Thermal Conductivity of the Toda Chain

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Heat Conduction

- Fourier's law of heat conduction $\mathbf{J}(\mathbf{x}, t) = -\kappa \nabla T(\mathbf{x}, t)$.
- For a 1–D finite system of length N in contact with two thermostats at temperatures $T_L \neq T_R$ with $\Delta T = T_L - T_R$

$$J_N = \kappa_N \frac{\Delta T}{N}$$

  where $\kappa_N = f(N, T_L, T_R)$ is the thermal conductivity.
- If $\lim\limits_{N\to\infty} \lim\limits_{\Delta T\to 0} \kappa_N = \kappa < \infty \Rightarrow$ Fourier's law
- Anomalous conductivity : $\kappa \sim N^{\alpha}$ with $\alpha > 0$
- We study the behavior of κ_N in a Toda chain subjected to a stochastic perturbation. In particular, we are interested in the dependence of α on the intensity of the stochastic perturbation.

Tools

Two main approaches

- non-equilibrium molecular dynamics with fixed temperatures at the boundaries
  - stochastic thermostats (Langevin, Maxwell)
  - deterministic thermostats (Nosé-Hoover)
- equilibrium method based on the following Green-Kubo formula

$$\kappa(N,T) = \frac{1}{NT^2}\int_0^\infty \langle J(0)J(t)\rangle dt$$

Both approaches are theoretically equivalent when $\kappa(N,T) < \infty$.

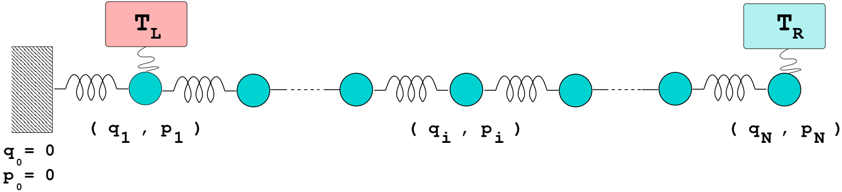
Previous Results

- Fourier's law is generally valid for 3-D systems, but this is not always the case in lower dimensions.
- Roughly speaking, we have normal transport in 1-D systems only in presence of stochastic perturbations destroying the conservation of (total) momentum and energy.
- In all other low-dimensional cases transport is anomalous.
- In particular for the Toda chain we have

$\kappa \sim N$	unperturbed case [a]
$0 \leq \kappa \leq C\sqrt{N}$	stochastically perturbed case [b]

[a] Zotos (2002)
[b] Basile *et al.*(2009)

Model Description



- $\{(q_i, p_i), i = 1, \ldots, N\} \in \mathbb{R}^{2N}$ (q_i displacement with respect to equilibrium and p_i momentum of the i-th oscillator)
- equal unit masses, first particle attached to a wall ($q_0 = 0$, $p_0 = 0$)
- $\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N} V(q_i - q_{i-1})$ with $V(r) = \frac{e^{-br} + br - 1}{b^2}$ and $b > 0$
- the Hamiltonian system is *completely integrable* [c]

[c] Hénon (1974)

Evolution equations

- Hamiltonian dynamics in the bulk, Langevin dynamics at the boundaries ($V'(q_{N+1} - q_N) = 0$)

$$
\begin{cases}
dq_i = p_i \, dt \\
dp_i = \Big(V'(q_{i+1} - q_i) - V'(q_i - q_{i-1}) \Big) dt \\
\qquad + \delta_{i,1} \Big(-\xi p_1 \, dt + \sqrt{2\xi T_{\mathrm{L}}} \, dW_{1,t} \Big) \\
\qquad + \delta_{i,N} \Big(-\xi p_N \, dt + \sqrt{2\xi T_{\mathrm{R}}} \, dW_{N,t} \Big)
\end{cases}
\qquad \forall i \in [1, N]
$$

- $T_L = T_R = T_{\mathrm{eq}} \Rightarrow$ invariant measure $\dfrac{e^{-\mathcal{H}/T_{\mathrm{eq}}} dq_1 \dots dq_N dp_1 \dots dp_N}{\mathcal{Z}}$
- If $T_L \neq T_R$ one can prove the existence and uniqueness of an invariant measure under some specific assumptions on the potential

