions among modes

$$H(p, q) = \frac{1}{2} \sum_{1 \leq x \leq L} p_x^2 + \omega_x^2 q_x^2 + g(q_{x+1} - q_x)^2 + \lambda q_x^4$$

disordered harmonic chain

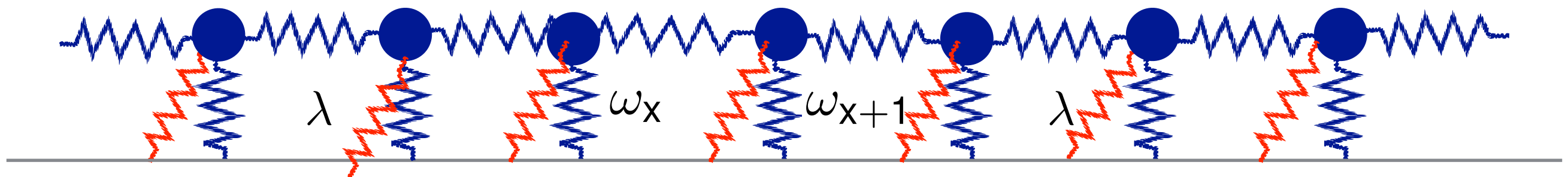
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localized system

anharmonic pinning

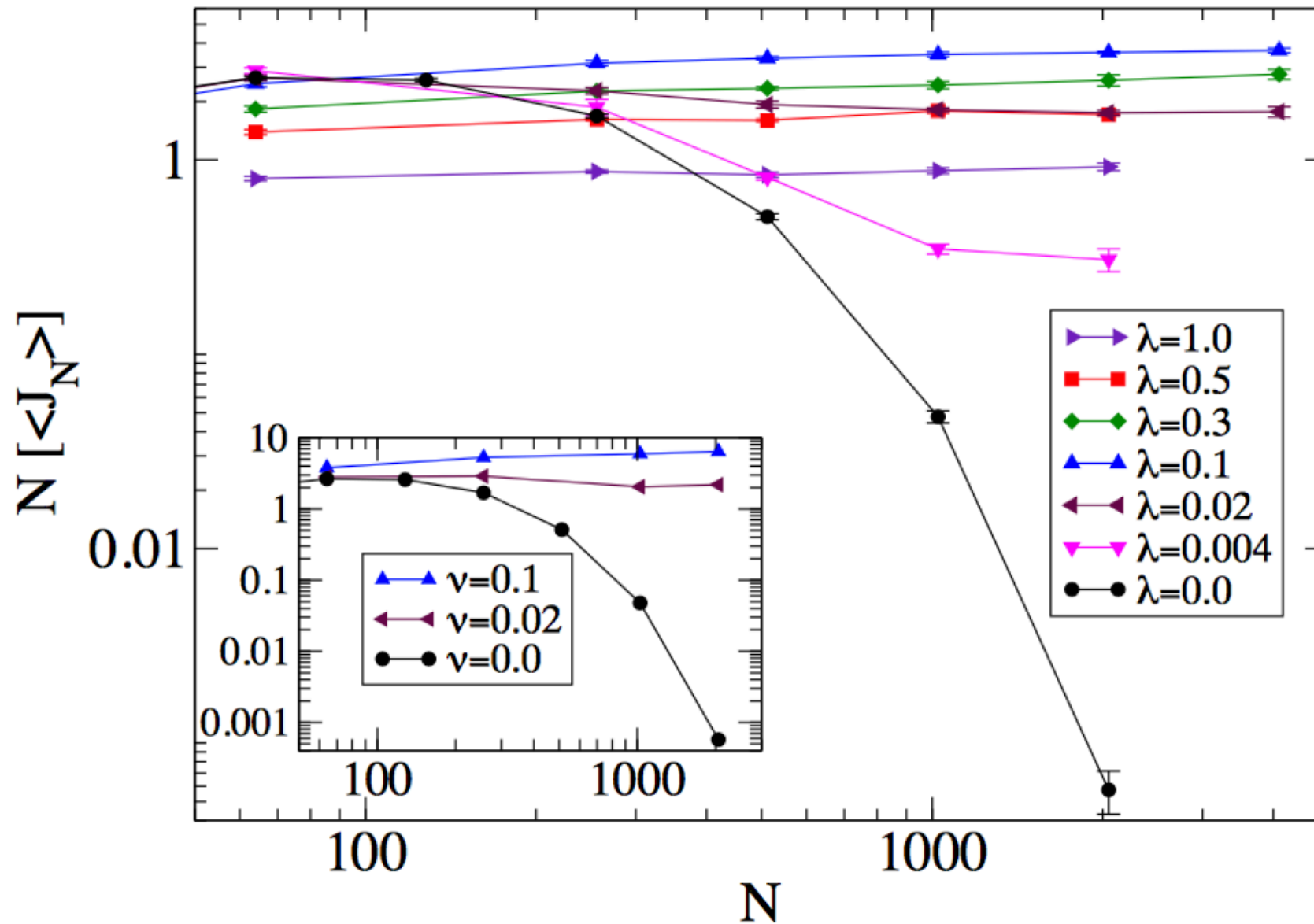
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interaction among modes



