Thermal transport in one-dimensional chains

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Transport phenomena

Transport phenomena are characterized by the general macroscopic relation

$$J = -\alpha \nabla \phi$$

$\nabla\phi$: forcing acting on the system
(ϕ = temperature, electrical potential, concentration)

J : response of the system
(current of energy, momentum, particle/mass)

α : transport coefficient
(thermal conductivity, mobility, viscosity)

Remarks:

1. The presence of currents characterizes out-of-equilibrium systems.
2. For small $|\nabla\phi|$, α can be considered constant.
3. From now on $\phi = T$ and dimension 1

Outline

- Transport properties for small $|\nabla T|$
  – the computation of the thermal conductivity in a 1-D system, the example of the Toda chain
- Properties of a system far from equilibrium
  – the case of the forced rotor chain
- Macroscopic diffusion in the forced rotor chain (work in progress)

Transport properties in the linear regime

Heat transport in one-dimension

Fourier's law

$$\mathbf{J}(\mathbf{x},t) = -\kappa \nabla T(\mathbf{x},t) \quad \xrightarrow{\text{1-D}} \quad J_L = -\kappa_L \frac{\Delta T}{L}, \quad L = \text{sys. length}$$

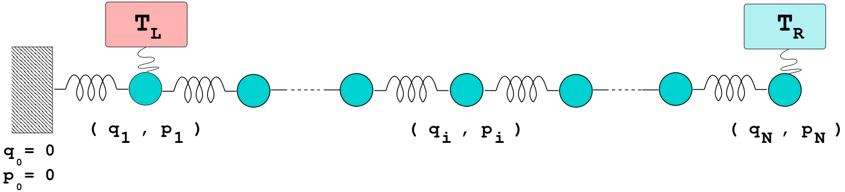
where k, κ_L are the thermal conductivities.

- Validity of Fourier's law : $\lim_{L\to\infty} \lim_{\Delta T\to 0} \kappa_L = \kappa < \infty$
- Anomalous conductivity: $\kappa_L \sim L^\alpha$, with $\alpha > 0$

Models: atom chains. Simple, but still complicated to study:

- issues with analytical approaches
  - nonlinear interactions
  - very degenerate noise
  - invariant measure unknown
- issues with numerical approaches
  - computational constraint (time step, finite comp. time, sys. size, ...)
  - large relative error (large systems $\Rightarrow$ small currents)

Microscopic model



- $\{(q_i, p_i), i = 1, \ldots, N\} \in \mathbb{R}^{2N}$, $r_i = q_i - q_{i-1}$
- unitary masses
- first particle attached to a wall ($q_0 = 0$, $p_0 = 0$), free/fixed BC on the right-end
- $\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N} U(q_i - q_{i-1})$ where $U(r)$ models the interaction
- $T_L = T_R = T \Rightarrow$ equilibrium with $\mu(\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}) = \mathrm{e}^{-\mathcal{H}/T}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{p}$

The system dynamics

Hamiltonian dynamics in the bulk, Langevin dynamics at the boundaries

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

→ $\xi > 0$ controls the coupling with the thermostats

→ Existence and uniqueness of the invariant measure can be proved for a certain class of $U \in C^{\infty}$ (1)

(1) Carmona (2007), Rey-Bellet (2006).

Computation of transport coefficients : two main approaches

Denoting by $J_N(q_t, p_t) = \sum_{i=1}^{N-1} j_i(q_t, p_t)/(N-1)$ the total average instantaneous current

Non-equilibrium computation for $\Delta T \ll 1$ (linear response regime)

$$\kappa_{N,\Delta T} = \frac{N}{\Delta T} \lim_{t \to +\infty} \frac{1}{t} \int_0^t J_N(q_s, p_s) \, \mathrm{d}s$$

Equilibrium computation based on the Green-Kubo formula

$$\kappa_{N,T}^{\mathrm{GK}} = \frac{(N-1)^2}{T^2} \int_0^\infty \mathbb{E}_{\mu_T} \Big(J_N(q_0, p_0) J_N(q_t, p_t) \Big) dt, \qquad \mu_T \propto \mathrm{e}^{-\mathcal{H}/T}$$

Both approaches are theoretically equivalent (if both $\kappa_{N,\Delta T}$ and $\kappa_{N,T}^{\mathrm{GK}}$ are finite).