Stochastic Perturbation

- Conservative noise: at times $t_i \overset{\text{iid}}{\sim} \text{Exp}(\gamma^{-1})$ *exchanges of momenta* between nearest neighbor atoms [d]
- Locally for $i = 2\ldots, N-1$

$$d\mathcal{E}_i(t) = dJ_{i-1,i}(t) - dJ_{i,i+1}(t)$$

where the local energy is

$$\mathcal{E}_i = \frac{p_i^2}{2} + \frac{1}{2}\Big(V(q_i - q_{i-1}) + V(q_{i+1} - q_i)\Big)$$

and the local current is

$$J_{i,i+1}(t) = \int_0^t \left(j_{i,i+1}^{\mathrm{ham}}(s) + \gamma\, j_{i,i+1}^{\mathrm{sto}}(s)\right) ds + M_{i,i+1}^{\gamma}(t)\,. \qquad (1)$$

with

$$j_{i,i+1}^{\mathrm{ham}} = -\frac{1}{2}(p_i + p_{i+1})V'(q_{i+1} - q_i), \qquad j_{i,i+1}^{\mathrm{sto}} = \frac{1}{2}\left(p_i^2 - p_{i+1}^2\right)$$

[d] Basile, Bernardin, Olla (2006) & (2009)

Thermal Conductivity

- Because of energy conservation, the expectation of the local current with respect to the stationary (unknown) measure is

$$\left\langle J_{i,i+1}(t) \right\rangle = t \left\langle j^{\mathrm{ham}}_{i,i+1} + \gamma j^{\mathrm{sto}}_{i,i+1} \right\rangle =: tJ^i_N \equiv tJ_N$$

- Computing the spatial mean of $\left\langle j^{\mathrm{ham}}_{i,i+1} + \gamma j^{\mathrm{sto}}_{i,i+1} \right\rangle$

$$J_N = \frac{1}{N-1} \sum_{i=1}^{N-1} \left\langle j^{\mathrm{ham}}_{i,i+1} \right\rangle + \frac{\gamma}{2} \frac{\left\langle p_1^2 \right\rangle - \left\langle p_N^2 \right\rangle}{N-1} = J_N^{\mathrm{ham}} + J_N^{\mathrm{sto}}. \quad (2)$$

- since $\kappa_N(T) = \lim_{\substack{T_L - T_R \to 0 \\ T_R \to T}} \dfrac{NJ_N}{T_L - T_R} = \kappa_N^{\mathrm{ham}}(T) + \kappa_N^{\mathrm{sto}}(T)$

$\Rightarrow$ $\kappa_N^{\mathrm{sto}}(T)$ bounded $\Rightarrow$ divergence relies only on $\kappa_N^{\mathrm{ham}}(T)$

Numerical Simulations: Integration Scheme (1)

We split the dynamics in two parts: Langevin dynamics + noise.

For the implementation of noise, we attach to each spring a clock τ_i^m, $i = 2, \dots, N-1$, and apply the following algorithm at each iteration $t_m = m\Delta t$

$m = 0$ draw $\tau_i^0 \overset{\text{iid}}{\sim} \mathcal{E}(\gamma^{-1})$

$m \geq 1$ $(\forall\, i = 2, \dots, N-1)$

if $\tau_i^m < \Delta t \;\Rightarrow$ exchange p_i and p_{i+1} and redraw $\tau_i^{m+1} \sim \mathcal{E}(\gamma^{-1})$

otherwise $\Rightarrow \;\tau_i^{m+1} = \tau_i^m - \Delta t$

Numerical Simulations: Integration Scheme (2)