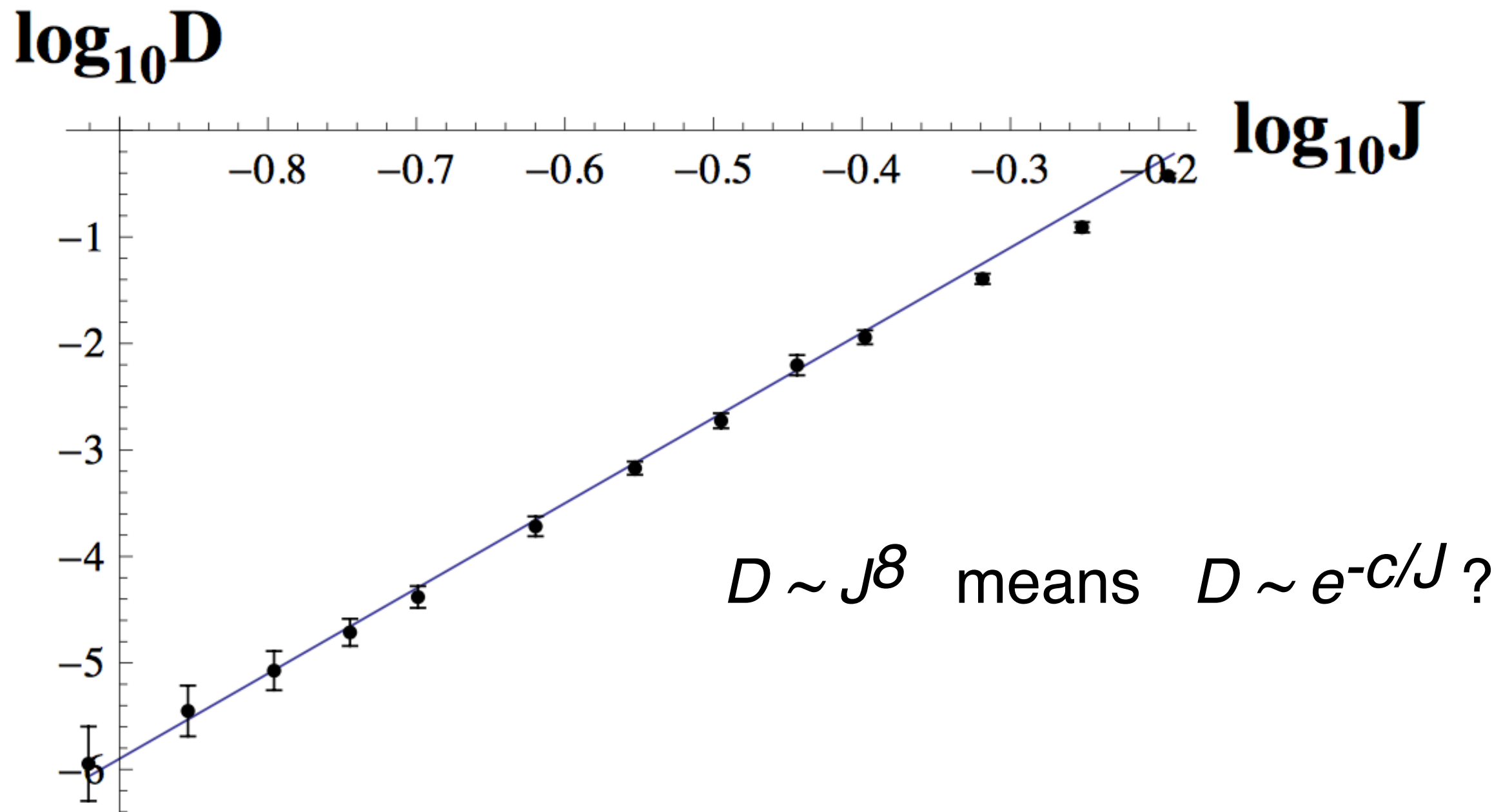
How about $\kappa(T)$?

