Sharp spectral gap for disordered and regular chain of oscillators

Joint work with S. Becker (Courant Institute)

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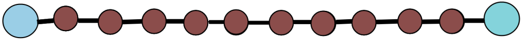
- Main interest: heat conduction models of atom chains
- Motivation: Hilbert's 6th problem, deriving macroscopic physical phenomena
- Fourier's law: $J(t,x) = -\kappa(T)\nabla T(t,x)$, κ: the conductivity
- Let N be the microscopic length of the system



- Assume system reaches a steady state μ - *Non-equilibrium steady state*
- Want $\kappa_N := \frac{\langle J_N \rangle_\mu}{((T_1 - T_2)/N)} \to \kappa \in (0, \infty)$.

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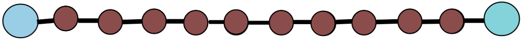

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Need to know:

- Properties of the steady state: Existence, Uniqueness, how fast we approach it
- Quantifying key quantities in terms of N

Model Description

Consider a model for heat conduction that consists of a 1-dimensional chain of N coupled oscillators in *phase space* $(p, q) \in \mathbb{R}^{2N}$ with Hamiltonian:

$$H(p,q) = \underbrace{\frac{1}{2}\sum_{i=1}^{N} p_i^2}_{\text{kinetic energy}} + \underbrace{\sum_{i=1}^{N} U_{pin}(q_i) + \sum_{i=1}^{N-1} U_{inter}(q_{i+1} - q_i)}_{\text{potential energy}}.$$

U_{pin}: pinning potential, U_{inter}: each one interacts with its neighbours.

- The two ends of the chain are in contact with heat baths at two temperatures T_1, T_2. The coupling reservoirs-chain: *Langevin* processes.

Model Description

Our system:

$$
\begin{aligned}
dq_i(t) &= p_i(t)dt \quad \text{for} \quad i = 1, \dots, N, \\
dp_i(t) &= (-\partial_{q_i} H)dt \quad \text{for} \quad i = 2, \dots, N-1, \\
dp_i(t) &= (-\partial_{q_i} H - \underbrace{\gamma_i p_i)dt}_{\text{friction term}} + \underbrace{\sqrt{2\gamma_i T_i} dW_i(t)}_{\text{stochastic term}} \quad \text{for} \quad i = 1, N.
\end{aligned}
\tag{1}
$$

- $z_t = (p_t, q_t)$ Markov process with generator

$$
\mathcal{L} = \sum_{i=1}^{N} (p_i \partial_{q_i} - \partial_{q_i} H \partial_{p_i}) - \gamma_1 p_1 \partial_{p_1} - \gamma_N p_N \partial_{p_N} + \gamma_1 T_1 \partial^2_{p_1} + \gamma_N T_N \partial^2_{p_N}.
$$

Set Up and assumptions

Note that this operator is

- not self-adjoint
- not elliptic (in fact hypoelliptic)
- not coercive (hypocoercive)
- the invariant measure does not have an explicit formula

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We restrict to the case when both potentials are quadratic (harmonic chain): $U_{pin}(q) = aq^2/2$, $U_{int}(q_i - q_j) = c(q_i - q_j)^2/2$.

- Generator is: $\mathcal{L}f(z) = -\langle z, M\nabla_z f\rangle + \langle \nabla_p, \mathcal{F}\Theta\nabla_p f\rangle$ where

$$M = \begin{bmatrix} \mathcal{F} & -I \\ B & 0 \end{bmatrix}, \mathcal{F} = \mathrm{diag}(\gamma_1, 0, \dots, 0, \gamma_N), \Theta = \mathrm{diag}(T_1, 0, \dots, 0, T_N).$$

$$B = -c\Delta^N + \sum_{i=1}^{N} a_i \delta_i$$

Set Up and assumptions

About the boundary conditions:

- Either *fixed* boundaries - edges attached to a wall: $q_0 = q_{N+1} = 0$ (Dirichlet b.c.)
- Or *free* boundaries: $q_0 = q_1, q_N = q_{N+1}$ (Neumann b.c.)