Computing $\kappa_{N,\Delta T}$ (1/2)

- Approximation: $(q^m, p^m) \approx (q_{m\Delta t}, p_{m\Delta t})$

- Integration scheme: analytic integration of the fluctuation-dissipation part

  + Strang splitting with Verlet scheme [(2)] for the Hamiltonian part

- Currents computation at iteration m : $(r_i = q_i - q_{i-1})$

  energy on site i : $$\varepsilon_i = \frac{p_i^2}{2} + \frac{1}{2}\Big(U(r_i) - U(r_{i+1})\Big)$$

  local energy conservation : $$\frac{\mathrm{d}\varepsilon_i}{\mathrm{d}t} = j_{i-1,i} - j_{i,i+1}$$

  instantaneaous energy current : $$j_{i,i+1} = -\frac{1}{2}(p_i + p_{i+1})U'(r_{i+1})$$

  total average instantaneous current : $$J_N = \frac{1}{N-1}\sum_{i=1}^{N-1} j_{i,i+1}$$

(2) Verlet (1967)

Computing $\kappa_{N,\Delta T}$ (2/2)

- Thermal conductivity : Computed by empirical average on M iterations

$$\widehat{\kappa}_{n,\Delta T} = \frac{1}{\Delta T}\left(\frac{1}{M+1}\sum_{0}^{M} J_N^m\right)$$

- Statistical error

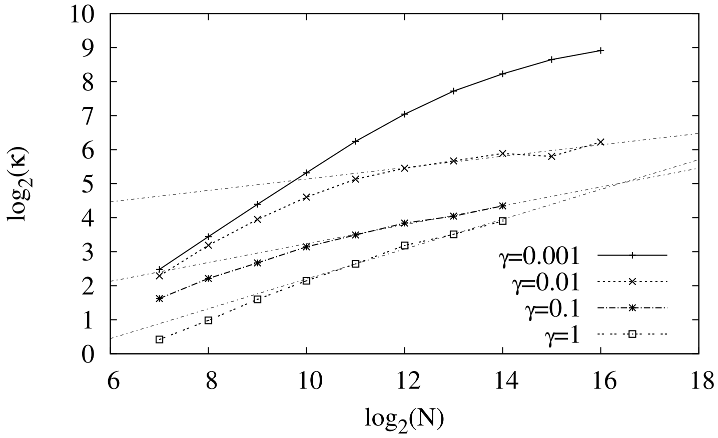
$$\kappa_{N,\Delta T} \simeq \kappa + \mathcal{O}\left(\frac{1}{\sqrt{(M\Delta t)}\,\Delta T}\right)$$

This means that $M\Delta t = \mathcal{O}((\Delta T)^{-2})$ and I have to keep $\Delta T \ll 1$ to remain in the linear response regime. . .

Example : $\kappa_{N,\Delta T}$ for the Toda chain

$$U(r) = \frac{e^{-br} + br - 1}{b^2} \text{ with } b > 0 + \text{stochastic perturbation of intensity } \gamma$$

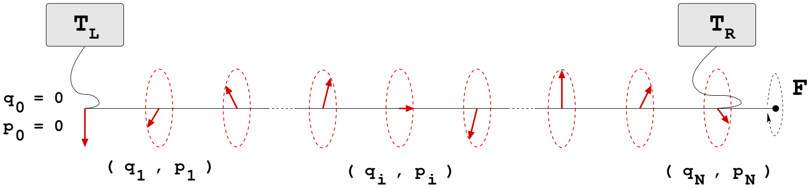
b=1, ξ=0.1



Out of the linear response regime

The rotor model [3]

N interacting rotors + temperature gradient + constant force.