Normal conductivity



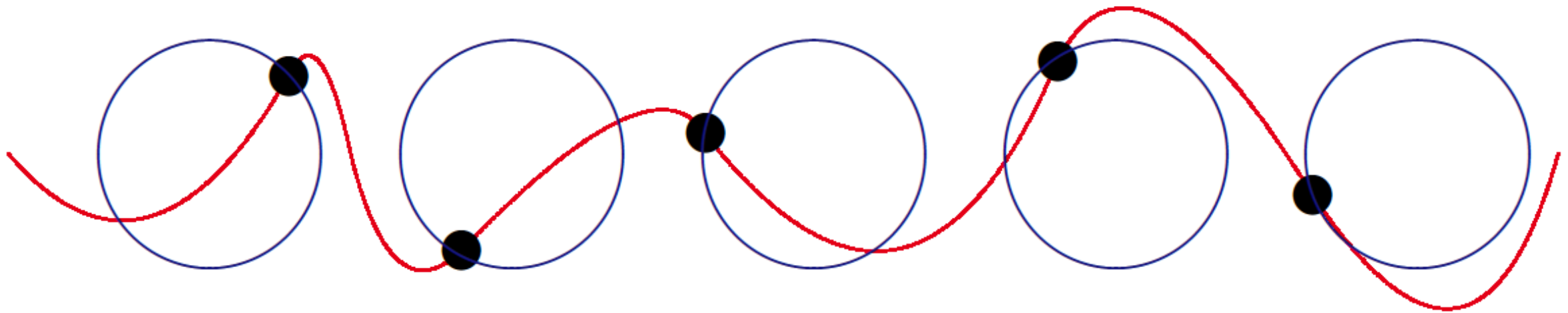
From Dhar and Lebowitz, PRL 2008

Small normal conductivity



From Oganesyan, Pal and Huse, PRB 2009

The rotor chain



$$H(\omega, \theta) = \sum_{x=1}^L \frac{\omega_x^2}{2} + g(1 - \cos(\theta_x - \theta_{x+1}))$$

For small g , ω_x are almost i.i.d. in the Gibbs state:
same phenomenology, cf. KAM, Nekhoroshev at finite L

III - Rigorous results

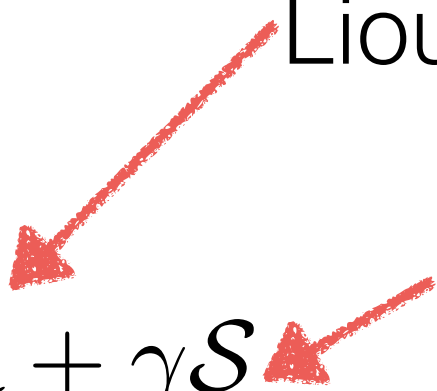
Difficulty and way out

Problem: We don't know whether $\kappa(T, \lambda) < +\infty$

Introduce some noise s.t.

- 1) Energy still conserved
- 2) Make G-K integral convergent
- 3) Not too large to keep Hamiltonian effects

E.g.: add velocity flip


$$\mathcal{L} = \mathcal{A} + \gamma \mathcal{S}$$

$$\mathcal{S}f(p, q) = \sum_x f(\dots, -p_x, \dots, q) - f(p, q)$$

Results

Chains like before:

$$H(p, q) = \sum_{x=1}^L \frac{p_x^2}{2m} + \frac{\omega_x^2 q_x^2}{2} + \lambda(q_x - q_{x+1})^4 \quad (\text{disordered})$$

$$H(\theta, \omega) = \sum_{x=1}^L \frac{\omega_x^2}{2} + \lambda(1 - \cos(\theta_x - \theta_{x+1})) \quad (\text{strongly anharmonic})$$

Theorem

$$\forall r \in \mathbb{N}, \exists C(r, T) \quad s.t. \quad \kappa(T, \lambda, \gamma) \leq C(r, T) \left(\frac{\lambda^{2r}}{\gamma} + \gamma \right)$$