• Aim: We show that the spectral gap of $\mathcal{L}$ is determined by the decay rate of the eigenstates of B for 3 different scenarios:

- Homogeneous chain
- Chain with a sufficiently strong impurity in the pinning potential of one particle - Schrödinger operator possesses both localised and extended states
- Chain with disordered pinning potential - Schrödinger operator has only exponential localised e-states in $d = 1$

Main Theorems (Becker-M. '21)

Spectral gap λ_N for **Homogeneous Networks**

- For the 1-dimensional oscillators chain: $N^{-3} \lesssim \lambda_N \lesssim N^{-3}$.
- If the friction/diffusion act on two particles located at the corners: $\lambda_N \lesssim N^{-3d}$.
- If the friction/diffusion act on two particles located at the center of two opposite edges of the network: $\lambda_N \lesssim N^{-3-(d-1)}$.

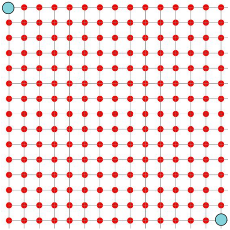


Figure: Spectral gap $\mathcal{O}(N^{-6})$.

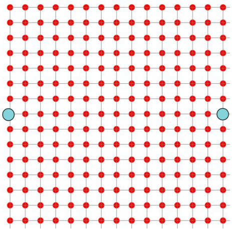


Figure: Spectral gap $\mathcal{O}(N^{-4})$.

Spectral gap for Non-Homogeneous Networks

- **Chain with impurity:** If the pinning strength $a_{c_d(N)} + 2d + \varepsilon \leq a_i$ at the center of the network, then $\lambda_N \leq \mathcal{O}(Ce^{-cN})$ for all $d \geq 1$.
- **Disordered chain:** If the pinning strengths are iid random variables according to some compactly supported density $\rho \in C_c(0, \infty)$, then $\lambda_N \leq \mathcal{O}(Ce^{-cN})$ for all $d \geq 1$.

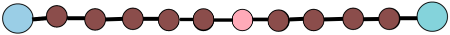


Figure: Chain with impurity: Spectral gap $\leq \mathcal{O}(e^{-cN})$.

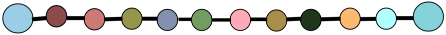


Figure: Disordered chain: Spectral gap $\leq \mathcal{O}(e^{-cN})$.

Longer range interactions

- What happens for longer-range interactions? Consider *Next-to-nearest-neighbor interactions* so that

$$V(q) = \sum_{i=1}^{N-1} \frac{(q_i - q_{i-1})^2}{2} + \omega \sum_{i=1}^{N-2} \frac{(q_i - q_{i-2})^2}{2}$$

and the quadratic form associated with this potential is

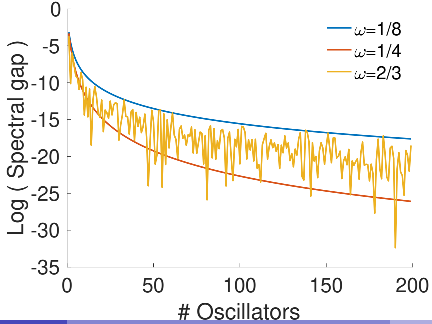
$$\Gamma = (1+4\omega)\Delta^N - \omega(\Delta^N)^2 + \omega \,\mathrm{diag}(L, 0, \ldots, 0, L)$$

• There is a critical value for $\omega = \frac{1}{4}$ where the gap exhibits different behaviours.

Theorem (Becker-M. '22)

Under Dirichlet b.c.:

- *There is an explicit countable dense subset of* $\{|\omega| > \frac{1}{4}\}$, *so that for* $N = N(\omega)$, *the generator of the* $N(\omega)$*-sized chain is not hypoelliptic.*
- *When* $\omega = \frac{1}{4}$, $N^{-4-\epsilon} \lesssim |\lambda_N| \lesssim N^{-4+\epsilon}$ *for every* $\epsilon > 0$, *i.e. the spectral gap* $\Re(\mu(N))$ *is upper bounded by* $N^{-4+\epsilon}$.
- *When* $\omega < \frac{1}{4}$, $N^{-3} \lesssim |\lambda_N| \lesssim N^{-3}$.



Merci de votre attention!!