- $q_i \in 2\pi\mathbb{T}$, $p_i \in \mathbb{R}$ with $i = 0, \dots, N$
- $r_i = q_i - q_{i-1}$, for $i = 2, \dots, N$, $r_1 = q_1$
- equal unitary masses
- first rotor attached to a wall ($q_0 = 0$, $p_0 = 0$), free BC on the last rotor
- $\mathcal{H} = \sum_{i=1}^{N} \left[\frac{p_i^2}{2} + U(q_i - q_{i-1}) \right]$ with $U(r) = 1 - \cos r$

(3) Iacobucci, Legoll, Olla, Stoltz (2011).

The system dynamics

Hamiltonian dynamics in the bulk, Langevin dynamics at the boundaries and mechanical forcing at the right end ($U'(q_{N+1} - q_N) = 0$))

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

- Average stationary energy current

energy on site i : $\varepsilon_i = \frac{p_i^2}{2m} + \frac{1}{2}\Big(U(q_i - q_{i-1}) - U(q_{i+1} - q_i) \Big)$

local energy conservation : $\frac{\mathrm{d}\varepsilon_i}{\mathrm{d}t} = j_{i-1,i} - j_{i,i+1}$

instantaneous energy current : $j_{i,i+1} = -\frac{1}{2}(p_i + p_{i+1}) U'(q_{i+1} - q_i)$

total average current : $J_N = \frac{1}{N-1} \sum_{i=1}^{N-1} \langle j_{i,i+1} \rangle$

About the system

$F = 0 \quad T_L = T_R = T_{eq}$ → equilibrium ⇒ stationary Gibbs measure with $\beta = T_{eq}^{-1}$

$T_L \neq T_R$ → finite thermal conductivity [4]

$F \neq 0 \quad T_L = T_R = \overline{T}$ → **out of equilibrium**

→ the stationary measure not explicitly known; existence proved [5] only for $N \leq 4$

→ highly non-linear temperature profiles

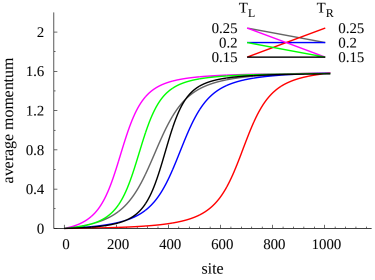
$F \neq 0 \quad T_L \neq T_R$ → forcing mechanisms not necessarily additive

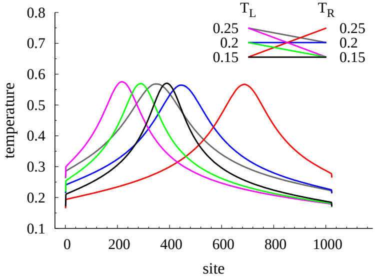
[4] Giardiná, Livi, Politi, Vassalli (2000), Gendelman and Savin (2000,2005), Yang and Hu (2005), Das and Dhar, arXiv:1411.5247 (2014).

[5] Cuneo, Eckmann & Poquet (2015); Cuneo & Eckmann (2016); Cuneo & Poquet (2017)

Highly non-monotonic "temperature" and momentum profiles

$T^{\mathrm{loc}}_{i,\mathrm{kin}} := \overline{(p_i^2)} - (\overline{p_i})^2$. Profiles for $N = 1024$, $F = 1.6$.





The macroscopic diffusion model

Macroscopic description of the model (work in progress)

Total energy and total momentum are conserved by the dynamics.

We introduce

- → $e(x,t)$ and $p(x,t)$, $t \in \mathbb{R}^+$ and $x \in [0,1]$, and $\beta(x,t) = T^{-1}(x,t)$
- → $u(x,t)$ internal energy. It holds (by thermodynamics)

$$u(x,t) = e(x,t) - \frac{p(x,t)^2}{2}$$

and at fixed (x,t), by thermodynamics

$$u(\beta) = \left(1 - \frac{I_1(\beta)}{I_0(\beta)}\right) + (2\beta)^{-1} \qquad \Rightarrow \qquad \beta(u)$$

where I_0, I_1 are modified Bessel function of the first kind

- → We thus obtain $T(x,t)$.