Results

Taking $\gamma = \lambda^r$ we get

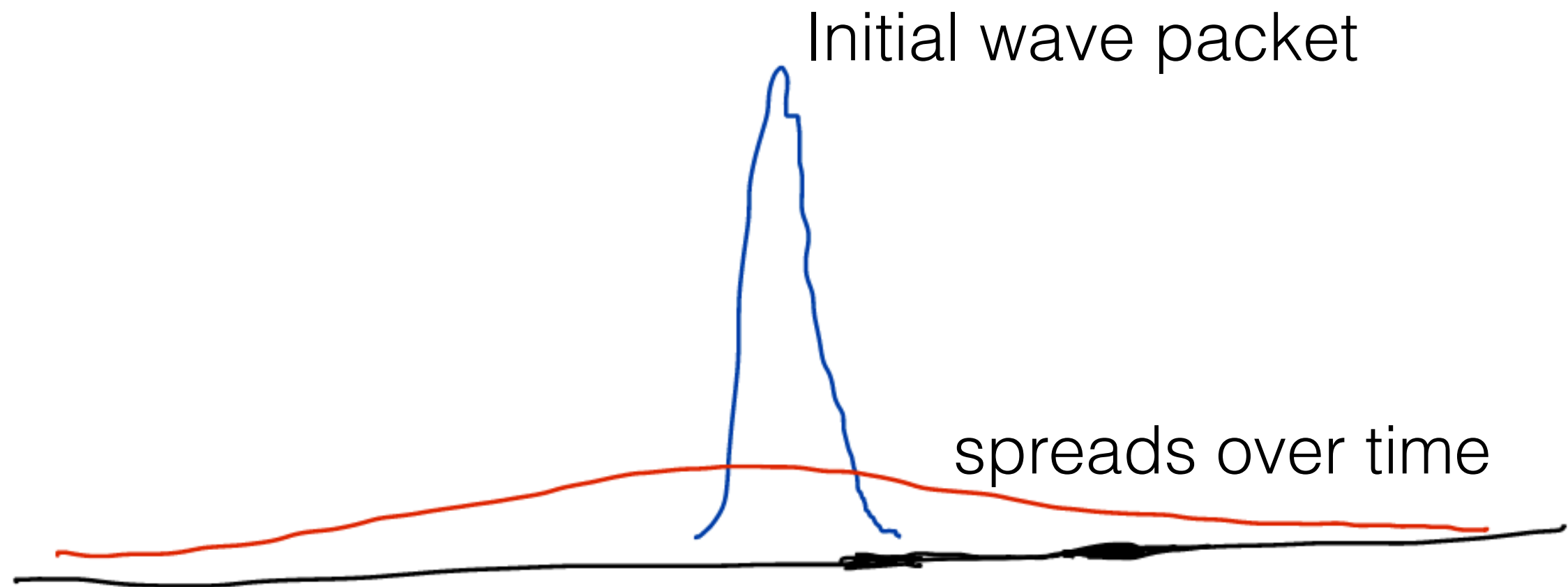
$$\kappa(T, \lambda, \lambda^r) \leq C(r, T) \lambda^r$$