Langevin dynamics: BBK scheme [e]

$$
\left\{
\begin{array}{rcl}
p_i^{m+1/2} & = & p_i^m - \dfrac{\Delta t}{2}\nabla_{q_i} V(q^m) + \delta_{i,1}\left(-\dfrac{\Delta t}{2}\xi p_1^m + \sqrt{\dfrac{\xi \Delta t}{2}\, T_l}\; G_1^m\right) \\
 & & +\delta_{i,N}\left(-\dfrac{\Delta t}{2}\xi p_N^m + \sqrt{\dfrac{\xi \Delta t}{2}\, T_r}\; G_N^m\right), \\
q_i^{m+1} & = & q_i^m + \Delta t\, p_i^{m+1/2}, \\
p_i^{m+1} & = & p_i^{m+1/2} - \dfrac{\Delta t}{2}\nabla_{q_i} V(q^{m+1}) + \delta_{i,1}\left(-\dfrac{\Delta t}{2}\xi p_1^{m+1} + \sqrt{\dfrac{\xi \Delta t}{2}\, T_l}\; G_1^m\right) \\
 & & +\delta_{i,N}\left(-\dfrac{\Delta t}{2}\xi p_N^{m+1} + \sqrt{\dfrac{\xi \Delta t}{2}\, T_r}\; G_N^m\right),
\end{array}
\right. \tag{3}
$$

where $G_k^m \overset{\text{iid}}{\sim} \mathcal{N}(0,1),\ k = 1, N$

[e] Brünger, Brooks, Karplus (1984)

Numerical Simulations: Implementation

Choice of the parameters and initial conditions:

- all simulations performed with $\underline{T_L = 1.05}$ and $\underline{T_R = 0.95}$
- $\underline{N = 2^7 \div 2^{17}}$, $\underline{\gamma \in \{10^{-3}, 10^{-2}, 10^{-1}, 1\}}$
- coupling with the thermostats: $\underline{\xi = 1}$ and $\underline{\xi = 0.1}$
- Toda potential: $\underline{b = 1}$ and $\underline{b = 10}$
- linear temperature profile imposed as initial condition by attaching each oscillator to a Langevin thermostat at a temperature $T_i = \frac{N-i}{N-1} T_L + \frac{i-1}{N-1} T_R$

Estimation of α on $T_{\mathrm{sim}} = M\Delta t$ (with $10^6 \leq M \leq 5 \times 10^7$) by

$$\overline{j_N(t_m)} = \frac{1}{N-2} \sum_{i=1}^{N-2} j_{i,i+1}^{\mathrm{ham},m} =: \overline{j_N^m}$$