Evolution

- It can be shown that $e(x,t)$ and $p(x,t)$ evolve following

$$\partial_t \begin{pmatrix} p \\ e \end{pmatrix} = \partial_x \left(K(\beta, p)\, \partial_x \begin{pmatrix} p \\ e \end{pmatrix} \right) , \qquad K(\beta, e) = \begin{bmatrix} K^{pp} & K^{pe} \\ K^{ep} & K^{ee} \end{bmatrix} ,$$

where K is the Onsager matrix, whose elements are Green-Kubo coefficients.

- Setting $K^{pp}(\beta, 0) \doteq K_1$ and $K^{ee}(\beta, 0) \doteq K_2$, it can be shown that

$$K^{pp}(\beta, p) \equiv K_1 \doteq K_1, \qquad K^{ee}(\beta, p) = K_2 + p^2 K_1$$

$$K^{pe}(\beta, p) = K^{ep}(\beta, p) = pK_1$$

The stationary problem

$$\partial_x (K_1\, \partial_x p + pK_1 \partial_x e) = 0$$

$$\partial_x (p[K_1\, \partial_x p + pK_1 \partial_x e] + K_2 \partial_x e) = 0$$

Numerical solution of the stationary problem

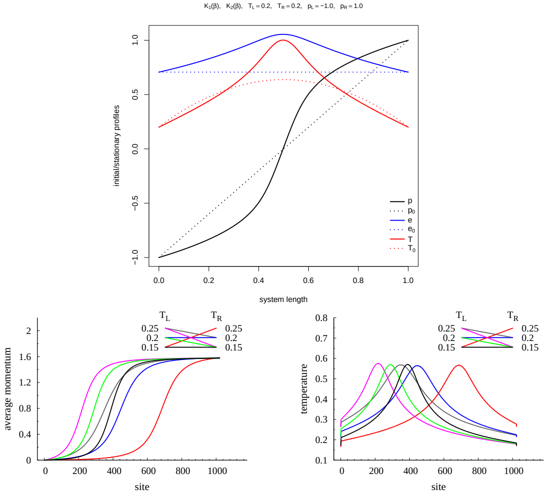
→ Compute K_1 and K_2 at equilibrium (........)

→ Solve the stationary problem with Dirichelet BC $p(0,0) = p_L$, $p(1,0) = p_R$, $T(0,0) = T_L$ and $T(1,0) = T_R$ by the following fixed point algorithm

1. find $\left\{p^{k,n}\right\}$ solutions of the first equation for fixed $\left\{e^{k,n-1}\right\}$;
2. find $\left\{e^{k,n}\right\}$ solutions of the second equation for fixed $\left\{p^{k,n}\right\}$;
3. compute $\left\{u^{k,n}\right\}$ as $u^{k,n} = e^{k,n} - (p^{k,n})^2/(2m)$;
4. find $\left\{\beta^{k,n}\right\}$ by numerically inverting the function
$$U_0\left(1 - \frac{I_1(U_0\beta^{k,n})}{I_0(U_0\beta^{k,n})}\right) + (2\beta^{k,n})^{-1} = u^{k,n}\,;$$
5. update $\left\{K_1^{k,n}\right\}$ and $\left\{K_2^{k,n}\right\}$;
6. if both
$$\left\|\left\{p^{k,n}\right\} - \left\{p^{k,n-1}\right\}\right\| \geq \varepsilon$$
and
$$\left\|\left\{e^{k,n}\right\} - \left\{e^{k,n-1}\right\}\right\| \geq \varepsilon$$
for a fixed ε go to 1, otherwise you have reached the steady state.

Stationary profiles (1/2)

$K_1(\beta)$ and $K_2(\beta)$ form Iubini et al (2016), $T_L = T_R = 0.2,\ p_L = -1.0,\ p_R = 1.0$.



Stationary profiles (2/2)

$K_1(\beta)$ and $K_2(\beta)$ form Iubini et al (2016), $T_L = 0.2$, $T_R = 0.5$, $p_L = -1.0$, $p_R = 1.0$.