From physics, we expect the noise to enhance transport, so we think

$$\kappa(T, \lambda, 0) \leq C(r, T) \lambda^r$$

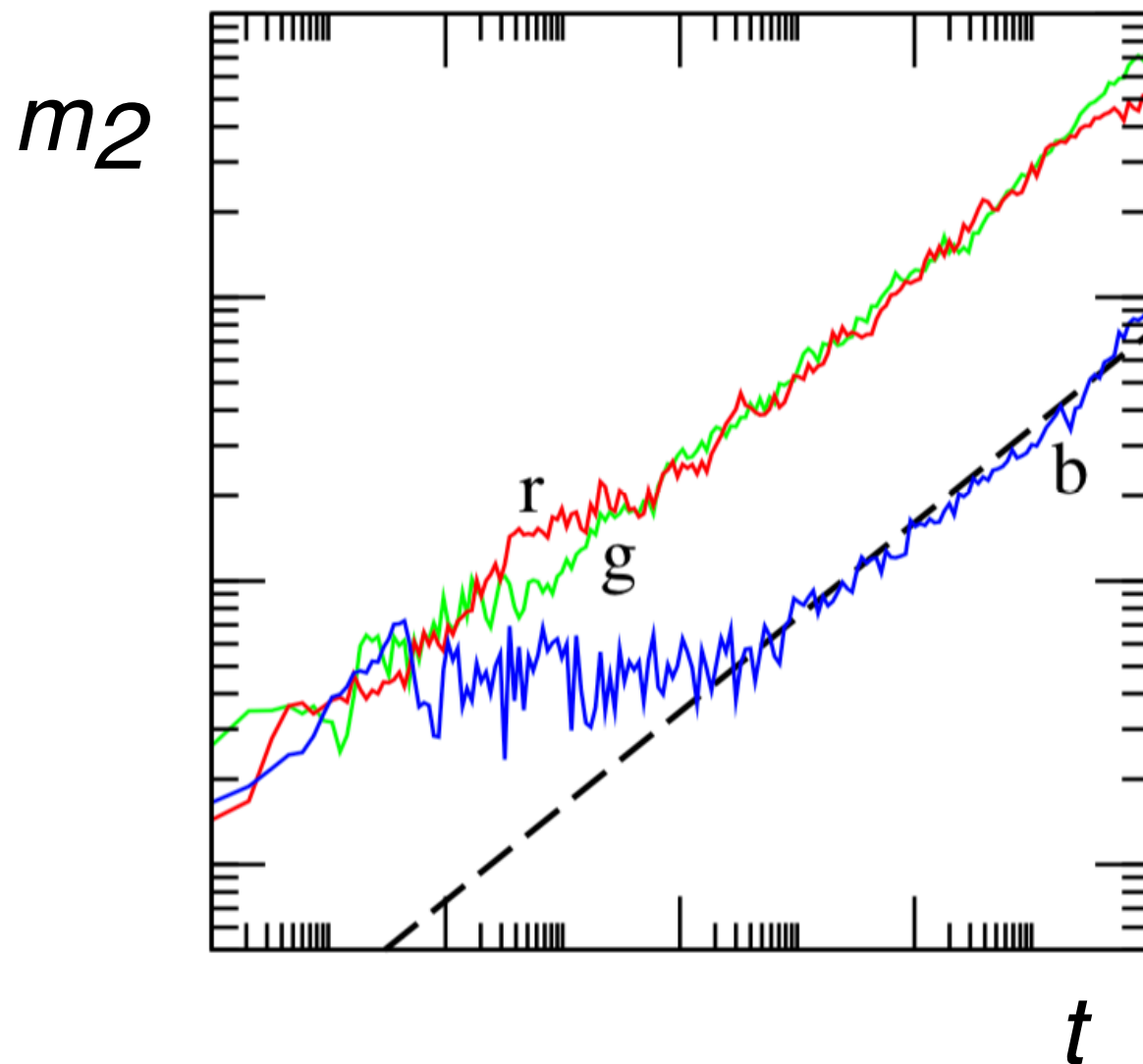
IV - Puzzles at $T=0$

Spreading at zero temperature



$$H(p, q) = \frac{1}{2} \sum_{1 \leq x \leq L} p_x^2 + \omega_x^2 q_x^2 + g(q_{x+1} - q_x)^2 + \lambda q_x^4$$

Spreading at zero temperature



..... $t^{1/3}$

$$m_2(t) = \sum_{x \in \mathbb{Z}} x^2 e_x(t)$$

From Flach, Krimer and Skokos, PRL 2009

This clashes with our result

We expect local equilibrium to set in, hence

$$\partial_t E = \partial_x \kappa(T, \lambda) \partial_x E, \quad T = T(E)$$

with $T(t, x) \rightarrow 0 \quad \forall x \quad as \quad t \rightarrow +\infty$

For this system:

$$\kappa(T, \lambda) = \overline{\kappa}(T\lambda)$$

i.e. low temperature = low effective anharmonic interactions

$m_2(t) \sim t^{1/3}$ only possible if $\overline{\kappa}(T\lambda)$ approach 0 **polynomially**

Way out?