$$\Downarrow$$

$$\widehat{J}_N^M = \frac{1}{M} \sum_{m=1}^{M} \overline{j_N^m}$$

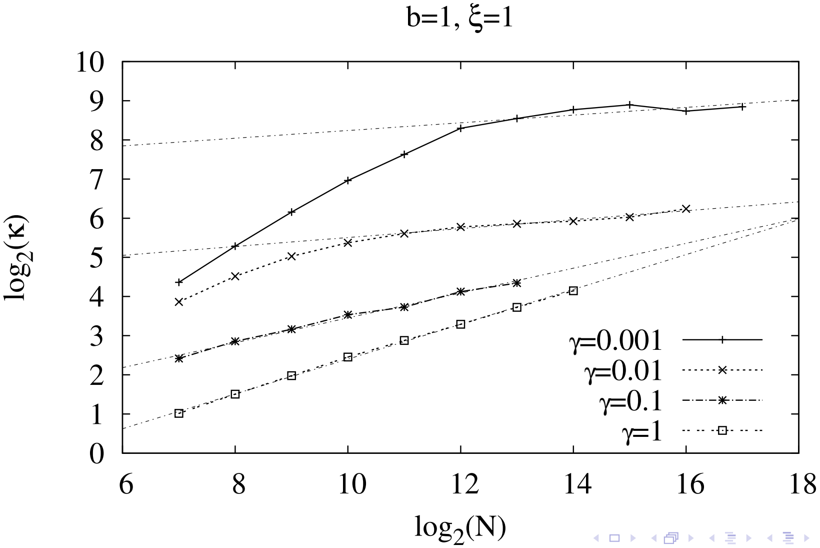
$$\Downarrow$$

$$\widehat{\kappa}_N^M = \frac{N \widehat{J}_N^M}{T_L - T_R} \sim N^{\alpha}$$

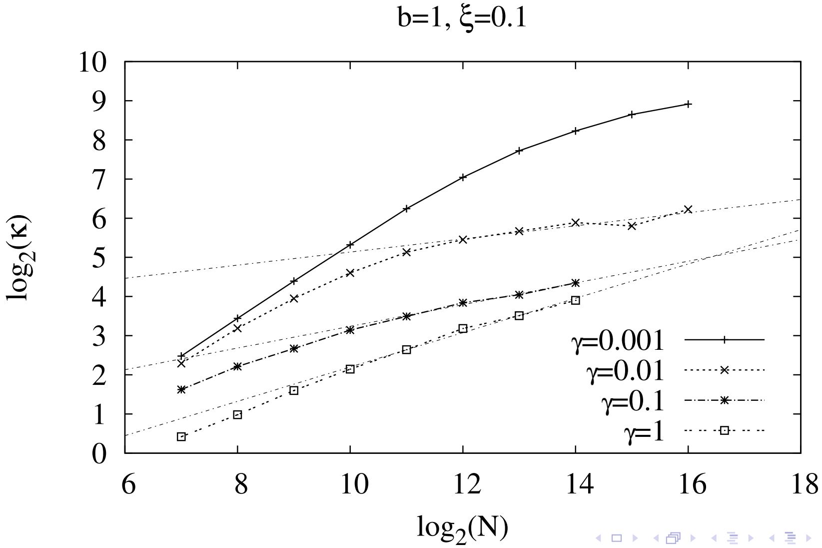
$$\Downarrow$$

$$\ln_2 \kappa_N^M = \alpha \ln_2 N + cost. \qquad [\text{linear fit}]$$

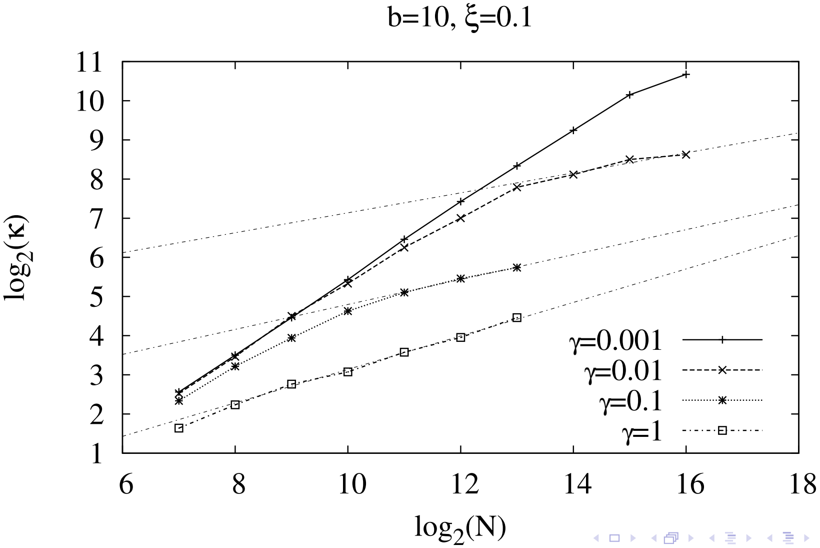
Numerical Results: Case $b = 1$, $\xi = 1$



Numerical Results: Case $b = 1$, $\xi = 0.1$



Numerical Results: Case $b = 10$, $\xi = 1$



Numerical Results: Linear Fit

A least square fit of the log-log diagram gives

γ	α $(b = 1,\ \xi = 1)$	α $(b = 1,\ \xi = 0.1)$	α $(b = 10,\ \xi = 0.1)$
0.001	0.10	–	–
0.01	0.11	0.17	0.25
0.1	0.32	0.30	0.32
1	0.44	0.44	0.43

Concluding Remarks

Our findings:

- ballistic transport broken as soon as $\gamma \neq 0$
- $\alpha \leq 0.5$ in accordance with the theoretical upper bound
- $\alpha \approx 0.5$ for $\gamma = 1$ in any parameter configuration (stochastic dynamics prevails)
- no universal α value
- for a fixed parameter configuration, α depends on γ in a monotonically increasing way