Our theorem does not apply directly to this set-up

Wait longer? $\sqrt{m_2(t)} \sim t^{1/6}$ **very slow!**

(may explain the apparent stability of this regime)

Main idea:

describe numerically how $\kappa(\lambda T)$ behaves,
that this is consistent with the scaling of m_2 ,
that it must change by virtue of a theorem

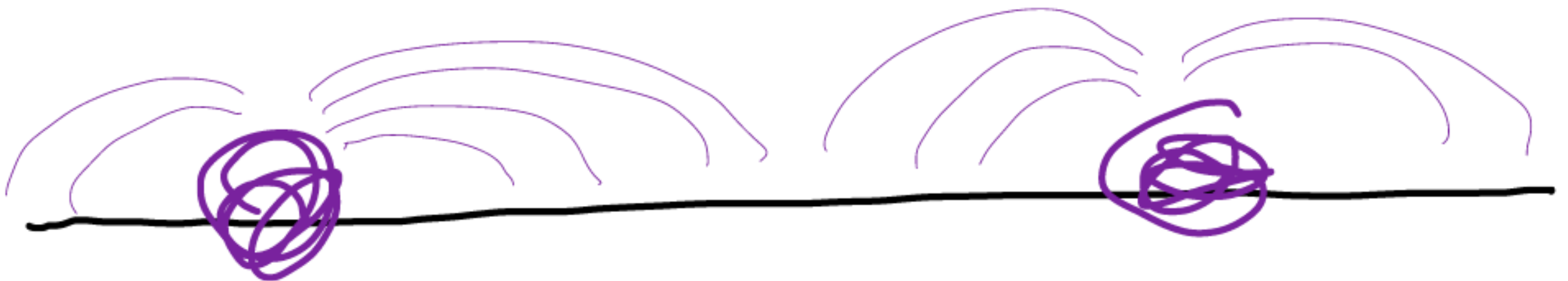
V - Many Body
Localization

Classical vs Quantum

For classical systems, why do we expect

$$\kappa(\lambda, T) > 0 \quad \text{for} \quad \lambda > 0 ?$$

Naive idea: a few oscillators can yield chaos:

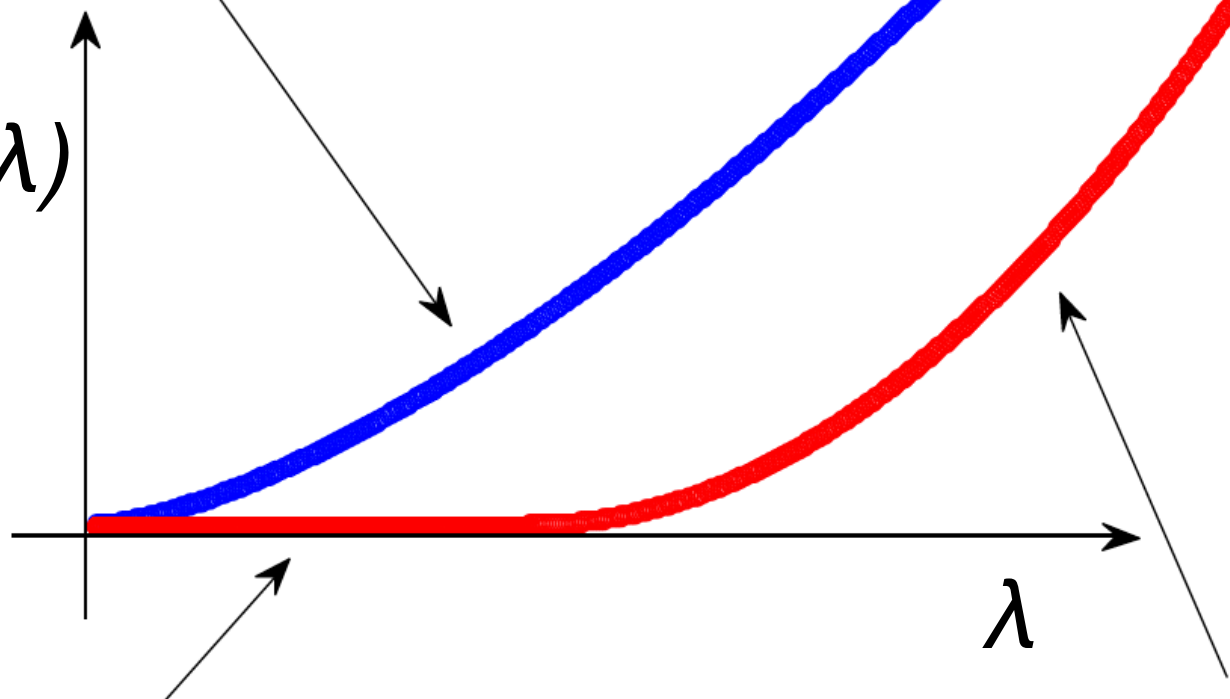


This does not need to be true for quantum systems!

Quantum vs Classical

Classical (conjecture)

$\kappa(\lambda)$



Quantum: localized (Imbrie and Spencer)

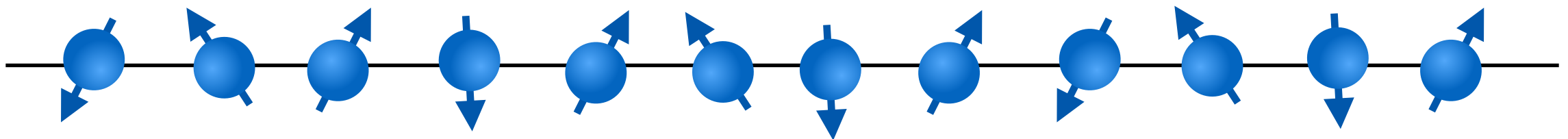
Quantum: delocalized phase (conjecture)

Many-body localized phase

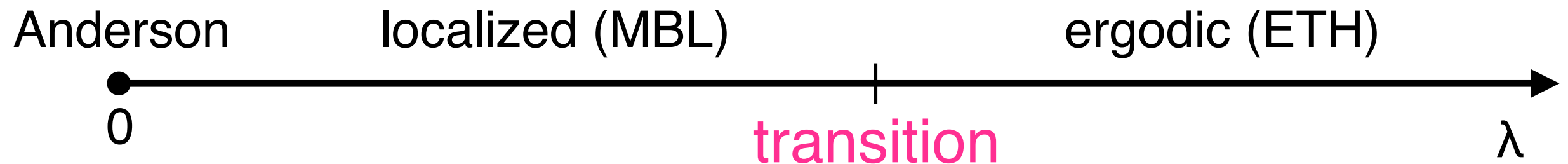
disordered quantum spin chain:

$$H = \sum_{i=1}^L h_i \sigma_i^{(z)} + J \sum_{i=1}^{L-1} \sigma_i^z \sigma_{i+1}^{(z)} + \lambda \sum_{x=1}^L \sigma_i^{(x)}$$

classical Ising model spin flip



Expected phase diagram



Localized means: eigenstates look still a bit like the eigenstates at $\lambda=0$:

2^L eigenstates of the classical Ising model:

$$| + + - + - + + \cdots + \rangle$$

Localized vs ergodic

Thermal: $\langle E | \sigma_0^{(z)} | E \rangle \sim \langle \sigma_0^{(z)} \rangle_{T(E)} \sim 0$

where ~ 0 holds at high temperature

Localized: $\langle E | \sigma_0^{(z)} | E \rangle \sim \pm 1 + \mathcal{O}(\lambda)$

This is like KAM: keeps memory of initial conditions forever

Green-Kubo formula

$T + \Delta T$

NESS

$T - \Delta T$

$$\langle J \rangle \sim \kappa(T) \cdot \frac{2 \Delta T}{L}$$

Physical limit:

$$\lim_{\Delta T \rightarrow 0} \lim_{L \rightarrow \infty} \frac{L \langle J \rangle}{2 \Delta T} = \kappa(T) \quad \text{Fourier}$$

Other limit:

$$\lim_{L \rightarrow \infty} \lim_{\Delta T \rightarrow 0} \frac{L \langle J \rangle}{2 \Delta T} = \underline{\kappa(T)}$$

$$(1) \quad (L-1) \langle J \rangle_{\text{NESS}} = \left\langle \sum_{x=1}^{L-1} j_{x, x+1} \right\rangle_{\text{NESS}} \\ = \underline{\langle J \rangle_{\text{NESS}}}$$

$$(2) \quad \Delta T = 0: \quad \underline{\langle \cdot \rangle_{\text{NESS}}} = \langle \cdot \rangle_T$$

$$\rho: \quad \langle f \rangle_{\text{NESS}} = \int f \cdot \rho \, dp \, dq$$

$$\rho = \rho_0 (1 + (\Delta T) \textcolor{red}{f} + \frac{(\Delta T)^2 f^2 + \dots}{\text{Forget}})$$

$$\rho_0 = \frac{1}{Z(\tau)} e^{-H/\tau}$$

(3) f ? ρ is invariant.

\mathcal{L} : generator

\mathcal{L}^+ : adjoint of \mathcal{L} w.r.t. ρ_0

$$\mathcal{L}^+ (1 + \Delta T f + O(\Delta T^2)) = 0$$

$$\mathcal{L} = \mathcal{L}_0 + \Delta T \mathcal{L}_1$$

$$\mathcal{L}_1 = \gamma \left(\frac{\partial^2}{\partial p_1^2} - \frac{\partial^2}{\partial p_L^2} \right)$$

$$(\mathcal{L}_0^+ + (\Delta T) \mathcal{L}_1^+) (1 + \Delta T f + O(\Delta T^2)) = 0$$

$$\mathcal{L}_0^+ 1 = 0 \quad \text{OK}$$

$$\mathcal{L}_0^+ f = -\mathcal{L}_1^+ 1$$

$$f = \underline{(-\mathcal{L}_0^+)^{-1} \mathcal{L}_1^+ 1}$$

$$4) \quad \frac{(L-1) \langle J \rangle_{\text{NESS}}}{2\Delta T} = \frac{\langle J \rangle_{\text{NESS}}}{2\Delta T}$$

$$\frac{dp}{dp_0} = \frac{\langle J \cdot (1 + \Delta T f + \underbrace{G(\Delta T^2)}) \rangle_T}{2\Delta T}$$

$$= \frac{\cancel{\langle J \rangle_T}}{\cancel{2\Delta T}} + \underbrace{\left(\frac{\langle J \cdot f \rangle_T}{2} \right)}_{\parallel} + \underbrace{G(\Delta T)}_{\rightarrow 0}$$

$\lim_{L \rightarrow \infty}$

$$K(T) = \frac{1}{2} \langle J \cdot (-Z_0^+) \underline{Z_1^{+1}} \rangle_T$$

$$(5) \quad Z_1^{+1} = \frac{1}{T^2} (\delta p_1^2 - \delta p_L^2)$$

$$= \frac{-1}{T^2} (j_{0,1} + j_{L,L+1})$$

$$K(T) = \frac{-1}{2T^2} \langle J_1 (-Z_0^+) \underline{(j_{0,1} + j_{L,L+1})} \rangle$$

(6) Energy conservation:

$$L_0 e_x = j_{x-1,x} - j_{x,x+1}$$

$\parallel \frac{d}{dt}$

$$\underline{L_0} (e_x + e_{x+1} + \dots + e_y) =$$

$$j_{x-1,x} - j_{y,y+1}$$

$$j_{0,1} = \frac{1}{L-1} \sum_{x=1}^{L-1} j_{x,x+1} + \underline{L_0^+ (e_1 + \dots + e_x)}$$

$$(7) \quad \langle J, \underbrace{(-L_0^+)^{-1} L_0^+}_{\substack{\parallel \\ p\phi(q)}} e_z \rangle_T$$

$$= \underbrace{\langle J, e_z \rangle_T}_{\parallel p^2} = 0$$

$$K(T) = \lim_{L \rightarrow \infty} \frac{1}{L-1} \frac{1}{T^2}$$

$$\langle J, (-L_0)^{-1} J \rangle$$

$$\tilde{J} = \frac{1}{\sqrt{L-1}} \sum_{x=1}^{L-1} j_{x,x+1}$$

$$\boxed{K(T) = \lim_{L \rightarrow \infty} \frac{1}{T^2} \langle J, (-L_0)^{-1} J \rangle}$$

$$8) \quad (-L_0)^{-1} = \int_0^\infty dt e^{t \underline{L_0}}$$

$$L_0 \uparrow = 0$$

$$\lambda \in \sigma(L_0), \operatorname{Re}(\lambda) \leq 2$$

$$\Rightarrow \kappa(T) = \lim_{L \rightarrow \infty} \frac{1}{T^2} \int_0^{\infty} dt \langle \tilde{J}, e^{t\mathcal{L}_0} \tilde{J} \rangle_T$$

$$= \lim_{L \rightarrow \infty} \frac{1}{T^2} \int_0^{\infty} dt \mathbb{E}_T (\tilde{J}(0) \tilde{J}(t))$$

$$= \lim_{L \rightarrow \infty} \left[\lim_{t \rightarrow \infty} \frac{1}{T^2} \mathbb{E}_T \left(\left(\frac{1}{\sqrt{t}} \int_0^t ds \tilde{J}(s) \right)^2 \right) \right]$$